Docking and Bioinformatics Tools to Guide Enzyme Engineering

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One general law, leading to the advancement of all organic beings, namely, multiply, vary, let the strongest live and the weakest die.

-Charles Darwin, The Origin of Species (1859)

Declaration

I, John Strafford confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.

Acknowledgements

I wish to thank my supervisors, Paul Dalby and David Jones, for their continued support throughout my PhD. I would also like to extend my thanks to all those in the Biochemical Engineering Department of UCL, in particularly Nigel Titchener-Hooker for his words of encouragement at difficult times.

I would not have been able to complete this work without the unending support of my girlfriend, Hannah Summers, who has kept me motivated and very happy throughout the last six years. I also need to give a massive thanks to my mum and my close family, who have always been there for me in the good, and the difficult times.

Last, but not least, I would like to thank the Biotechnology and Biological Sciences Research Council for funding my PhD.

Abstract

The carbon-carbon bond forming ability of transketolase (TK), along with its broad substrate specificity, makes it very attractive as a biocatalyst in industrial organic synthesis. Through the production of saturation mutagenesis libraries focused on individual active site residues, several variants of TK have been discovered with enhanced activities on non-natural substrates. We have used computational and bioinformatics tools to increase our understanding of TK and to guide engineering of the enzyme for further improvements in activity.

Computational automated docking is a powerful technique with the potential to identify transient structures along an enzyme reaction pathway that are difficult to obtain by experimental structure determination. We have used the AutoDock algorithm to dock a series of known ketol donor and aldehyde acceptor substrates into the active site of *E. coli* TK, both in the presence and the absence of reactive intermediates. Comparison of docked conformations with available crystal structure complexes allows us to propose a more complete mechanism at a level of detail not currently possible by experimental structure determination alone.

Statistical coupling analysis (SCA) utilises evolutionary sequence data present within multiple sequence alignments to identify energetically coupled networks of residues within protein structures. Using this technique we have identified several coupled networks within the TK enzyme which we have targeted for mutagenesis in multiple mutant variant libraries. Screening of these libraries for increased activity on the non-natural substrate propionaldehyde (PA) has identified combinations of mutations that act synergistically on enzyme activity. Notably, a double variant has

been discovered with a 20-fold improvement in k_{cat} relative to wild type on the PA reaction, this is higher than any other TK variant discovered to date.

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Abbreviations

2OXO: 2-oxoisovalerate dehydrogenase
AA: Acetaldehyde
ALS: Acetolactone synthase
BAL: Benzyaldehyde lyase
BFDC: Benzoylformate decarboxylase
DE: D-erythrose
DE4P: D-erythrose-4-phosphate
DG: D-glyceraldehyde
DG3P: D-glyceraldehyde-3-phosphate
DHAS: Dihydroxyacetone synthase
DHP: 1,3-dihydroxypentan-2-one
DR: D-ribose
DR5P: D-ribose-5-phosphate
DX5P: D-xylulose-5-phosphate
DXPS: D-xylulose-5-phosphate synthase
E4P: Erythrulose-4-phosphate
epPCR: Error-prone polymerase chain reaction
GA: Glycolaldehyde
GXC: Glyoxylate carboligase
HPA: Hydroxypyruvic acid
HPLC: High performance liquid chromatography
IEMR: Immobilised enzyme microreactor
IPDC: Indolepyruvate decarboxylase
ISPR: *In situ* product removal
MSA: Multiple sequence alignment
NMR: Nuclear magnetic resonance
PA: Propionaldehyde
PCR: Polymerase chain reaction
PDC: Pyruvate decarboxylase
PFRD: Pyruvate ferrodoxin reductase
PhPDC: Phenylpyruvate decarboxylase
PKL: Phosphoketolase
PO: Pyruvate oxidase
PPDC: Phosphopyruvate decarboxylase
R5P: Ribose-5-phosphate
SCA: Statistical coupling analysis
SPDC: Sulfopyruvate decarboxylase
ThDP: Thiamine diphosphate
TK: Transketolase

1 Introduction

Transketolase (TK) is a key constitutive enzyme in metabolic regulation, providing a link between the pentose phosphate pathway and glycolysis through the production of 3 and 6 carbon sugars (glyceraldehyde-3-phosphate and fructose-6-phosphate respectively) (Figure 1.2 a and b) [1]. Found in the non-oxidative branch of the pentose phosphate pathway, TK catalyses the reversible transfer of two carbon ketol groups between several donor and acceptor substrates. In addition to supplying substrates for glycolysis, TK controls the supply of ribose-5-phosphate (R5P), essential for biosynthesis of nucleotides and nucleic acids, and catalyses the production of erythrulose-4-phosphate (E4P) which is utilised by microorganisms in the shikimate pathway for the biosynthesis of aromatic amino acids.

Transketolase was first purified from *Saccharomyces Cerevisiae* [2] and requires divalent cations and thiamine diphosphate (ThDP) for its activity [3]. There is a high level of sequence identity between the TK proteins of different organisms with many residues displaying complete invariance [4]. A second TK encoding gene was identified in *Escherichia Coli* in 1993 [5], this gene was named tktB to distinguish it from tktA. tktA and tktB share high sequence identity (74%) but tktA encodes the major TK activity in *E. coli*. All future references to *E. coli* TK refer to tktA encoded transketolase. In all structures solved to date, TK exists as a homodimer with two identical active sites positioned at the interface between the subunits.

The reaction catalysed by TK proceeds via a Ping Pong Bi Bi mechanism: two substrates are converted into two products as the ThDP cofactor within the enzyme active site shuttles between a free and a substrate modified intermediate state [6].

The Ping Pong Bi Bi model describes a specific type of Bi Bi mechanism in which substrates and products are bound and released sequentially and the enzyme shuttles between a free and a substrate modified intermediate state (Figure 1.1).

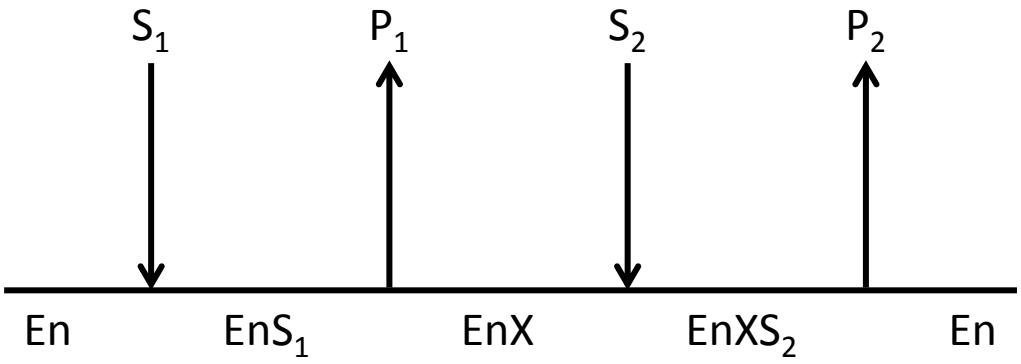

Figure 1.1 Kinetic Scheme of a Bi Bi Ping Pong Mechanism. In the Bi Bi Ping Pong model the enzyme shuttles between a free and a substrate modified intermediate state. In contrast to the standard Bi Bi model, substrates and products are bound and released sequentially in the Ping Pong model

Enzymatic thiamine catalysis is recognised as proceeding through two intermediate states: the ylide of ThDP in which the C2 proton of the thiazolium ring is abstracted, and the 2-α carbanion which is formed following nucleophilic attack by the ylide C2 on the donor substrate [6]. The α-carbanion is stabilised by the thiazolium ring which acts as an electron sink. Further stabilisation is provided by interconversion of the α-carbanion into a neutral enamine, creating a resonance hybrid. Following formation of the intermediate, the two carbon unit is transferred from the carbanion to the acceptor substrate forming a ketose with an extended carbon skeleton through nucleophilic attack. The ThDP in TK is bound in a V conformation which brings the 4-amino group of the pyrimidine ring into close proximity with the C2 carbon atom of the thiazolium ring, this conformation is essential for catalysis [7].

Broad substrate specificity, stereospecificity and stereoselectivity have made TK an attractive target for applications in organic synthesis [8]. The reversible reaction catalysed by TK *in vivo* has been utilised in a synthetic manner, but if the natural ketol donor is replaced with hydroxypyruvic acid (HPA), carbon dioxide is released as a by-product rendering the reaction irreversible and far more industrially useful (Figure 1.2 c). The industrial applicability of TK has been further adapted by engineering the protein sequence of the enzyme to improve attributes such as substrate specificity and enantioselectivity [9-11]. This thesis explores the potential of computational applications to direct and optimise the engineering of this enzyme towards even greater improvements.

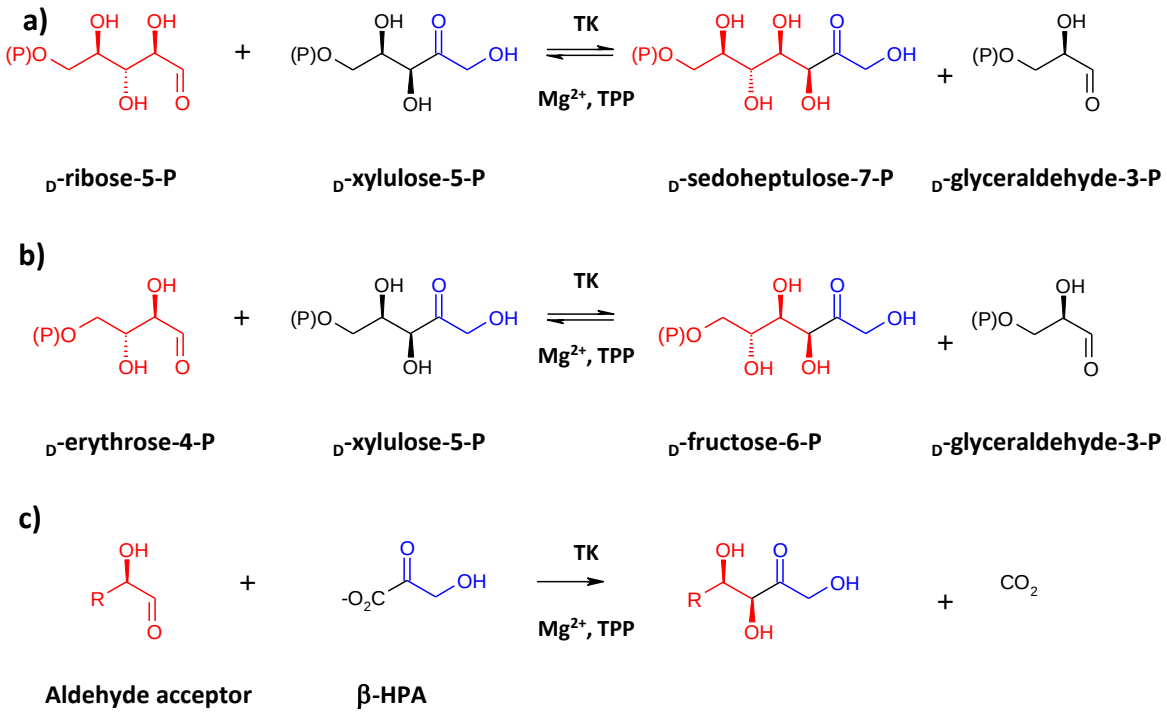

Figure 1.2 *In vivo* and *In vitro* reactions catalysed by transketolase. Reactions (a) and (b) occur *in vivo* in the non-oxidative branch of the pentose phosphate pathway and are reversible. (c) *In vitro* the ketol donor is generally replaced with β-HPA, rendering the reaction irreversible through elimination of CO_2. Various aldehyde acceptors are accepted by TK but TK preferentially accepts α-hydroxylated aldehydes with the (R)-configuration.

1.1 Transketolase structure and mechanism

1.1.1 Transketolase structure

The first transketolase structure was solved for yeast TK in 1992 [12] this was refined to 2Å in 1994 [13] (1TRK). Since then, several other transketolase structures have been solved for TK. The *E. coli* TK structure was solved in 1994 [14] (1QGD), Maize TK in 2003 [15] (1ITZ) and *Leishmania Mexicana* TK in 2004 [16] (1R9J). Several further yeast TK structures have also been solved in the quest to refine our functional understanding of this catalyst. These include Apo TK [17], D-ethrythrose-mutants of TK [19] (1AYO) and several complexes of TK with ThDP analogues [20] (1TKA, 1TKB, 1TKC). More recently, *E. coli* TK structures were determined in covalent complexes with DX5P (2R8O) and DF6P (2R8P), and in non-covalent complex with DR5P (2R5N) [21].

The majority of detailed structural analysis and functional studies have been carried out on the yeast TK protein. Yeast and *E. coli* TK share a very high level of sequence identity and all homologous TK structures defined show near identical conformations of functional residue side chains. The vast majority of functional residues identified in yeast TK are 100% conserved in all TK proteins sequenced so far. We can therefore utilise the data and information gathered for yeast TK and apply it in our study of *E. coli* TK. Throughout this thesis, except where scientific evidence is based solely on yeast TK, numbering refers to *E. coli* TK and is based on the PDB structure 1QGD. Where yeast TK numbering is used, residues are underlined and numbering is based on the PDB structure 1TRK (in these situations *E. coli* numbering is also reported in brackets). Key functional residues are listed in

Table 1.1 together with the corresponding *E. coli* and yeast numbering for reference.

In all TK structures solved to date, TK is a homodimer consisting of two subunits each of 70-74 kDa (Figure 1.3 a). ThDP binds along with the metal ion cofactor at the interface between these two subunits. Each subunit of TK is made up of three domains, the N-terminal domain or the PP domain, the middle domain or Pyr domain, and the C-terminal domain (Figure 1.3 b). Each of the domains is of α/β type and the PP and Pyr domains are structurally similar when superimposed upon each other. The following structural analysis of transketolase is based on the structure for *E. coli* TK [14], but could equally be applied to the structure of yeast TK due to the high degree of structural equivalence.

The PP domain of *E. coli* includes residues 2-317 and comprises of a five stranded parallel β sheet with several helices on either side and some on top of the sheet. The α/β connection after the third strand contains a hairpin loop 187-191, this loop is involved in binding the cofactor and has been shown to be mobile in the apo-transketolase of yeast [17]. In the holo-enzyme of yeast TK, Asp 192 (190) and Ile 191 (189) are in contact with the metal ion and the cofactor. These interactions keep the hairpin in a closed conformation, enclosing the cofactor and shielding it from solvent [14].

The Pyr domain includes residues 318-527. This domain is made up of a parallel β-sheet of six strands. As mentioned above, the Pyr domain is structurally similar to the PP domain. The similarity between these two structural motifs is most pronounced in the last four α/β units of the two domains. Like the PP domain, the

Pyr domain forms interactions with the THDP cofactor through the loops at the carboxy ends of the β-sheet [14].

The C-terminal domain of TK consists of a mixed β-sheet with one antiparallel strand followed by four parallel strands. This domain is not involved in binding the ThDP cofactor and contributes less to the dimer interface interactions than do the other domains. Recent results [22] have demonstrated that the C-terminal domain is not essential for catalysis. The function of this domain remains unknown but it has been suggested that it may have a regulatory or a cellular localisation role.

The interface between the subunits of TK consists of a buried region representing approximately 18% of the accessible surface area of one free monomer [13]. Interactions between the two equivalent PP domains consist of tight packing interactions between the equivalent helices that link β-strands two and three and the equivalent helices that link strands three and four. The main interactions between the Pyr domains of each subunit are limited to the equivalent helices that link strands four and five of the Pyr β-sheet. This dimeric configuration positions the loops at the carboxy ends of the PP β-sheet facing the loops at the carboxy ends of the Pyr β-sheet of the other subunit. The region where these loops come together constructs the ThDP binding site and the active site of TK.

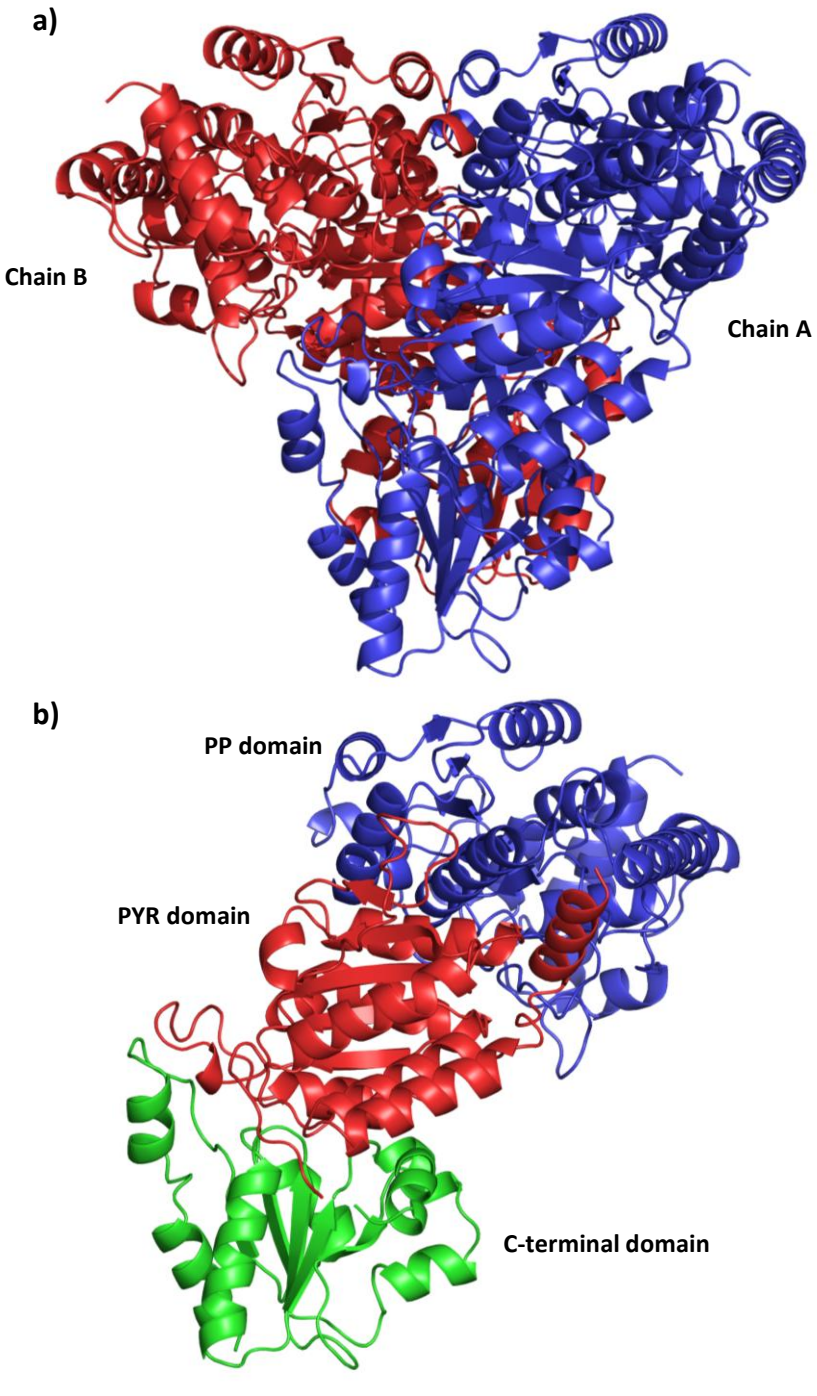

Figure 1.3 (a) *E. coli* transketolase homodimeric structure (1QGD) coloured by chain. (b) Chain A of *E. coli* transketolase coloured by domain.

	TK Numbering		
Residue	*E. coli*	*S.cerevisiae*	Proposed function
His	26	30	Interacts with substrates
His	66	69	Interacts with cofactor and substrates
His	100	103	Interacts with substrates
Gly	114	116	Interacts with pyrimidine ring (4'-NH_2)
Leu	116	118	Interacts with pyrimidine ring (N3')
Asp	155	157	Metal ion ligand
Asn	185	187	Metal ion ligand
Ile	187	189	Metal ion ligand (main chain oxygen)
Ile	189	191	Contact with metal ion and cofactor
Asp	190	192	Contact with metal ion and cofactor
His	261	263	Interacts with cofactor and substrates
Arg	358	359	Interacts with phosphate of substrates
Leu	382	383	Interacts with cofactor thiazolium ring
Ser	385	386	Interacts with phosphate of substrates
Val	409	Ile 416	Interacts with cofactor thiazolium ring
Glu	411	418	Protonates N1' nitrogen pyrimidine ring
Phe	434	442	Interacts with pyrimidine ring
Phe	437	445	Interacts with pyrimidine ring
Tyr	440	448	Interacts with pyrimidine ring
His	461	469	Interacts with phosphate of substrates
Asp	469	477	Interacts with substrates
His	473	481	Interacts with substrates
Arg	520	528	Interacts with phosphate of substrates

Table 1.1 Key functional residues identified in yeast and *E. coli* transketolase with corresponding numbering. All residues are conserved apart from Val 109 in *E. coli* TK, the equivalent of which is Ile 416 in yeast TK.

1.1.2 Cofactor binding

ThDP binds in a deep cleft at the interface of the two TK subunits. Bound ThDP is totally isolated from the surrounding solvent apart from the reactive C2 carbon atom of the thiazolium ring. Unlike the structure of free ThDP, the bound cofactor is strained into a V-conformation. This brings the pyrimidine ring 4'-NH2 group into close proximity with the reactive C2 carbon and contributes to the catalytic mechanism of all ThDP dependent enzymes (Figure 1.4).

Conserved *E. coli* TK residues His 66 and His 261 form hydrogen bonds with the diphosphate group of ThDP. Two oxygen atoms of diphosphate together with Asp

155, Asn 185 and the main chain oxygen of Ile 187 are ligands of Ca^{2+} and create further indirect interactions [14].

Whilst the diphosphate of ThDP forms interactions with one subunit of TK, the thiazolium and pyrimidine rings of the cofactor are bound in a cleft between the subunits. The thiazolium ring forms hydrophobic interactions with conserved residues Leu 116 and Ile 189. The C4 methyl group of the thiazolium ring interacts with the side chains of Leu 382 and Val 409 [14].

The pyrimidine ring is stacked with the ring system of Phe 437 and forms further interactions with conserved residues Phe 434 and Tyr 440. Main chain atoms of Gly 114 and Leu 116 form H-bonds with the pyrimidine ring 4'-NH2 group and the N3' nitrogen atom respectively. The N1' nitrogen atom of the pyrimidine ring forms a H-bond with Glu 411 [14]. This interaction is very important in the molecular mechanism of enzymatic thiamine catalysis [23].

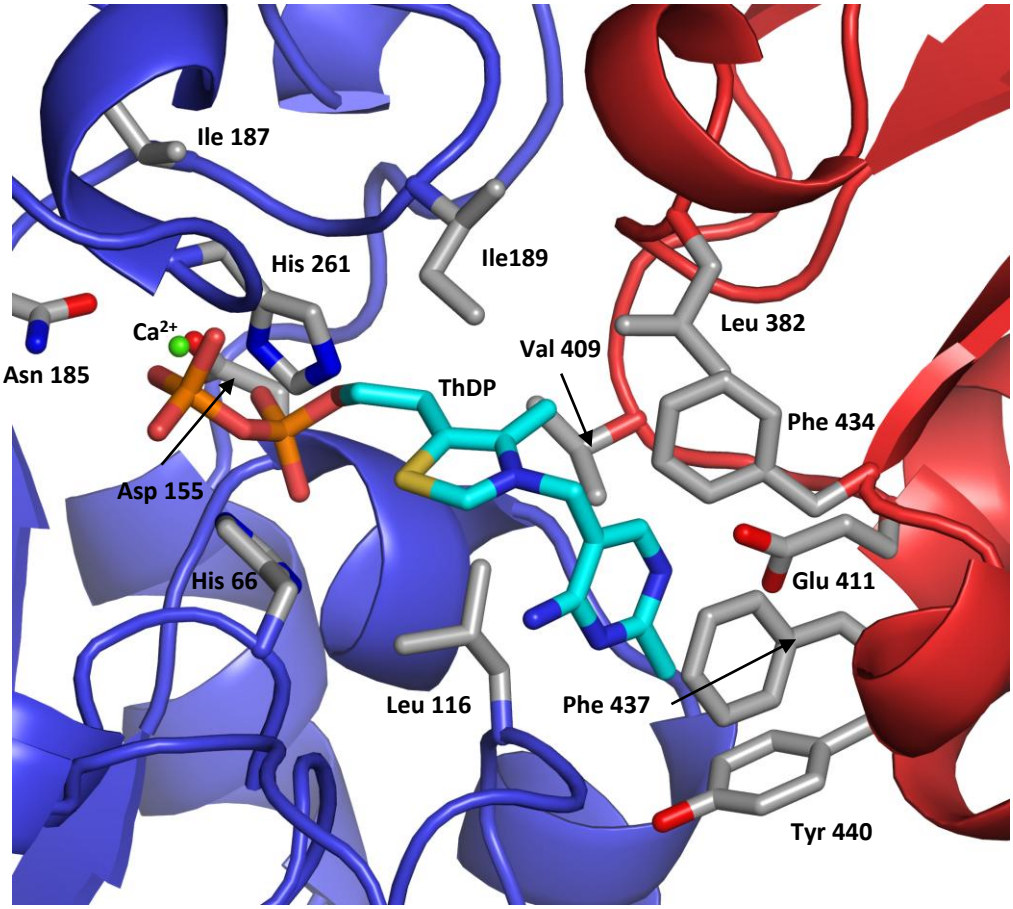

Figure 1.4 ThDP bound in one active site of *E. coli* TK with the Ca^{2+} metal ion. The active site is formed between the PP domain of chain A (blue) and the PYR domain of chain B (red). Interacting residues are labelled.

1.1.3 Substrate binding and recognition

The active site binding cleft of TK is a deep funnel leading towards the exposed reactive C2 of ThDP. Conserved loops make up the walls of this binding funnel. Two conserved arginine residues are positioned at the entrance to the binding funnel. The middle of the binding channel contains several conserved residues including Asp 469, Ser 385 and His 461. Towards the base of the binding cleft, near the thiazolium ring of ThDP, there is a cluster of histidine residues on one side and there are also several conserved hydrophobic residues [14].

The crystal structure of the acceptor substrate, DE4P, bound in yeast TK gives insight into the residues involved in substrate binding and recognition [18]. The phosphate group of the acceptor substrate forms interactions with several conserved residues near the entrance of the binding funnel. Arg 359 (358), Arg 528 (520), Ser 386 (385) and His 469 (461) form interactions with the substrate phosphate group. These interactions position the substrate in the binding channel in the correct orientation, the long side chains of the arginine residues may also provide some flexibility to allow the substrate to move towards the reactive C2 of ThDP [18]. Asp 477 (469) forms polar interactions with the C2-hydroxyl group of the substrate and the aldehyde oxygen atom is within H-bonding distance of His 30 (26) and His 263 (261) (Figure 1.5) [18].

In order to further elucidate the role played by the arginine and histidine residues at the entrance to the binding funnel, these residues have been subjected to site directed mutagenesis in yeast TK [18]. Substitution of residues Arg359 (358), Arg528 (520) and His469 (461) for alanine did not have a great effect on catalytic activity (residual catalytic activities were 31%, 17% and 77% respectively) but did increase K_m values for donor substrate, and in particular acceptor substrates, significantly. Consistent with the crystal structure of DE4P bound in the TK active site, these results support a role for these residues in binding the phosphate group of substrates.

The pattern of H-bonds formed by Asp 477 (469), His 30 (26) and His 263 (261) with the acceptor substrate is consistent with the enantiosensitivity TK displays towards D-threo configured donor substrates. Inversion of the stereocentres in the favoured

configuration would disrupt this H-bond network and reduce enzyme affinity for substrate. The potential of forming a H-bond with Asp 477 (469) also explains the preference for α-hydroxylated acceptor substrates. Replacement of Asp 477 (469) with alanine in yeast TK resulted in an enzyme with severely impaired catalytic activity [24]. Kcat/Km for this variant is reduced relative to wild type TK for D-α-hydroxyaldehydes (DE4P, DR5P) and this reduction is equivalent to the reduction in Kcat/Km for the wild type enzyme with 2-deoxyaldoses or L-α-hydroxyaldehydes [24].

Yeast TK residues His 30 (26) and His 263 (261) have also been mutated to alanine [19]. These residues are within H-bonding distance to the carbonyl oxygen of the acceptor substrate and their mutation to alanine has a large effect on k_{cat} [19].

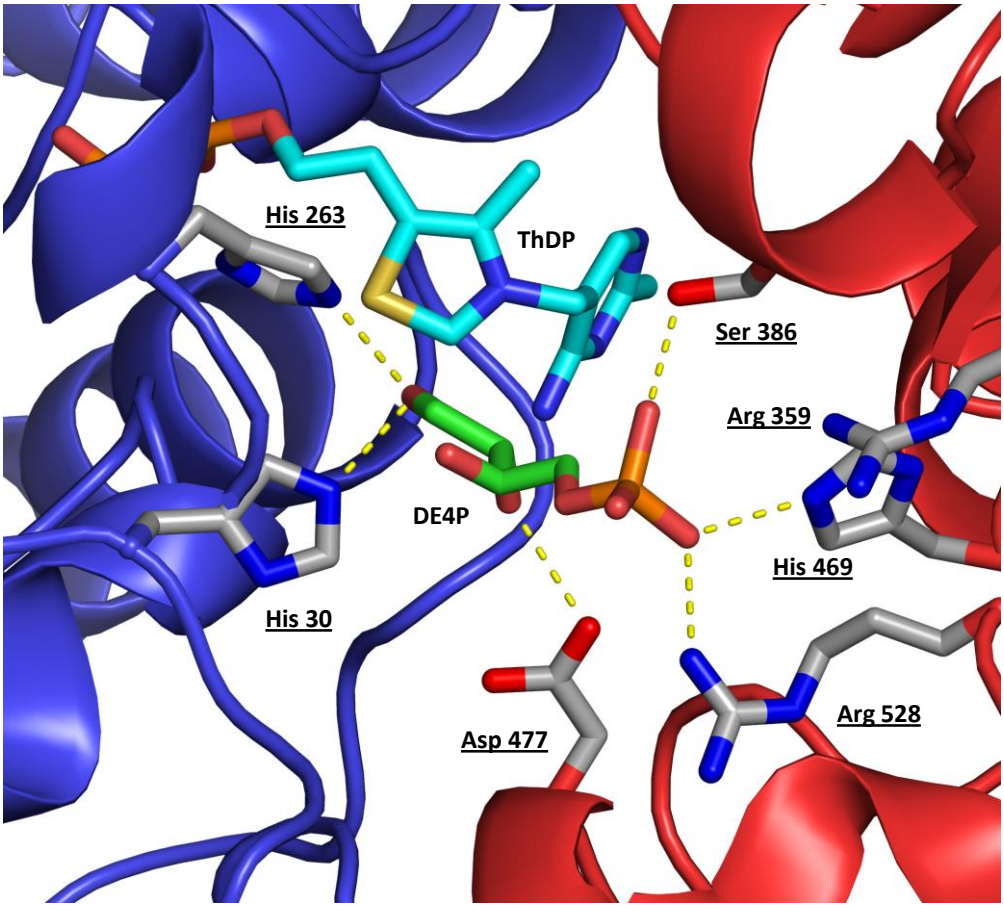

Figure 1.5 DE4P bound by yeast TK. The active site is formed at the interface of the PP domain of chain A (blue) and the PYR domain of chain B (red). Residues from both chains make key interactions with DE4P. Interacting residues are labelled with yeast TK numbering. Hydrogen bonds are displayed by yellow dashed lines.

A cluster of histidine residues is located towards the base of the binding funnel close to the reactive C2 of ThDP. Based on the structures of TK and acceptor substrate (DE4P) bound TK, histidine residues His 69 (66) and His 103 (100) were predicted to form H-bonds with the C1-hydroxyl group of the donor sugar phosphate [18]. In support of this role, replacement of His 69 (66) or His 103 (100) with alanine had little effect on the K_m values for acceptor substrates but significantly increased those of donor substrates [19, 25]. These mutants also displayed a significant decrease in catalytic activity. Although hydroxypyruvate is a donor substrate for TK, pyruvate is not. The recognition of the C1-hydroxyl group of the donor by these two histidine residues might explain this molecular selectivity. In

a crystal structure of the covalent enamine intermediate bound in yeast TK [7], His 103 (100) formed a H-bond with the β-hydroxyl oxygen of the intermediate. The β-hydroxyl oxygen also interacted with His 69 (66), indirectly through a water molecule. These interactions further support a role for His 69 (66) and His 103 (100) in discrimination between hydroxypyruvate and pyruvate.

Recent structures determined of covalent intermediates in *E. coli* TK support the structural studies above and the conserved function of residues between yeast and *E. coli* TK [21]. DX5P and DF6P covalent intermediates adopted very similar extended conformations in the active site of *E. coli* TK, forming at least 11 well defined hydrogen bonds with the side chains of active site residues. The C1-hydroxyl and C2-hydroxyl groups of both substrates formed interactions with His 473 and the 4'-amino group of the ThDP pyrimidine ring. The C1-hydroxyl group also formed a hydrogen bond with His 100. The C3-hydroxyl groups interact with the two histidine residues His 261 and His 26 and the C4-hydroxyl group interacts with Asp 469 and His 26 (Figure 1.6). Phosphate interactions were mediated by residues His 461, Ser 385 and Arg 358 with the phosphate group of DF6P slightly closer to these residues due to the longer carbon chain. The additional C5-hydroxyl group of DF6P interacts with Ser 385.

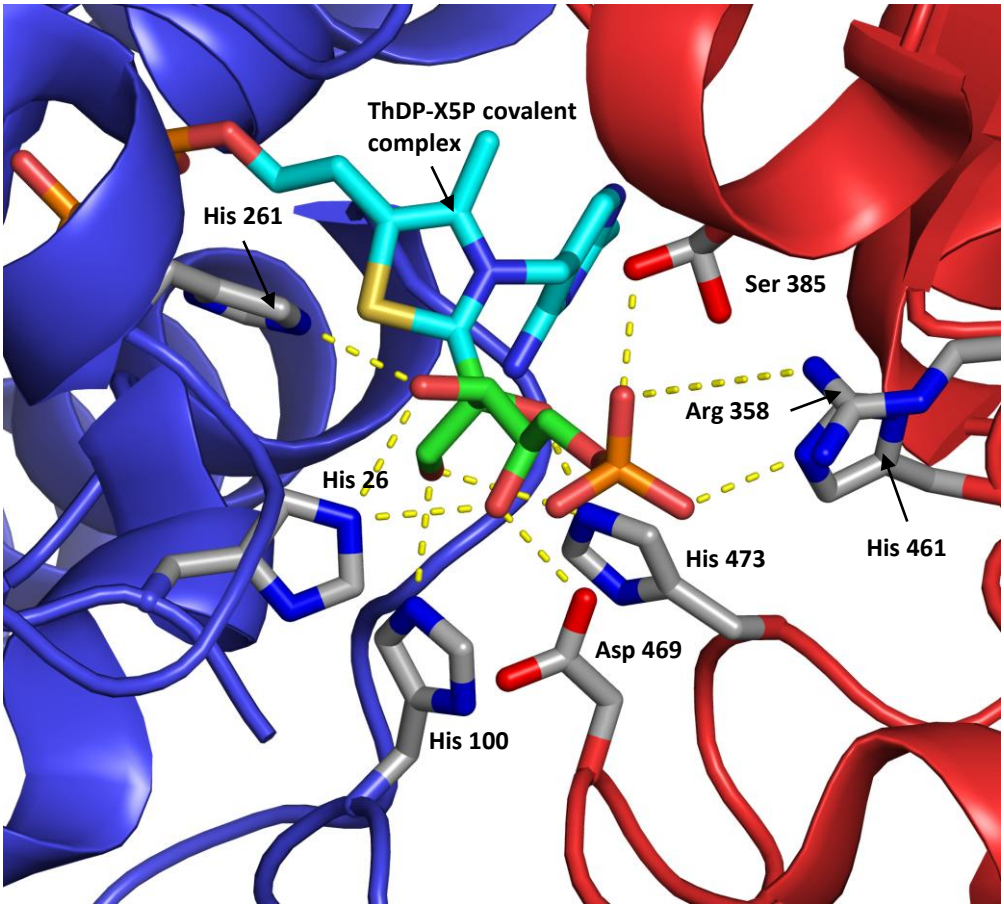

Figure 1.6 Structure of the covalent complex formed between X5P and ThDP in the active site of *E. coli* TK. The PP domain of chain A is coloured blue and the PYR domain of chain B is coloured red. Residues forming interactions with the complex are labelled. Hydrogen bonds are displayed by yellow dashed lines.

1.1.4 Molecular mechanism of Transketolase

Transketolase catalyses the transfer of a two carbon unit from a ketose donor to an aldose acceptor, the reaction proceeds through two major steps. In the first step, the donor substrate is cleaved to produce an aldose and a covalent intermediate, ThDP α-carbanion. The second step is initiated by nucleophilic attack by the α-carbanion on the acceptor substrate, resulting in a ketose product with an extended carbon skeleton. This reaction mechanism, described in further detail bellow, was proposed by Schneider and Lindqvist (1993) [6] (Figure 1.1Figure 1.7).

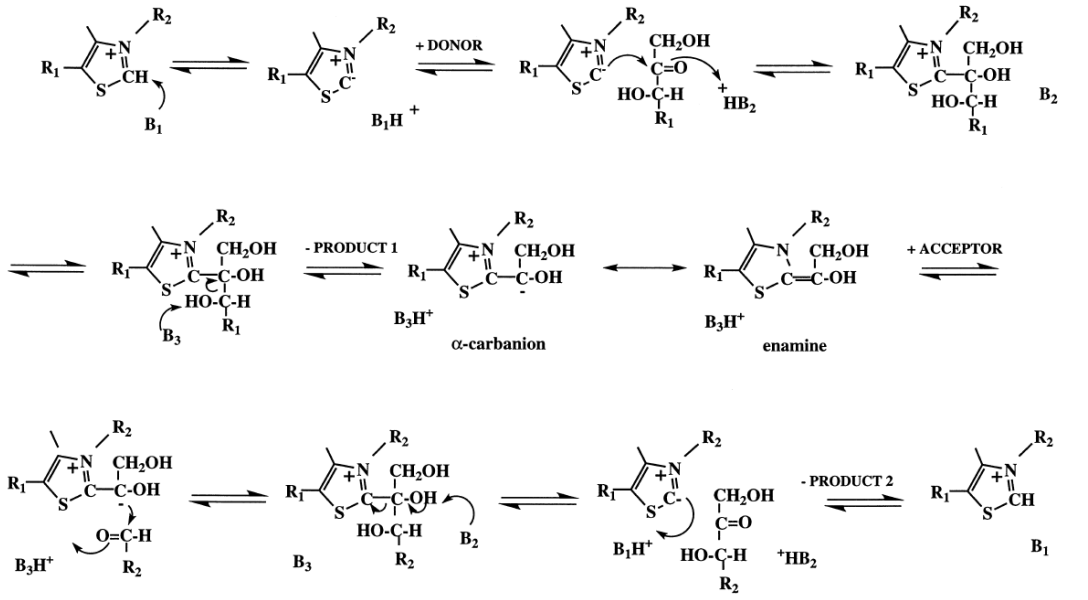

Figure 1.7 Reaction mechanism of transketolase, reproduced from Biochemica et Biophysica Acta (1385 387-398) with permission from author and publisher. B_1 represents the 4'-imino group of the pyrimidine ring; B_2 represents either His 473 or the 4'-imino group of ThDP; B_3 represents either His 26 or His 261.

Prior to the first step in catalysis, the C2 carbon of the thiazolium ring must be deprotonated in order to create an ylide that can attack the donor substrate. Evidence suggests that the deprotonation of C2 is catalysed by the cofactor itself [23]. The transketolase molecule contributes to cofactor deprotonation by maintaining the V-conformation of ThDP, which brings the 4'-NH2 group into close proximity with the C2 carbon, and through protonation of the N1' nitrogen of the pyrimidine ring. The N1' nitrogen is protonated by a H-bond with Glu 411, this interaction alters the pKa of the 4'-NH2 group and leads to the production of a 4'-imino group which is sufficiently basic to deprotonate the C2 carbon of the thiazolium ring [6].

Once the C2 carbon has been deprotonated, the carbanion formed attacks the carbonyl oxygen of the donor substrate to create a high energy intermediate. During covalent bond formation between ThDP and the donor substrate, a proton

donor is required to stabilise the negative charge forming at the carbonyl oxygen. His 473 and the charged 4'-imino group of ThDP are possible proton donors at this step in the reaction. While site directed mutagenesis of the His 481 (His 473) in yeast TK suggested a role in transition state stabilisation, the lack of conservation of this histidine residue across other TK enzymes suggests that the 4'-imino group may be responsible for the majority of transition state stabilisation.

The final steps in TK catalysis require an acid/base catalyst that can deprotonate the hydroxyl group of the substrate at C3, catalysing the cleavage that produces the α-carbanion intermediate, and act as a proton donor to the carbonyl oxygen of the acceptor substrate as it is attacked by the α-carbanion. Both His 26 and His 261 are within H-bonding distance from the C3-hydroxyl group of the reaction intermediate and the carbonyl oxygen of the acceptor substrate. Replacement in yeast of either of these residues by alanine severely impairs catalytic activity and they may act together as the acid/base catalyst in the reaction [19].

Crystal structures of the covalent high energy intermediates formed with DX5P and DF6P in *E. coli* TK reveal a conformation in which the newly formed C2-Cα bond is out-of-plane with the thiazolium ring by 25-30^{o} (Figure 1.8) [21]. This strained conformation will be relieved upon product elimination conceivably providing the driving force for the reaction. Density functional theory (DFT) calculations supported the above out-of-plane conformation, demonstrating that this conformation is energetically favourable relative to a model with a co-planar C2-Cα bond [21]. No structural rearrangements were seen in the active site following intermediate formation, suggesting that the active site is poised for catalysis such

that the substrate binding energy and the enthalpic energy gain following covalent bond formation between ThDP and the donor substrate can be channelled directly into the formation of the high energy, strained intermediate.

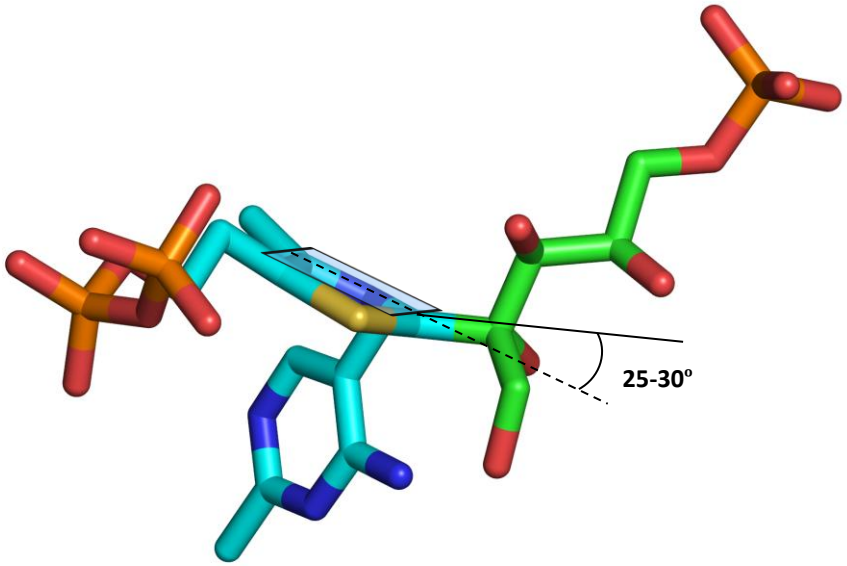

Figure 1.8 Covalent complex of X5P and ThDP isolated in the active site of *E. coli* TK. The strained angle of the out-of-plane C2-Cα bond is displayed relative to the thiazolium ring of ThDP.

1.2 Transketolase as a biocatalyst

In vivo, trasketolase catalyses the transfer of a 2-carbon ketol unit from D-xylulose-5-phosphate to D-ribose-5-phosphate, generating D-sedulose-7-phosphate and D-glyceraldehyde-3-phosphate. The carbon-carbon bond formation catalysed by TK is both stereospecific and stereoselective, making this a very attractive enzyme for the industrial production of complex organic structures. Unlike traditional chemical methods for organic synthesis, enzymatic catalysis does not require complex protection and de-protection steps, additional advantages include greater chiral control and milder reaction conditions.

The reversible reaction catalysed by TK *in vivo* has been utilised for industrial applications but the usefulness of the biocatalyst can be enhanced by replacing the D-xylulose-5-phosphate (X5P) ketol donor with β-hydroxypyruvate (HPA). Use of HPA results in the elimination of CO_2 thereby rendering the reaction irreversible [26].

In addition to varying the ketol donor, much work has been carried out exploring the substrate specificity of TK for aldehyde acceptors. Although TK favours aldehydes containing an α-hydroxylated group in an (R)-configuration [27], specificity with respect to the aldehyde is relatively broad with both non-phosphorylated and phosphorylated aldehydes of varying sizes being accepted [28]. Steric hindrance appears to impact on relative activity with cyclic aldehydes and aldehydes containing bulky groups displaying lower activities.

The broad nature of aldehyde substrate specificity is advantageous for the application of TK in organic synthesis as it provides flexibility in the nature of structures that can be produced. The broad specificity also provides a good starting point for engineering TK to improve activity on non-natural substrates.

Early work in the development of TK as a biocatalyst utilised commercially available *S. cerevisiae* TK, and spinach TK extracted from spinach leaves. These sources are readily available but do not offer the scale required for an industrial process. In 1993, Hobbs *et al* developed an efficient and reliable source of TK by introducing the previously cloned *E. coli* TK gene fragment into a high copy number plasmid and transforming this into *E. coli* [29]. The resulting transformants overexpressed TK with superior specific activity to that obtained previously from *E. coli* TK. Evaluation

of the substrate specificity of *E. coli* TK demonstrated a similar profile to yeast TK and the same preference for α-hydroxylated aldehydes with an (R)-configuration [29]. An additional benefit of *E. coli* TK was its increased activity with HPA (60 U/mg protein) relative to yeast (8.6 U/mg protein) or spinach (2 U/mg protein) [1, 28, 30].

1.2.1 Use of Transketolase in enzymatic syntheses

Transketolase has been used successfully in various organic syntheses of both natural and unnatural complex, chiral compounds. The compounds produced using transketolase are expensive and would require complex multi-step synthesis if produced using traditional chemical methods. Some of the compounds synthesised by transketolase cannot be produced chemically.

In an early example, D-[1,2-$^{13}C_2$]-xylulose was produced from [2,3-$^{13}C_2$]-hydroxypyruvate and D-glyceraldehyde using spinach transketolase [31]. The isotopic labelling of sugars is useful for the study of metabolism and structure. Introduction of two adjacent ^{13}C labels is particularly useful due to ^{13}C-^{13}C coupling. Transketolase has also been utilised to produce glycosidase inhibitors fagomine [32] and 1,4-dideoxy-1,4-imino-D-arabinitol [33], which have applications as agrochemicals and therapeutic agents.

Commercially available TK was used together with chemical steps to produce α-exo brevicamycin, a beetle pheromone with applications in pest control. In this example TK was used to convert a racemic mixture of 2-hydroxy butyraldehyde and HPA into the key tri-hydroxy ketone intermediate in the process [34].

Production of expensive food additives has also utilised TK. Spinach TK was used to produce 6-deoxy-L-sorbose, a precursor for synthetic furaneol, an aromatic product with a caramel like flavour. In the above synthesis, serine glyoxylate amino transferase was used to prepare HPA and 4-deoxy-L-threose was obtained by microbial isomerisation of 4-deoxy-L-erythrulose [35].

Multi-enzyme approaches have been successfully applied to the production of sugars 4-deoxy-D-fructose 6-phosphate and D-xylulose 5-phosphate. In the first example, 4-deoxy-D-fructose 6-phosphate was synthesised in a process including four steps and two enzymatic reactions. Epoxide hydrolase was first used to obtain (3S)-1,1-Diethoxy-3,4-epoxybutane which was subsequently opened by inorganic phosphate to produce 2-deoxy-D-erythrose 4-phosphate. This aldehyde was then reacted with L-erythrulose in the presence of yeast TK to introduce the second chiral centre [36].

In the second example, D-xylulose-5-phosphate, a valuable substrate required for enzymatic assays, was prepared in gram quantities through a one-pot procedure incorporating fructose 1,6 bisphosphate aldolase followed by *E. coli* TK [37]. The aldolase was initially used to produce D-glyceraldehyde-3-phosphate and dihydroxyacetone phosphate (DHAP) through retro-aldolization of D-fructose-1,6-bisphosphate. The D-glyceraldehyde-3-phosphate produced was then coupled with HPA by *E. coli* TK to produce X5P. Zimmermann *et al* also incorporated triosephosphate isomerase (TPI) to equilibrate the two products of the retro-aldolization thereby increasing the overall yield. Thanks to recent advances in

synthesis [38], DHAP is now available as a starting point, opening up a new route to the synthesis of X5P using just TPI and TK [39].

Finally, transketolase was utilised to catalyse the key asymmetric step in a process to produce N-hydroxypyrrolidine, a glucosidase inhibitor. In this synthesis TK was used to couple (+-)-3-*O*-benzylglyceraldehyde with HPA to yield 5-*O*-benzyl-D-xylulose in multigram quantities [40].

1.2.2 Optimisation of process for industrial application

To utilise TK in large scale industrial enzymatic syntheses, limitations in the process must be identified and overcome to ensure product purity and maximise yield and efficiency. Limitations in TK biocatalysis include stability of the enzyme (reactive α-hydroxy aldehydes inactivate TK [41]), and product inhibition. More general process options also need to be optimised during process development to ensure maximum yield, minimum cost and scalability.

One strategy to overcome the problem of substrate deactivation of TK is to minimise substrate concentration by carrying out the reaction in an enzyme membrane reactor. Applied to the production of L-erythrulose from GA and HPA this strategy was able to increase the half-life of TK from 5.6 hours (repetitive batch reactor) to 106 hours (enzyme membrane reactor). This improvement in stability resulted in an increase in space time yield from 28 g/L/d to 45 g/L/d [41].

An alternative approach to increasing enzyme stability is to immobilise the enzyme on a support. GA is believed to deactivate TK by forming Schiff bases with amino acid side chains on the surface of the enzyme. Formation of Schiff bases can alter

the three dimensional structure of proteins. Stabilisation of TK by immobilisation can be explained by the prevention of the formation of Schiff bases, or by rigidifying the three dimensional structure of TK. Applied to the production of L-erythrulose from GA and HPA, immobilisation of TK on commercially available supports (Amberlite XAD-7 and Eupergit C) increased the stability of TK by 80- and 100-fold respectively. Immobilisation was unable to prevent inactivation by oxidation but this could be reduced by the inclusion of a stabilising solute such as mercaptoethanol [42]. Immobilisation confers additional benefits on process productivity: allowing the enzyme to be retained in the bioreactor, extracted from the product stream, and/or reused.

In situ product removal (ISPR) has been explored as a means to overcome limitations introduced by product inhibition. L-erythrulose was successfully removed using an immobilised phenylboronate resin, however there were also considerable levels of nonspecific substrate binding to the resin which reduced the actual yield. To overcome the problem of nonspecific binding, a fed batch system was utilised. The fed batch mode gave the added benefit of reducing the deactivation of TK by GA. The rate of deactivation of TK by substrate is much higher than by the synthesised product [41], therefore in practice the reduction in aldehyde toxicity overcame the benefits of product removal and negated the need for ISPR [43].

Work has also been carried out to explore more general process development strategies to optimise yield, cost and scalability. The synthesis of X5P using TK and TPI has been utilised as a model reaction to investigate the potential of

semiquantitative process screening, to speed up process development for multienzyme biocatalytic processes. This approach has the potential to reduce the number of process options that need to be screened, applied to the synthesis of X5P the strategy successfully identified new biocatalytic routes and processes for further investigation [44].

As an alternative to reducing the number of process options to screen, high-through microwell based based methods can be used to screen multiple process options in parallel. For TK process characterisation a more efficient alternative to microwells has recently been developed in the form of an immobilised enzyme microreactor (IEMR). The microreactor developed is composed of a 25 cm long fused silica capillary with a 200 μm internal diameter. His-tagged TK is reversibly immobilised inside the capillary via Ni-NTA linkages. His-tagged TK is expected to be kinetically identical to un-tagged protein based on the location of the His tag and on previous kinetic characterisation. The reactor can be operated in stop flow or continuous flow mode and product is analysed by HPLC. For high throughput screening of different process options or different enzyme variants the IEMR has several advantages over traditional microwell approaches, these include reduction in reactant volume, enhanced productivity, reduced reaction time and increased reusability [45].

1.2.3 Transketolase enzyme engineering

Although TK displays broad substrate specificity, non-natural aldehyde substrates are converted at far lower rates than the phosphorylated, α-hydroxylated natural substrates. The production of non-phosphorylated chiral products is one of the

major advantages of TK over other enzymes such as aldolases, it would therefore be advantageous to increase the activity of TK on these non-natural substrates.

In addition to process engineering, enzyme engineering can be applied to TK to further optimise the biocatalyst for industrial applications. The good structural and mechanistic understanding of TK and its broad substrate specificity make the wild type enzyme a good candidate for enzyme engineering. However, the two-substrate mechanism of TK complicates engineering as any change can result in positive or detrimental effects to the binding of either substrate. In recent years TK has been engineered to improve its activity on non-phosphorylated and non-hydroxylated substrates. The enzyme has also been engineered to improve or reverse its stereoselectivity with these non-natural substrates.

Early work on TK engineering focussed on improving activity in the model reaction of GA and HPA to produce L-erythrulose. Variants with up to 5-fold improvements in activity against GA were identified by screening a library of single point mutants generated by saturation mutagenesis of nineteen positions. Residues were selected for mutagenesis based on structural and phylogenetic criteria. Two sets were included: residues within 4 Å of bound substrates, and phylogenetically varied residues within 10 Å of TPP. Following the screen, twelve variants were identified with enhanced specific activity on GA relative to wild type TK. Six of the nineteen residue libraries yielded variants with improved activity.

The greatest improvements in activity against GA were associated with variations at residues His 461, Arg 520 and Ala 29. His 461 and Arg 520 interact with the phosphate group of natural substrates, mutation of these residues could improve

GA accessibility to the active site by removing a charged group or by reducing the steric bulk around the entrance to the active site. The third position identified, Ala 29, is harder to rationalise as it is in the active site second shell and is in direct contact with the terminal phosphate group of TPP. Overall, residues with high sequence entropy were more likely to confer enhanced activity on GA following mutagenesis. The important exceptions to this rule were the three residues known to interact with the phosphate group of natural substrates. Saturation libraries of His 461, Arg 358 and Arg 520 all yielded at least one mutant with increased specific activity on GA despite the low sequence entropy at these positions. Interestingly the most successful mutations were non-natural variants [9].

In addition to increasing activity on non-phosphorylated substrates it would be advantageous to extend the applicability of TK by enhancing activity on aliphatic, non-hydroxylated aldehydes. Typically, activity of wild type TK on these substrates is only 5%-35% of that for α-hydroxylated aldehydes such as GA. The active site variant libraries described above were screened for TK catalysed production of 1,3-dihydroxypentan-2-one (DHP) using the aldehyde substrate propioanldehyde (PA).

Twenty-six distinct mutants were identified with increased specific activity on PA relative to wild type. These variants represented eight of the nineteen residue libraries. Five of the eight libraries yielding enhanced activity on PA had been previously identified through screening for enhanced activity on GA. These included the group of residues which interacts with the phosphate group of natural substrates, Arg 358, His 461, and Arg 520. The phylogenetically variant residues in the active site second shell, Ala 29 and Asp 259, were also identified. A third group

of residues not previously identified yielded variants with the greatest increase in activity on PA. This group was made up of conserved residues His 26, Asp 469 and His 100. These residues form a pocket in the active site and directly interact with the hydroxyl group at C2 of erythrose-4-phosphate. The greatest increase in activity on PA was observed with D469T which demonstrated a 5-fold improvement in specific activity over wild type [10].

Variation of phylogenetically variant residues or those interacting with the phosphate group of natural substrates led to enhanced activity on both GA and PA [10, 46]. In contrast, mutation of hydroxyl interacting residues produced variants with enhanced substrate specificity for PA over GA. The D469Y mutant displayed the greatest substrate specificity, with a 64-fold higher activity on PA relative to GA [10].

Wild type TK catalyses the production of L-erythrulose from GA and HPA with 95% ee, but 3S-DHP is only produced in 58% ee using PA and HPA. To identify variants with increased stereoselectivity for the production of 3S-DHP, Smith *et al* screened the three variant libraries of residues that interact with the hydroxyl group of natural substrates, His 26, Asp 469 and His 100. Significant increases in stereoselectivity were obtained with the D469E variant which produced 3S-DHP in 90% ee. Interestingly the majority of His 26 variants lead to the formation of 3R-DHP and H26Y produced 3R-DHP in 88% ee [11].

This work was extended to establish the enantioselectivity of wild type TK and selected variants on linear aliphatic aldehydes of increasing length and cyclic aldehydes. Compared to wild type TK, D469E TK produced products in greater yields

for the longer chain and cyclic aliphatic aldehydes although yield did decrease as chain length increased. Although yields were lower, D469E displayed enhanced stereoselectivity with longer chain aldehydes and over 99% ee for cyclic aldehydes cyclopropanecarbaldehyde and cyclopentanecarbaldehyde. H26Y gave product with lower yields but the reversal of ee was maintained across all the aldehydes tested, with the highest ee noted for butanal at 92% [47].

Although work to date has been limited to single point variants and residues in close proximity to the active site, considerable success has been achieved in the engineering of TK. Activity on both non-phosphorylated and non-hydroxylated aldehydes has been improved by 5-fold relative to wild type, and enantioselectivity has also been improved for the non-natural substrates. Surprisingly, a single point mutation was also able to reverse the enantioselectivity of the enzyme. The variants identified further expand the potential applications of TK for industrial synthesis applications. However, there is significant potential to further engineer TK to the point where non-natural substrates convert at the same rate and with the same exquisite stereoselectivity as the natural substrates.

1.3 Current methods in enzyme engineering

Directed evolution can be used to engineer the catalytic properties of enzymes and has been used successfully to modify properties such as specificity, selectivity and enantioselectivity. The general process of directed evolution can be broken down into three steps; generation of a variant library, screening for a desired property and selection of positive variants for the next cycle. Although most directed evolution experiments follow this overall process, there are many different ways to carry out each step. The main limitation in directed evolution is the size of the library that can be screened. Typically, libraries of 10^3 to 10^6 variants can be screened using high-throughput techniques and robotic equipment. In some cases a desired attribute can be linked to a growth advantage in bacteria, allowing significantly larger libraries (up to 10^{9-13}) to be screened. Unfortunately for most directed evolution experiments this cannot be applied and we are limited to libraries containing thousands rather than millions of variants. In some situations we are limited to even smaller libraries, for example where a suitable colorimetric or fluorogenic assay is not available.

The limitation in the size of libraries means we can only sample a tiny fraction of the possible sequence space. A protein with 300 amino acids has 20^{300} distinct possible sequences so even with a large screening effort of 10^6 variants we can only sample a minute fraction of the potential sequence space. The strategy chosen to produce the variant library must therefore be selected very carefully in order to target the best section of sequence space for the desired property.

1.3.1 Error-prone polymerase chain reaction

The most commonly used method to produce a library is error-prone polymerase chain reaction (epPCR). Error-prone PCR involves the introduction of random copying errors through imperfect reaction conditions (e.g. by adding Mn^{2+} or Mg^{2+} to the PCR reaction mixture) usually with the aim of introducing approximately one mutation each time the gene is copied [48]. Such a technique applied to a 300 amino acid protein will produce a library of 5,700 potential variants, easily screenable even accounting for the oversampling required. In such examples it is usually possible to find a variant with improved properties although several cycles may be required as multiple variations are usually needed to generate the required level of improvement in a particular property. Previous experiments have demonstrated that on average 30% - 50% of random mutations are deleterious, 50% - 70% are neutral, and just 0.01% - 0.5% are beneficial [49]. In our example of a 300 amino acid protein we could expect to find 1 – 30 beneficial mutations in the 5,700 variant library.

Using epPCR the full length of the protein sequence can be probed; but the cycling nature of directed evolution, and the introduction of one change at a time, means that an evolutionary trajectory is entered once the first variant has been selected. This trajectory theoretically limits the potential optimal sequence that can be achieved. If all the individual variations that constitute an improved activity are independently beneficial and additive in nature then this is not a problem because all trajectories should arrive at the same optimal solution. Unfortunately, variation

at one site in a protein sequence often requires the simultaneous variation at another site to be beneficial.

Following several rounds of selection directed evolution experiments often plateau with further rounds failing to generate improvements. This has been suggested to represent protein sequences becoming stuck on fitness peaks in sequence space. Usually this can be overcome by one or two rounds of selection for stabilising mutations, it is hypothesised that the accumulation of beneficial mutations gradually reduces stability until no further mutations can be tolerated [49]; introduction of stabilising mutations allows the protein to tolerate further mutations. We can envisage a situation where an incredibly beneficial variant is so destabilising that it cannot be introduced without the simultaneous introduction of a specific stabilising variation, which by itself may have no impact on the stability of the wild type sequence. In such a situation, it would be impossible to identify the beneficial variant even following pre-stabilisation of the protein fold.

1.3.2 Saturation mutagenesis

Another common method of library generation is saturation mutagenesis. This approach requires the selection of one, or a small number of sites in the protein sequence; randomised codons are then used in PCR primers to generate all the possible variants at the individual sites. Single site libraries created in this manner are small enough to allow the use of conventional GC or HPLC methods for screening and therefore allow selection for properties that are intractable with high throughput techniques. However, as more sites are added to the library, the size quickly becomes intractable to screening. Complete saturation at three sites would

create 7,999 potential variant sequences (including 57 single point mutants and 1,083 double mutants), four sites results in approximately 1.6 x 10^5 possible sequences, representing the approximate upper limit even for high throughput screening techniques. Such a mutagenesis strategy generally requires structural information and a good understanding of the functionally important residues. Sites are normally selected based on their proximity to the active site and on their hypothesised role in specific elements of the reaction being catalysed.

Saturation mutagenesis overcomes some of the issues which limit epPCR, allowing multiple amino acids to be varied simultaneously means we can identify combinations of variations that may be deleterious or neutral in isolation. Reetz *et al* identified multiple beneficial variants by saturated mutagenesis of three positions in the epoxide hydrolase enzyme from *Aspergillus niger* (ANEH), variants were screened for activity on a new substrate. 5000 variants were screened resulting in 26 unique hits. Twenty two (85%) of the resulting hits were triple mutants and four (15%) were double mutants; none were single mutants [50]. The authors did not create double and triple mutant cycles to investigate whether the multiple beneficial variants were synergistic or additive in nature but it is interesting that no single variants were identified by the screen.

1.3.3 Limitations in enzyme engineering

Many variations and combinations of the above methods have been used in directed evolution experiments. A further method, DNA shuffling, represents another technique used for library generation but this is not covered in detail here. For each enzyme engineering experiment a choice of technique is made in an effort

to maximise the proportion of beneficial variants in the limited library size. However, no one method has proved universally superior to the others and each has its own benefits and limitations.

In examples where mutagenesis is focused on residues likely to confer beneficial properties, positions are usually selected based on their proximity to the active site. Where an attempt is made to introduce multiple mutations, such sites are often selected based on their proximity to each other [51]. Such a simple selection strategy illustrates the limitations of current enzyme engineering approaches. Enzyme properties such as substrate specificity are sometimes determined by sites distant from the active site. Hedstrom *et al* successfully engineered Trypsin serine protease to accept Chymotrypsin substrates, but to do so required mutation of both the binding pocket and distributed surface loops which don't interact directly with the substrate. A particular residue (172) was identified as a determinant of substrate specificity through interaction with both the binding pocket residues and surface loops [52, 53]. Using proximity to the active site to select residues for mutagenesis, it would not be possible to engineer a Trypsin enzyme to accept Chymotrypsin substrates.

Modern computational techniques such as structural modelling and statistical coupling analysis provide a new resource to refine our choice of enzyme residues to target in enzyme engineering experiments. In addition to supporting library design, structural modelling can be used to rationalise positive hits identified in a successful enzyme engineering campaign. This new information can be cycled around for further potential benefit in later rounds of design. Statistical coupling analysis has

the potential to identify relationships between residues that are not apparent from examination of the structure. Such information could lead to the production of multiple variant libraries that are not limited to a proximal shell around the active site. In the following sections these techniques are discussed in further detail.

1.4 Computational methods for enhanced of enzyme engineering

1.4.1 Computational structural modelling

Crystal structures provide a great deal of information that can be utilised in the generation of hypotheses on enzyme mechanism and to guide the design of variant libraries for enzyme engineering. Protein crystallisation does however have various limitations- the time required to produce crystals is often limiting; the nature of the crystallisation process renders it impossible to derive reactive structures that only exist transiently; this process also limits crystal structures to static structure solutions, crystal structures often fail to indicate the dynamic nature of a particular protein structure. Computational docking of ligands in protein active sites allows us to address some of the issues that limit crystal structures of proteins and extends the use of structure data. With a protein structure as a starting point, computational docking allows us to generate multiple structures representing the likely conformations of different ligands bound in the active site of the protein in a fraction of the time required to achieve this experimentally. We can also model the structures of intermediate, transient, structures within the protein active site. This would not be possible experimentally. Computational modelling has even been extended to design *de novo* functional enzymes, Baker *et al* have utilised computational enzyme design to produce both kemp elimination catalysts [54] and a Diels-Alderase [55].

Computational automated docking involves searching for a conformation of a ligand in an active site that has minimal energy. The energy of the ligand in the context of

the active site is calculated using a molecular mechanics forcefield with parameters for all the different types of interaction that contribute to the bound energy of the ligand. There are two main categories of automated docking methods: matching methods and docking simulation methods. In matching methods, a model of the active site is created and rigid ligands are docked into this model. Dock is a good example of an automated docking algorithm using a matching method. In contrast to matching methods, docking simulation methods involve exploration of flexible ligand translations and orientations until an ideal conformation is found within the protein active site. Docking simulation methods are more computationally intensive than matching methods but this is not a problem unless a large chemical database of lead compounds needs to be screened against an active site. Docking simulation methods allow the docking of a flexible ligand and the use of a more detailed molecular mechanics forcefield which can more accurately calculate the binding energy of the ligand.

Although other programs such as DOCK are available for ligand-protein docking, Autodock is the best known example of a docking simulation method. This program couples a well optimised empirical molecular mechanics forcefield with an efficient search algorithm. These attributes, together with the fact that Autodock is freely available, have led to a good support network for this program and many publications utilising it. Docking simulation aims to identify the minimum energy binding conformation in a huge energy landscape, resulting in a very computationally intensive problem requiring sophisticated search algorithms to reduce the search space to a tractable size. Autodock (Version 3.0.5) uses a

Lamarckian genetic algorithm and an empirical free energy function to find the minimal energy binding conformation

A genetic algorithm is a search technique that utilises the principles of biological evolution to find a solution which exhibits maximum fitness. In the genetic algorithm used by Autodock, the state of the ligand in the context of the protein is defined by a set of state variables which describe the translation, orientation and conformation of the ligand. Each state variable corresponds to a gene in the genetic algorithm. The state of the whole ligand corresponds to the genotype, and the atomic coordinates of the ligand correspond to the phenotype. Finally, the fitness of the ligand state is defined by the total interaction energy of the ligand with the protein.

The genetic algorithm initiates with a random set of genotypes which makes up the population. Individuals with better fitness in the initial population are allowed to reproduce whereas others die. Reproduction involves the mating of random pairs of individuals, during this process crossover takes place with new individuals inheriting genes from either parent. Some of the offspring also undergo random mutation where one gene changes by a random amount.

Autodock 3.0.5 combines a genetic algorithm with a local search method which performs energy minimisation. The genetic algorithm stage is a global search of the energy landscape and allows transitions over energy barriers which may separate energy valleys. The local search method uses the same forcefield as the genetic algorithm to make fine adjustments and find the energetic minimum within the energy trough. The step size of the local search method is adaptive, becoming

smaller in response to a series of consecutive successes. Following a local search the individual can be replaced by the result of the local search. As the local search is carried out at the phenotypic level, this is an example of an inverse mapping function, a genotype can be derived from a given phenotype. The term "Lamarckian genetic algorithm" refers to Jean Baptiste de Lamarck's belief that phenotypic characteristics acquired during an individual's lifetime can become inheritable traits [56].

The scoring function used by Autodock to represent fitness is based on an empirical free energy function that can reproduce experimentally derived binding constants of ligands. The energy function consists of five entropic terms which represent Van der Waals forces, H-bonding, electrostatic forces, entropy of the ligand and solvation. Coefficients for each of these terms have been determined using linear regression from a set of protein ligand complexes with known binding constants. Autodock utilises a fast grid based method for energy evaluation in which ligand-protein pairwise interaction energies are precalculated and used as a look up table during the simulation. Summations are performed for all ligand (i) and protein (j) atom pairs as well as all ligand atom pairs three or more bonds apart (Equation 1.1).

$$\Delta G = \Delta G_{vdw} + \Delta G_{Hbond} + \Delta G_{elec} + \Delta G_{tor} + \Delta G_{sol}$$

$$\Delta G_{vdw} = \sum_{i,j}\left(\frac{A_{ij}}{r_{ij}^{12}}\frac{B_{ij}}{r_{ij}^{6}}\right)$$

$$\Delta G_{Hbond} = \sum_{i,j} E(t)\left(\frac{C_{ij}}{r_{ij}^{12}}\frac{D_{ij}}{r_{ij}^{10}} E_{Hbond}\right)$$

$$\Delta G_{elec} = \sum_{i,j}\frac{q_i q_j}{\varepsilon(r_{ij})r_{ij}}$$

$$\Delta G_{tor} = N_{tor}$$

Equation 1.1 Energy function utilised by Autodock 3.0.5 calculations of binding energy.

The three terms that describe the interaction energies of atom pairs include a Lennard Jones 12-6 van der waals term, a directional 12-10 H-bonding term in which E(t) is a directional weight based on the angle between the H-bond donator and the H-bond acceptor atom, and a coulombic electrostatic potential with a distance cut off. Ligand binding is accompanied by unfavourable entropy as the ligands conformational degrees of freedom are reduced. This contribution to the total binding energy is proportional to the number of SP3 bonds in the ligand and is represented by Ntor. The grid based method for energy evaluation used by Autodock limits the choice of solvation terms to use as most of these methods are based on surface area calculations. Autodock uses the pairwise volume based method of Stouten *et al*, in which the percentage of volume around a ligand atom that is occupied by protein atoms is weighted against the atomic solvation parameter of the ligand atom [57]. This gives the desolvation energy contribution from the ligand atom upon binding.

1.4.2 Statistical coupling analysis

There are many examples of epistatic coupling within proteins. Signalling proteins such as GPCRs rely on information transfer between distant residues [58, 59], the exquisite specificity of antibodies generated through B-cell maturation is often determined by residues distant from the antigen binding site [60], co-operative binding of oxygen in haemoglobin is mediated by networks of interacting residues [61-64]. In all of these examples, energy transduction mechanisms have evolved which make possible the highly adapted functions of these varied proteins.

Identification of these interacting networks of residues could enable enhanced engineering of new properties into protein scaffolds.

A new method termed Statistical Coupling Analysis (SCA) has been developed to identify epistatically coupled networks of residues [65]. SCA utilises evolutionary data contained within multiple sequence alignments (MSA's) to identify co-evolved positions within a protein sequence. The method is based on two hypotheses, firstly that without evolutionary constraint, the amino acids at a specific position in an MSA will approach their mean distribution in all proteins. Secondly, that functional coupling of two positions in a protein should mutually constrain their evolution. If two positions are functionally coupled, alteration of the distribution of amino acids at one site (by the removal of sequences from the MSA) should results in a change in the distribution of amino acids at the other site. Importantly, this does not require that the level of conservation change at the second site, just that the distribution of amino acids be altered [65].

In the first application of the SCA technique, Lockless *et al* applied the method to the identification of coupled sites within the PDZ domain, a small protein binding motif [65]. PDZ domains can be divided into two classes based on their target sequence specificity. The identity of the residue at position 76 in the PDZ domain is known to be an important determinant of this property. Lockless *et al* constructed a multiple sequence alignment consisting of 274 eukaryotic PDZ domains, including 4 PDZ domains with known structures. This MSA was then perturbed by removing all the sequences apart from those with a histidine at position 76. In response to this perturbation, the distributions of amino acids at several other positions in the MSA

were found to be altered. These sites are statistically coupled to position 76. Positions identified included both sites in close proximity to position 76 and other surface residues which are involved in sequence recognition. Coupling to proximal cooperative surface sites can be explained by energy propagation through the bound substrate. A third, unexpected, class of residues were also identified by SCA; these sites were a long distance from position 76 and were found in the core or on the opposite surface of the PDZ domain. Although the mechanism and function of this coupling is unknown, pathways of sterically connected, coupled residues were identified that connect position 76 to these distant residues. These pathways may represent routes of signal transduction through the tertiary structure of the protein. Lockless *et al* went on to verify the coupling interactions identified through thermodynamic mutant cycle analysis. This verification demonstrated good correlation between the statistically coupled sites and the thermodynamically coupled sites including those both proximal and distant from position 76.

Since this early demonstration of statistical coupling analysis, the technique has been applied to several different protein folds including G-protein coupled receptors, haemoglobin and serine proteases [66]. In these examples, Suel *et al* hypothesised that if networks of coupled residues exist and are conserved, perturbations at positions within the network should redundantly identify each other. In each of the examples above, Suel *et al* carried out global perturbation analysis and displayed the resulting statistical coupling energies on a matrix with perturbations represented by columns and positions represented by rows. Using

two-dimensional cluster analysis, global patterns of statistical coupling could be identified in the protein folds.

Of particular interest is the analysis of statistical coupling in serine proteases. A multiple sequence alignment was constructed consisting of 616 chymotrypsin serine proteases. Global SCA was carried out involving 69 site specific perturbations. Iterative two-dimensional clustering of the resulting matrix identified two distinct clusters, each containing positions that demonstrate similar patterns of coupling. One of the clusters was found to encompass both the S1 binding pocket and the surface loops known to determine substrate specificity. Residue 172 was also present in this cluster. Although distant from the active site and the binding pocket, SCA was able to identify positions known to determine substrate specificity.

Substrate specificity of the transketolase enzyme has previously been modified using saturation mutagenesis. Improved specific activity towards non-natural substrates such as glycoaldehyde [9] and propionaldehyde [10] has been engineered into transketolase by targeting residues in close proximity to the TPP cofactor. Phylogenetic information was also used to select residues but in both cases no residues more than 10Å from the ThDP cofactor were modified. In the examples above, single point variant libraries were constructed and screened using a colorimetric assay or conventional HPLC. Although hits were identified for different non-natural substrates within these libraries, the screening process limited the number of residues that could be probed and multiple simultaneous mutations could not be assessed. Statistical coupling analysis was able to identify

sites in chymotrypsin that appear to have co-evolved to determine substrate specificity. Identification of such networks in the transketolase enzyme may allow screening to be directed towards areas of sequence space unidentifiable by traditional structure and phylogeny directed selection methods.

1.5 Conclusions

The natural activity of transketolase can be applied to many applications where regio- and stereo-specific carbon-carbon bonds need to be created. This activity is hugely sort after in the synthesis of fine chemicals and pharmaceuticals. In addition to the added specificity afforded by transketolase over more traditional chemical processes, the use of a biocatalyst reduces the need for harsh reaction conditions, organic solvents, and multistep processes. To date, all biotransformations using transketolase have used the wild type molecule, an enzyme which has evolved over millions of years to catalyse two specific reactions *in vivo*. Through protein engineering, the tools exist to tailor-make transketolase variants with improved properties desirable to the fine chemical and pharmaceutical industries.

Arguably the most powerful method in enzyme engineering is directed evolution. However, limitations in library size impose limits on the sequence space that can be searched using this technique. Effort is being made to reduce these size limitations through advancements in high throughput screening and improved ligation steps. But, as long as there is any limit at all in library size, it will be necessary to target the sequence space to be searched to areas most likely to lead to functional improvements. Various strategies can be adopted to select residues to target; from simple spatial constraints to more complex phylogenetic strategies, such as common ancestor rebuilding. We can also take a rational approach to choose changes that are likely to improve characteristics. Most of these selection methods utilise one branch of knowledge and data. Here we attempt to utilise sophisticated computational techniques to merge information sources, creating a more

sophisticated knowledge base that can be used to direct the creation of more intelligent variant libraries.

Crystal structures of proteins represent one of the richest data sources available to us as enzyme engineers. But, these structures are limited to long-lived, static targets through the nature of crystallisation. Our understanding of the nature of non-covalent interatomic interactions and data from ligand binding experiments allow us to computationally model the energy landscape of substrate-protein interactions, and predict conformations in which substrates are likely to bind. This extends our understanding of function and structure beyond what is possible with X-ray crystallography alone. Computational docking of substrates can identify residues directly involved in substrate interactions as well as rationalising the results from previous library screens.

The second great data source available to protein engineers is the vast, ever growing, collection of sequence data. Using statistical coupling analysis we can delve into this data and discover energetic coupling between sites within proteins. The true power of this technique becomes apparent when the networks of energetic coupling are superimposed onto the three-dimensional structure of the protein. Using the results from computational docking of substrates together with the knowledge of coupled networks of sites in the protein structure we can start to target our variant library very efficiently.

Structural and sequence data represents the culmination of a 3.5 billion year experiment in evolution. It is evolution which ties each of these data sets inextricably together. Random mutation of sequence affects the structure of

proteins, altering the chemical properties of active sites, leading to changes in the function of enzymes. These changes in enzyme function drive evolution. Only when each class of data is viewed in the context of the others does its true potential become apparent. Using the most modern computational methods, we hope to develop rich, combinatorial, information which can help direct the production of variant libraries to those regions which hold the most potential for improved activities.

2 Mechanistic analysis of *Escherichia coli* transketolase by *in silico* docking of substrates in the active site

2.1 Introduction

The carbon-carbon bond forming ability of TK, along with its broad substrate specificity, makes it very attractive as a biocatalyst in industrial organic synthesis [8, 39, 67]. If the ketol donor in the reaction is replaced by hydroxypyruvic acid (HPA) the reaction is rendered irreversible by the release of carbon dioxide . The use of α-hydroxyaldehydes as acceptors together with HPA as the ketol donor allows the creation of enantiomerically pure chiral triols. The potential for producing non-phosphorylated products simplifies their isolation and avoids the requirement to remove phosphate from the product [8, 67]. The TK enzyme from *E. coli* is a preferable biocatalyst to that from yeast due to the higher specific activity of *E. coli* TK towards HPA [68]. Therefore, it is useful to establish that the structural and mechanistic information gained for yeast TK is equally applicable to TK from *E. coli*, for which there is also a crystal structure available [14]. Considerable mechanistic detail has been obtained for *S. cerevisiae* and *E. coli* TK from crystal structures and NMR experiments [7, 18, 21]. Crystal structures have been obtained for the DE4P acceptor substrate bound to the yeast-TK active-site [18], and also for the enamine intermediate formed upon reaction of the yeast enzyme with the DX5P donor substrate [7]. More recently, *E. coli* TK structures were obtained in covalent complexes with DF6P (2R8P.pdb) and DX5P (2R8O.pdb) prior to enamine formation, as well as a non-covalent complex with the cyclic form of DR5P (2R5N) [21].

Despite these impressive structural studies, there is still little information regarding the mode of binding for the donor substrate before it reacts to form the covalent complex and subsequent enamine intermediate, or for the aldehyde acceptor binding in the presence of the enamine intermediate. While crystal structures offer valuable insights into how ligands interact with protein binding-pockets, the binding of enzyme substrates is more challenging as the substrate will usually only bind transiently in the correct conformation before reaction occurs. Notably, for the crystal structure of DE4P bound to the TK active-site [18], the original aim was to solve the structure with DF6P, but the electron density of the resulting structure revealed that the donor substrate had been cleaved into DE4P by TK during the crystal formation process. This exemplifies the difficulties in obtaining structures of substrates bound in active sites.

There is considerable interest in the further development of TK as an efficient biocatalyst, with rational mutagenesis and directed evolution approaches previously having resulted in mutants with altered or improved activity [9], substrate specificity [10, 69] and enantioselectivity [11]. However, further protein engineering to accept an even broader range of substrates would benefit from methods to rationalise the behaviour of existing mutants in structural terms, and to understand how non-natural substrates bind to the active site of this enzyme. Unlike DE4P, many of the non-natural aldehyde acceptor substrates so far examined for biocatalysis with TK, do not contain a phosphate group or an α-hydroxyl group, which are both known to have an important role in substrate recognition [18]. Furthermore, the engineering of TK variants that are less

susceptible to substrate or product inhibition will require a better understanding of the roles played by various residues within the enzyme active-site.

Automated computational docking presents an alternative and complementary means to x-ray crystallography for probing the binding of reactive substrates in short-lived conformations, and also for studying the many non-natural substrates and products, for which crystallography would be time-consuming. Computational automated docking involves searching for the conformation of a ligand bound within in an enzyme active-site that has minimal energy. AutoDock is the best known example of a docking simulation method in which the active site is created and ligands are docked into an enzyme active-site model with an accurate calculation of the binding energy. Flexible ligand translations and orientations are explored until an ideal conformation is found within the protein active site [70]. The observation that very little structural change occurs in the TK active site upon formation of covalent complexes with substrates [21], suggests that it would be an excellent system for docking different substrate complexes without requiring the modelling of amino-acid sidechains for induced fit.

Here we show that automated docking can produce accurate models of substrates bound in the active site of TK. The accuracy of our results is demonstrated by comparison of a computationally derived structure with the crystal structure of DE4P in yeast TK. Further validation is provided by a correlation of experimentally derived Km values for yeast TK, with those calculated from computationally derived docking energies in AutoDock. Having demonstrated the accuracy of the approach we explored the differences and similarities between the binding of DE4P in the

active-sites of *E. coli* TK and yeast TK, and the impact this may have on function. We then examined the binding of natural and non-natural substrates in *E. coli* TK in non-covalently associated complexes that are too reactive to be obtained by crystallography. We also discuss the implications on the potential nucleophilic attack of the deprotonated ThDP cofactor upon the ketol substrate at an unusual Bergi-Dunitz angle, and also the mechanism for ring opening of the cyclic form of D-ribose-5-phosphate. These results will have a significant bearing on attempts to further engineer TK as a biocatalyst for organic synthesis, as well as generating useful hypotheses for future experimental studies to understand the enzyme mechanism of TK.

2.2 Materials and methods

2.2.1 AutoDock 3.0.5

The open source AutoDock software version 3.0.5 was used for all the automated docking reported. AutoDock combines a Lamarckian Genetic algorithm with an empirical free energy function to obtain ligand docked conformations [70]. Substrate docking models were obtained using the *E. coli* TK structure 1qgd.pdb with a cubic grid in the active site of sides 80 Å. Defaults were used for docking each substrate except for the following: the maximum number of energy evaluations was increased to 1 million, the number of genetic algorithm runs was increased from 10 to 200, and the grid spacing used was 0.375 Å. AutoDock performed a cluster analysis to each final conformation obtained from the 200 GA runs such that two conformations with an RMSD less than 0.5 Å are stored in the same cluster. Clusters are output in ranked order of increasing energy following completion of analysis. Manual visual analysis of docked conformations and further analysis of the docked conformations was carried out with Pymol and Ligplot.

2.2.2 Docking of D-erythrose 4-phosphate in yeast TK

D-erythrose 4-phosphate (DE4P) was removed from the yeast TK PDB file 1NGS. AutoDock was used to re-dock the substrate back into the binding site. Grid centre and size used for AutoDock run: (-12.645, 56.02, 19.419) 80 Åx80 Åx80 Å.

2.2.3 Docking of D-erythrose 4-phosphate in *E. coli* TK

DE4P was docked into the binding site of *E. coli* TK (1QGD). Grid centre and size used for AutoDock run: (-10.6, 27.6, 36.4) 80 Åx80 Åx80 Å.

2.2.4 Creation of a model of the ThDP-enamine intermediate in *E. coli* TK

The ThDP-enamine intermediate was docked into *E. coli* TK (1QGD). Grid centre and size for AutoDock run: (-10.0, 28.1, 36.0) 80 Åx80 Åx80 Å.

2.2.5 Docking DE4P and glycolaldehyde in ThDP-enamine complexed forms of yeast and *E. coli* TK

DE4P was docked into the yeast ThDP-enamine-TK complex (1GPU) and in the modelled *E. coli* ThDP-enamine-TK complex. Glycolaldehyde (GA) was docked into the modelled *E. coli* ThDP-enamine-TK complex. Grid centres and sizes were (-6.6, 56.7, 18.4) 60 Åx60 Åx60 Å for DE4P in yeast ThDP-enamine-TK, and (-11.4, 26.3, 36.4) 60 Åx60 Åx60 Å for DE4P and GA in *E. coli* ThDP-enamine-TK.

2.2.6 Docking of natural and non-natural aldehyde substrates into *E. coli* TK

PDB files for the ten TK substrates for which there are published K_m values, and also fluoropyruvate, found to be a potential inhibitor (unpublished data), were generated using the Dundee PRODRG server [71]. Each substrate was docked into the active site of *E. coli* TK. Preliminary docking identified two docking regions within the binding funnel of *E. coli* TK for some of these substrates. Grid sizes and positions were altered to obtain docked conformations for each substrate in the binding region closest to the ThDP cofactor. For some substrates the grid centres were adapted to avoid inaccessible pocket "traps" within the protein. Grid centres and sizes were as follows (grid centres in brackets):

Hydroxypyruvate:	(-15.991 21.945 37.096)	60 Å x 60 Å x 60 Å
Acetaldehyde:	(-18.344 24.016 40.547)	60 Å x 60 Å x 60 Å
D-erythrose 4-phosphate:	(-18.344 24.016 40.547)	40 Å x 40 Å x 40 Å
D-erythrose:	(-18.344 24.016 40.547)	40 Å x 40 Å x 40 Å
D-glyceraldehyde 3-phosphate:	(-10.586 27.153 35.586)	80 Å x 80 Å x 80 Å
D-glyceraldehyde:	(-18.344 24.016 40.547)	40 Å x 40 Å x 40 Å
D-ribose 5-phosphate:	(-10.586 27.153 35.586)	80 Å x 80 Å x 80 Å
D-ribose:	(-10.586 27.153 35.586)	80 Å x 80 Å x 80 Å
Glycolaldehyde:	(-15.991 21.945 37.096)	60 Å x 60 Å x 60 Å
Xylulose 5-phosphate:	(-10.586 27.153 35.586)	80 Å x 80 Å x 80 Å
Fluoropyruvate:	(-15.991 21.945 37.096)	60 Å x 60 Å x 60 Å

Docking energies (ΔG) were converted to a K_m values using $\Delta G = -RT.\ln(K_m)$, where R is the gas constant and T is the temperature in Kelvin.

2.2.7 PyMol Molecular Graphics System

All visualisations of docked conformations were produced using PyMol, available from http://www.pymol.org [72].

2.3 Results and discussion

2.3.1 Automated docking of D-erythrose-4-phosphate in the active site of yeast TK

Nilsson *et al* (1997) previously solved the crystal structure for a substrate protein complex of DE4P bound in the active site of yeast TK [18]. The original aim of their crystallisation was to solve the structure with DF6P but the electron density of the resulting structure would not fit a six-carbon chain and the conclusion was drawn that the donor substrate had been cleaved into DE4P by TK during the long period necessary for crystal formation. This cleavage would also yield the α,β-dihydroxyethyl thiamine diphosphate intermediate but this would degrade in a few hours into ThDP and glycolaldehyde explaining the lack of an intermediate in the electron density map.

To assess the accuracy and potential of automated computational docking on the substrates of TK we initially docked DE4P into the empty active site of yeast holo-TK, to recreate the substrate-holoenzyme complex. AutoDock accurately predicts the binding conformation of DE4P producing a docked structure within 1.65 Å RMSD of the crystal structure (Figure 2.1). The hydrogen bonding network of the docked substrate is accurately predicted by AutoDock, supporting the role and evolution of this network in determining the stereospecificity of TK. In the crystal structure the C1 aldo carbon atom of the acceptor substrate is positioned 4.16 Å away from the reactive C2 carbon of the thiazolium ring of ThDP. This distance is sufficient to allow the presence of an enamine intermediate in a reactive conformation with the acceptor substrate. The computationally docked

conformation positioned the C1 aldo carbon 4.81 Å away from the thiazolium ring of ThDP. Although AutoDock docked DE4P slightly further away from the ThDP reactive centre, it was still within an acceptable distance to react in the presence of the intermediate.

The main discrepancy between the experimentally determined structure and that created by computational docking was the position of the phosphate group. In the computational docking the phosphate group of DE4P was pulled closer to the side chains of the Arg 358, Arg 520, Ser 385 and His 461 residues (*E. coli* numbering) at the entrance to the binding funnel (by just over 1 Å). This has the effect of pulling DE4P slightly out of the funnel away from the ThDP cofactor (Figure 2.1). The interaction between the phosphate group and the positively charged arginine residues of yeast TK is strongly affected by the electrostatic interactions between these groups. The force field of AutoDock includes a term to model electrostatic interactions but the discrepancy between the modelled and the crystal structures may be explained by errors in the electrostatic term of the forcefield. While all of the thirty ligand-protein complexes used to calibrate the AutoDock forcefield included H-bond interactions, only a small proportion involved electrostatic interactions of explicitly charged groups [70]. Electrostatic interactions between these groups would also be strongly influenced by pH which may further explain the slight discrepancy. However, the TK structure itself was resolved to 2.4 Å and so a 1 Å shift is acceptable within error. Despite the possible error in the modelling of phosphate binding, the results show that AutoDock is capable of reproducing accurate docked conformations of substrates in the active site of TK.

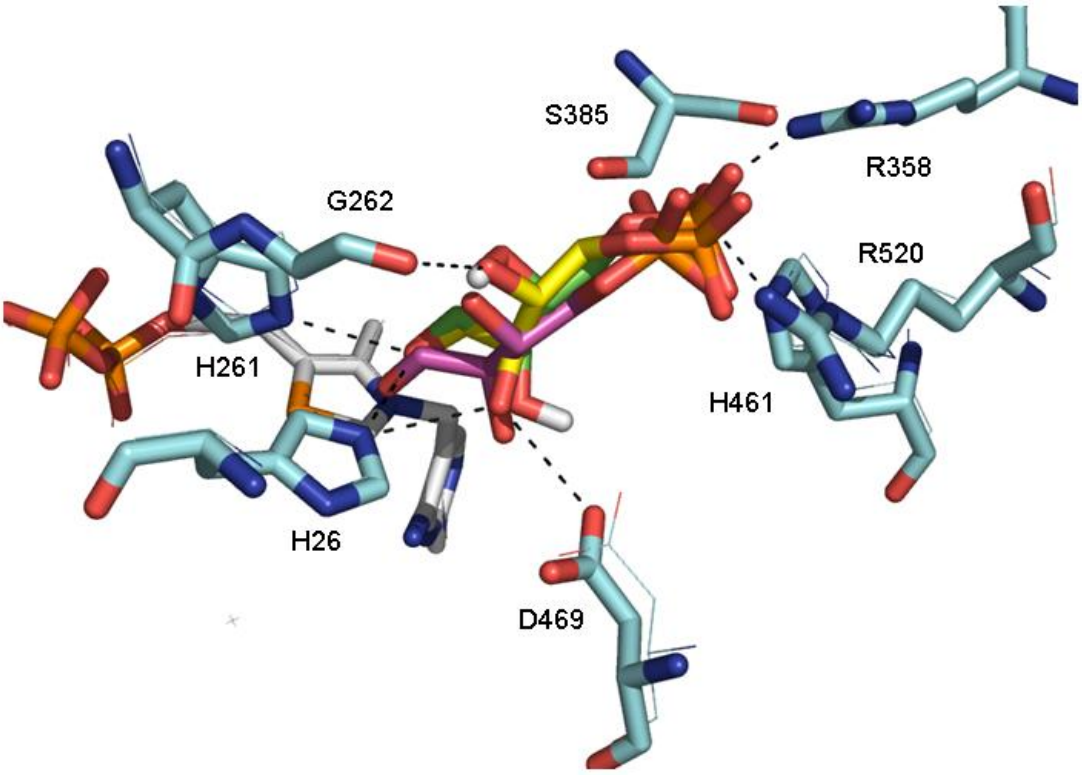

Figure 2.1 Comparison of D-erythrose-4-phosphate (DE4P) binding in yeast and *E. coli* transketolases. *E. coli* TK residues are shown as blue sticks and the aligned yeast TK residues are shown as lines. Three DE4P structures are compared: (magenta) crystal structure in yeast (1NGS); (yellow) docked into the uncomplexed *E. coli* TK structure (1QGD); (green) re-docked into the yeast TK structure (1NGS).

2.3.2 Automated docking of D-erythrose-4-phosphate in the active site of *E. coli* TK

The active sites of yeast and *E. coli* TK, including the orientation of conserved residues, are nearly identical. For *E. coli* TK, structures are available in covalent complexes with DF6P (2R8P.pdb) and DX5P (2R8O.pdb), as well as a non-covalent complex with the cyclic form of DR5P (2R5N) [21]. However, no crystal structure exists for the non-covalent complex of *E. coli* TK with DE4P. If *E. coli* TK binds DE4P in the same conformation as for yeast TK then mechanistic insights derived from studies of yeast TK could be used with confidence to infer equivalent mechanistic details in the *E. coli* protein. This would be of great value as much of the work on the function of TK to date has been carried out on the yeast enzyme.

DE4P was docked into the active site of *E. coli* TK (1QGD) using AutoDock. Many of the docked conformations predicted by AutoDock involved an inversion of the DE4P, with the phosphate group oriented towards the ThDP and the carbonyl active centre of DE4P pointing out of the active site in an un-reactive conformation. This could be explained by the error in the handling of phosphate interactions. Like the arginine residues at the entrance to the active site normally involved in phosphate binding, the ThDP molecule carries an explicit positive charge. Hypothetically, the DE4P may actually be able to bind in this orientation and form an un-reactive inhibitory complex. If this is not an artefact of computational docking it may therefore have implications for substrate inhibition of TK at high concentrations.

AutoDock also docked DE4P in the reactive orientation in *E. coli* TK (Figure 2.1). This conformation is very similar to that of DE4P bound in yeast TK (compared in Figure 2.1). The phosphate group is positioned close to the entrance of the active site and interacts with residues Arg 358, Arg 520, Ser 385 and His 461. These interactions are equivalent to those maintaining the position of the DE4P phosphate group in yeast TK. The carbon chain of DE4P extends down the active site of *E. coli* TK forming a hydrogen-bonding network with the side chains of several conserved residues. The C3 hydroxyl group forms an interaction with the backbone oxygen of Gly 262 that is not seen in the yeast TK bound structure. Like yeast TK, the conserved Asp 469 residue of the *E. coli* enzyme interacts with the C2 hydroxyl group of DE4P but an additional interaction is formed through His 26. The C1 aldo oxygen atom interacts with residues His 261 and His 26 in *E. coli* as

observed in yeast TK, to position the C1 aldo carbon at 4.89 Å away from the C2 atom of the ThDP thiazolium ring.

The general binding conformation for DE4P in *E. coli* TK is the same as that for yeast TK. The minor differences in the hydrogen bonding network do not change the favoured stereospecificity of the recognition and these interactions could be transiently present in the yeast structure with only a small degree of dynamic movement. The conformation of DE4P docked in *E. coli* TK supports the hypothesis that the conserved residues of the TK active sites of *E. coli* and yeast TK have the same roles in substrate binding.

2.3.3 Modelling the enamine intermediate in *E. coli* TK and docking of D-erythrose-4-phosphate into the yeast and *E. coli* TK-ThDP-enamine complexes

We have demonstrated the ability of AutoDock to accurately model the binding conformation of DE4P in yeast TK and shown that the same binding conformation is formed in *E. coli* TK. However, in the TK catalysed reaction, DE4P cannot bind productively until an enamine intermediate has first been formed between the ThDP cofactor and the ketol donor substrate. It is possible that the binding conformation of DE4P in the TK active site is different in the presence of this intermediate. Due to the reactive nature of the intermediate, DE4P would not bind and exist in the presence of the enamine intermediate for long enough to obtain crystals for structural analysis. Currently, the only way to solve the structure for DE4P bound in the presence of ThDP-enamine intermediate is to model this structure computationally. In the yeast-TK crystal structure of the ThDP-enamine

intermediate there were no significant variations in the orientations or positions of active site residue side chains relative to the ThDP bound structure. The ThDP-enamine intermediate could therefore be confidently docked into the known *E. coli* holo-TK structure using AutoDock to obtain a model of the *E. coli* TK-ThDP-enamine complex.

As seen in Figure 2.2, the complex obtained for *E. coli* TK-ThDP-enamine was nearly identical to the solved structure of the yeast TK-ThDP-enamine complex (1GPU) [7]. All the major functional interactions were present in the modelled complex, including the Glu 411 (Glu 418 in yeast TK) interaction with N1' of the pyrimidine ring [73]. The ketol donor derived enamine intermediate is co-ordinated by hydrogen bonds to the conserved *E. coli* histidine residues His 100 and His 473. The only difference between the TK-enamine interactions of yeast and TK is that in the yeast-TK complex His 481 (His 473 in *E. coli*) interacts with both hydroxyl groups of the enamine whereas in the *E. coli* complex His 473 only interacts with the α-hydroxyl group. Some other minor differences are present in the hydrogen-bonding network of the di-phosphate group but none of these differences significantly alter the position of ThDP-enamine relative to the TK molecule (Figure 2.2).

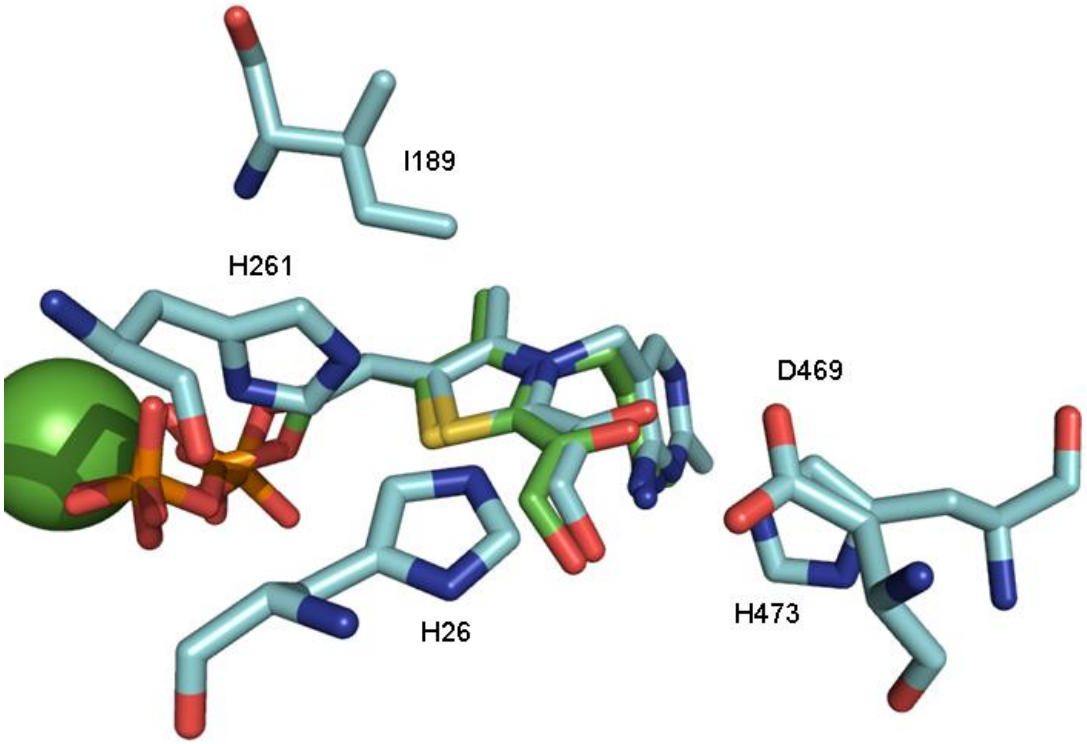

Figure 2.2 Comparison of the ThDP-enamine intermediate in yeast and *E. coli* transketolases. The ThDP-enamine intermediate in yeast TK (blue sticks) is from an available structure (1GPU), whereas that for *E. coli* TK was obtained by docking (green sticks) in 1QGD. The bound calcium ion is shown as a green sphere.

Following the creation of the *E. coli* TK-ThDP-enamine complex model, AutoDock was used to obtain docked conformations of DE4P in both the yeast (crystal structure) and the *E. coli* (modelled) TK-ThDP-enamine complexes. In each case the DE4P molecule docked in the same conformations as previously observed in Figure 2.1, in the absence of the enamine intermediate. The hydrogen bonding interactions between the TK and DE4P observed in the absence of the enamine are also preserved along with the few differences between yeast and *E. coli* TK described above. The DE4P carbonyl C1-atom is placed within 3.44 Å and 4.28 Å of the enamine α-carbon in the yeast TK and *E. coli* TK models respectively. As well as positioning the carbonyl group of DE4P in close proximity to the α-carbon of the enamine, the hydrogen-bonding network described orientates the carbonyl group

for the formation of the S-enantiomer product upon carbon-carbon bond formation as expected for TK (see Figure 2.4 a) [74].

2.3.4 Docking of other substrates in *E. coli* holo-TK

AutoDock has proven accuracy in predicting the binding affinities of ligand-protein complexes. Published kinetic data including K_m values are available for several substrates in the reaction catalysed by *E. coli* TK [1]. Ten substrates, namely glycolaldehyde (GA), β-hydroxypyruvate (HPA), D-xylulose-5-phosphate (DX5P), D-ribose-5-phosphate (DR5P), D-glyceraldehyde-3-phosphate (DG3P), D-erythrose-4-phosphate (DE4P), acetaldehyde (AA), D-ribose (DR), D-glyceraldehyde (DG), D-erythrose (DE), were docked in the binding site of *E. coli* TK and their K_m values were calculated from the binding affinities reported by AutoDock.

Initial docking using a grid that encompassed the entire binding funnel of *E. coli* TK revealed two regions in which substrates could bind in the active site of the enzyme. Following the identification of these separate binding sites, grid sizes and positions were altered to remove the non-productive and higher energy binding region, which was in the active-site funnel but further out from the ThDP molecule and the active centre of the enzyme. Such a site which involved mainly protein backbone interactions may prove to be physiologically relevant, for example resulting in substrate or product inhibition, but was not studied further here.

The calculated K_m values for the docked substrates were compared against the experimentally determined values previously published [1] as shown in Figure 2.3. The calculated K_m values we obtain from the binding energies of substrates in the

active site of TK were obtained only using the acyclic and monomeric forms of substrates. However, the values of K_m can be affected in some cases by the equilibrium between dimeric, monomeric, cyclic and linear forms which decreases the availability of the reactive substrate. DR5P, DR and DE can all form ring structures and the proportion of acyclic monosaccharides in aqueous solution have been determined respectively as 0.6% [75], 0.05% [76] and 12.1% [77]. These equilibria were used to adjust the experimental Km data obtained by Sprenger and co-workers as presented in Table 2.1 and Figure 2.3. A recent crystal structure of *E. coli* TK bound to DR5P has shown that the substrate can bind directly in the cyclic form. Therefore, the adjustment of Km values above assumed that the ring opening of the sugars is not rate limiting, and therefore does not affect the observed K_m. Other substrates such as glycolaldehyde and D-glyceraldehyde form dimers at high concentrations but in dilute aqueous solutions they become essentially monomeric and so the experimental data for these substrates were not adjusted [77]. The calculated and experimental log(K_m) values correlate well with a Pearson R^2 value of 0.82 indicating that the AutoDock algorithm is capable of predicting the conformations and binding energies of a broad range of mostly natural substrates. In all cases except DR5P, the calculated Km values are lower than the experimentally determined values indicating a systematic underestimation of Km values by AutoDock.

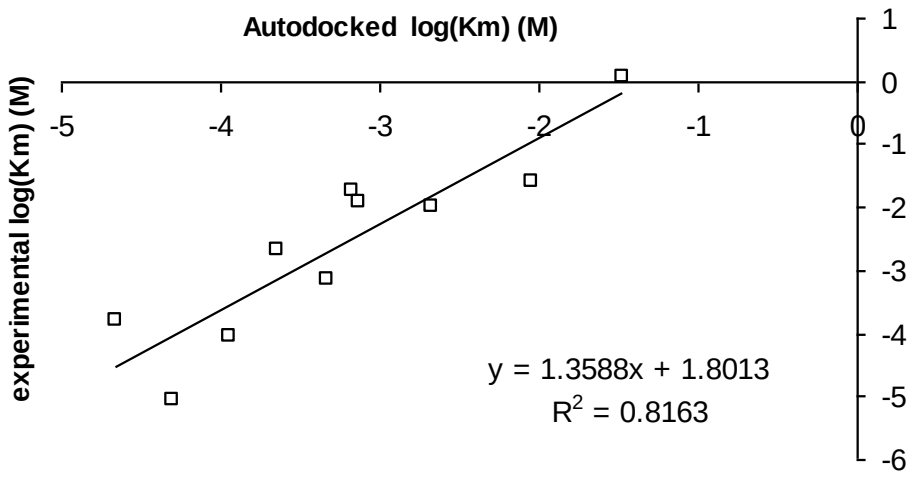

Figure 2.3 Comparison of log(K_m) values obtained experimentally and calculated from the docking energies reported by AutoDock for ten substrates of TK. All values were taken from Sprenger *et al* [1], except the values for HPA and GA which were averaged with those from Hibbert *et al* [9]. Values for D-ribose, D-ribose-5-P and erythrose, were adjusted by experimentally determined equilibrium constants for the fraction of the acyclic forms [75-77].

Substrate	K_m (calc) (mM)	K_m (exp) [a] (mM)	Distance to nucleophile [g] (Å)
D-Ribose	0.47	0.7 [b]	2.64
D-Ribose-5-phosphate	0.05	0.0084 [c]	3.13
D-Erythrose	0.67	18.15 [d]	3.93
D-Erythrose-4-phosphate	0.12	0.09	4.28
D-Glyceraldehyde	2.10	10 [e]	2.33
D-Glyceraldehyde-3-phosphate	0.23	2.1 [e]	5.01
Glycolaldehyde	9.14	24.5 [f]	2.66
Acetaldehyde	33.6	1200	2.69
β-Hydroxypyruvate	3.61	11.65 [f]	3.14
D-Xylulose-5-phosphate	0.022	0.16	4.73

Table 2.1 Comparison of *E. coli* TK K_m-values obtained by docking with those from experiment. [a] Experimental data obtained by Sprenger *et al* [1]. [b] adjusted by equilibrium for 0.05% acyclic form [76]. [c] adjusted by equilibrium for 0.6% acyclic form [75]. [d] adjusted by equilibrium for 12.1% acyclic form [77]. [e] Experimental data obtained with D,L racemate. [f] average of independent values from Sprenger *et al* [1] (glycolaldehyde 14 mM, β-Hydroxypyruvate 18 mM) and Hibbert *et al* [9] (glycolaldehyde 35 mM, β-Hydroxypyruvate 5.3 mM). [g] distances measured between either a) aldehyde carbon atom of aldol acceptor and the ThDP-enamine nucleophile, or b) carbonyl carbon atom of ketol donor and the ThDP thiazolium C2 nucleophile.

Examination of the structures of each substrate bound in the active site of *E. coli* TK reveals the same general binding conformation as seen for DE4P described above (Figure 2.4 a-b and Figure 2.5 a). Notably, all phosphorylated substrates docked with the phosphate group interacting with the conserved Arg 358, Arg 520, Ser 385 and His 461 residues at the entrance of the binding funnel as expected. This

conformation orientates the substrates so that their active centres are positioned within the binding funnel in an active conformation, but also creates small differences in their proximity to the ThDP/enamine depending on chain length which plays a role in substrate preference. The distance from the aldehyde carbon atom to the enamine nucleophile for phosphorylated substrates decreases progressively as the chain length increases from the three-carbon DG3P, and four-carbon DE4P, to the preferred five-carbon DR5P which has the shortest distance of 3.13 Å (Table 2.1). The phosphorylated substrates had generally lower experimental and predicted K_m values (Table 2.1) which can be explained by this strong interaction at the entrance to the binding cleft. When overlaid with the docked enamine structure (Figure 2.4 a) the phosphorylated aldol acceptors are all positioned and oriented with the Re-face of their aldehydic carbonyls ready for nucleophilic attack by the nearby α-carbon of the enamine to give products of the S-enantiomer.

Docking of the non-phosphorylated aldol acceptors was found to be dominated by hydrogen-bonding to His 26, His 261 and, with the exception of acetaldehyde, Asp 469 (Figure 2.4 b). Interestingly, D-ribose forms a hydrogen bond to Arg 520 via the C5-hydroxyl group in the absence of the phosphate, though this does not fully compensate for the much tighter binding achieved with the phosphate in DR5P. As for the phosphorylated aldehydes, an overlaid structure of the docked enamine (Figure 2.4 b) shows that the non-phosphorylated aldol acceptors are also all positioned and oriented with the Re-face of the aldehyde carbonyl prone to

nucleophilic attack by the nearby α-carbon of the enamine to give the S-enantiomer products.

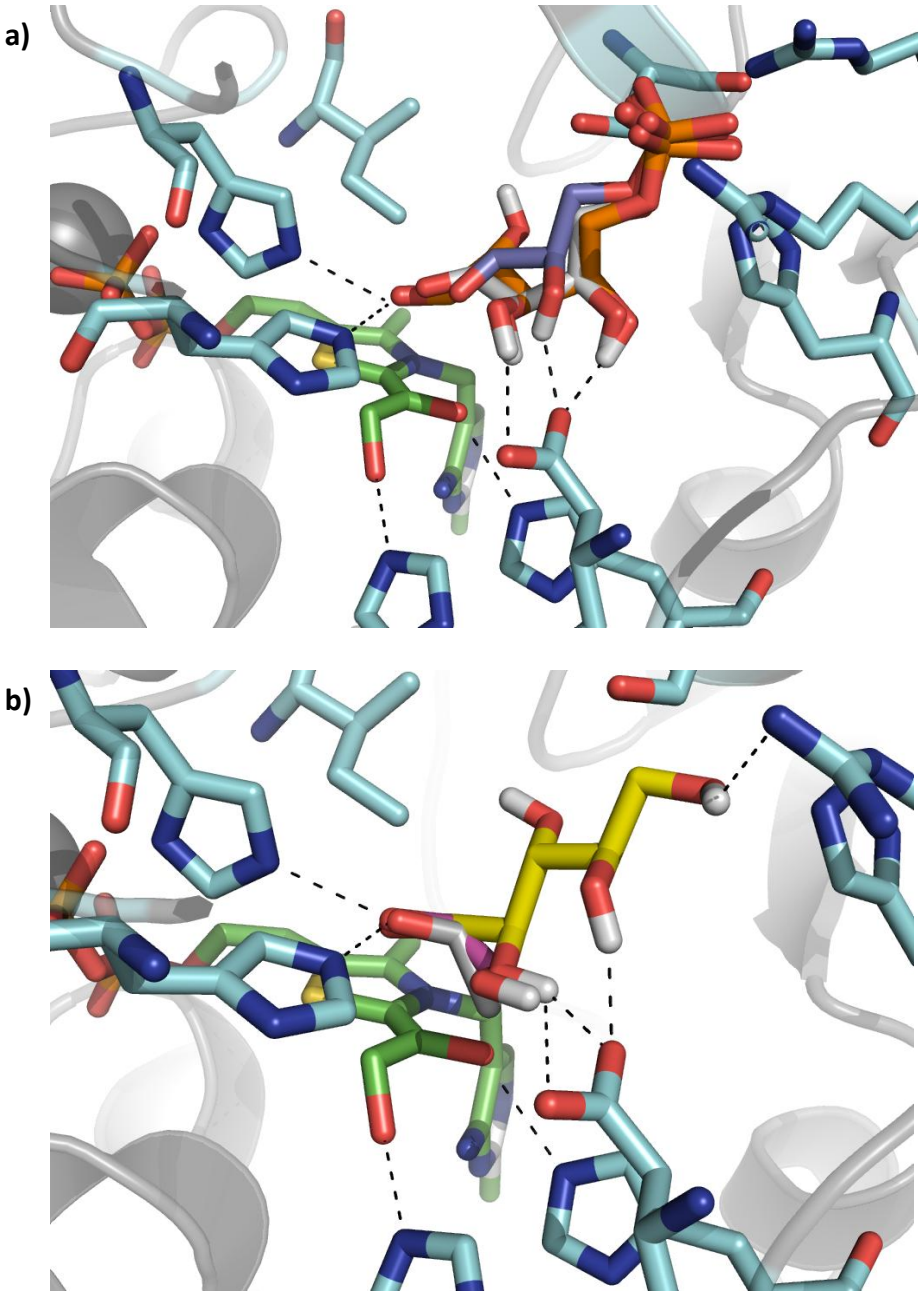

Figure 2.4 Comparison of the docking of phosphorylated and non-phosphorylated aldol acceptor and ketol donor substrates in *E. coli* TK. The enamine intermediate (not present during docking) is overlaid for reference in each panel (green sticks). a) Phosphorylated aldol acceptor substrates. DE4P (grey), G3P (dark blue) and DR5P (orange) are each oriented to present the *Re* face of their *aldo* carbonyls to give the expected *S*-enantiomer products. The phosphate binding location is highly defined in the R520 and R358 pocket, and creates differences in the proximity of the *aldo* carbonyl to the Cα enamine carbon depending on substrate chain length. b) Non-phosphorylated aldol acceptor substrates. Acetaldehyde (grey), Glycolaldehyde (magenta), and Ribose (yellow) are also oriented to present the *Re* face of their *aldo* carbonyls to give the expected *S*-enantiomer products. Non-phosphorylated substrate binding is dominated by hydrogen-bonding to H26, H261, and D469 (except acetaldehyde and ribose which hydrogen-bonds to R520 even without the phosphate).

2.3.5 Comparison of docked and crystallized DR5P conformations

Asztalos and co-workers previously obtained a structure of *E. coli* TK with a mixture of both the cyclic and acyclic forms of DR5P bound in the active site [21]. However, the apparently ambiguous electron density due to low occupancy of the acyclic form, positioned it such that it would clash sterically with our modelled enamine intermediate, indicating that this might not be the exact productive binding conformation. While modelling of the yeast TK enamine structure coordinates by Asztalos *et al* found the acyclic DR5P to approach the enamine Cα at a distance of 1.6 Å with a favourable angle of 112° for the C1 aldo carbon relative to the C2-Cα of the enamine, inspection of their structure indicates that the enamine would be poised to attack the incorrect Se face of the C1 aldo carbonyl. Our docked acyclic DR5P gives a more plausible (or earlier) conformation for binding prior to a productive reaction in which the reactive enamine is 3.13 Å from the Re face of the aldehyde carbon atom of DR5P. The aldehyde O-atom is coordinated by His 26 (3.0 Å) and His 261 (2.8 Å), the C2 hydroxyl hydrogen bonds with Ser 385 (3.0 Å), the C3 (2.6 Å) and C4 (2.8 Å) hydroxyl groups both hydrogen bond with Asp 469, and the phosphate is coordinated to Arg 358, Arg 520, Ser 385 and His 461 as usual. The contacts observed in the binding of the cyclic form by Asztalos *et al* are different to those in our modelled acyclic form with the C1 to C3 hydroxyl groups being rotated around the protein side-chains by one position (Figure 2.5 b-c). Comparison of the two suggests that TK binds the cyclic DR5P, catalyses the ring opening, and then re-arranges the position of the aldehyde closer to the enamine prior to reaction.

His 261 is highly polarised by the phosphate in ThDP (2.7 Å) making it a good base for catalysis of the ring opening via deprotonation of the C1-hydroxyl group in DR5P which is 3.33 Å away. Ser 385 was also found in two occupancies with the first coordinating the DR5P phosphate [21], and the second in position to stabilise the protonation of the furanose O-atom of DR5P during ring opening. As the aldehyde forms at C1 upon ring opening, the hydrogen bond to His 261 is retained via the O-atom which moves by 3.2 Å into the position previously occupied by the C2 hydroxyl group, and forms an additional hydrogen bond with His 26. This movement is facilitated by a 180° rotation of the C2-C3 bond, as suggested by Asztalos *et al*, but forms a new hydrogen bond between the C2 hydroxyl group and Ser 385. Meanwhile the hydrogen bond between Asp 469 and the C3 hydroxyl group becomes shorter by 0.15 Å and the C3-C4 bond rotates by 180° to form a new hydrogen bond between the C4 hydroxyl group and Asp 469. Collectively these hydrogen bond exchanges serve to unwind the now acyclic DR5P backbone and free up the space near His 26 and the enamine-ThDP intermediate for the newly formed C1 aldehyde.

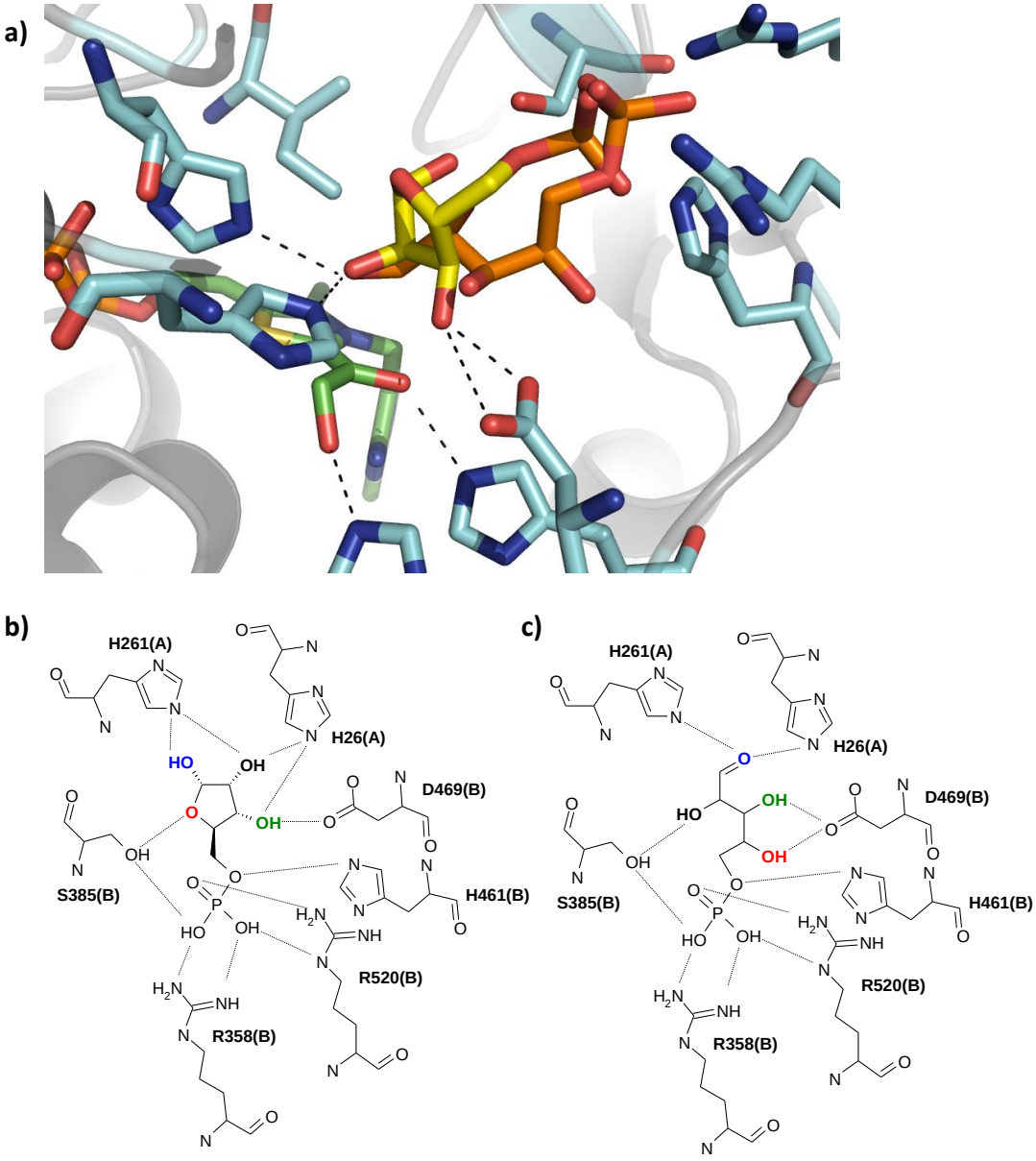

Figure 2.5 a) Cyclic and acyclic forms of DR5P. Cyclic DR5P (yellow) from a TK crystal structure [21] and the modeled acyclic DR5P (orange). b) and c) Hydrogen bonding network changes upon ring opening of DR5P. Cyclic (left) and acyclic (right) forms of DR5P with hydrogen bond interactions with transketolase shown schematically as dashed lines.

2.3.6 Glycolaldehyde docking

Glycolaldehyde (GA) is one of the smallest aldehydes accepted by TK and the reaction of GA with TK has been studied extensively [1, 26, 41, 74, 78]. As for DE4P, the docking of GA was performed both in the presence and absence of the modelled enamine. Comparison of the two docks indicated that they differed by an RMSD of only 0.53 Å and that their hydrogen bonding interactions were identical.

As with the other aldehydes, GA binding presented the Re face of the aldehyde to the nucleophilic enamine such that it would give the expected L-erythrulose product (Figure 2.6 a). Overall the very small differences, for both GA and DE4P docked with and without the enamine, indicate that the productive positioning of the aldehyde acceptors relative to the enamine is sufficiently optimised through specific interactions other than those to the enamine in the active site. This observation is analogous to that by Asztalos *et al* where the active site is catalytically poised to maximally translate substrate binding interactions directly into the strained tetrahedral intermediate with the ketol donor. It is possible then that the reaction between aldol acceptor and the enamine may introduce a similarly strained conformation, driven by optimised substrate interactions without the need for induced fit or the unfavourable flexibility this introduces.

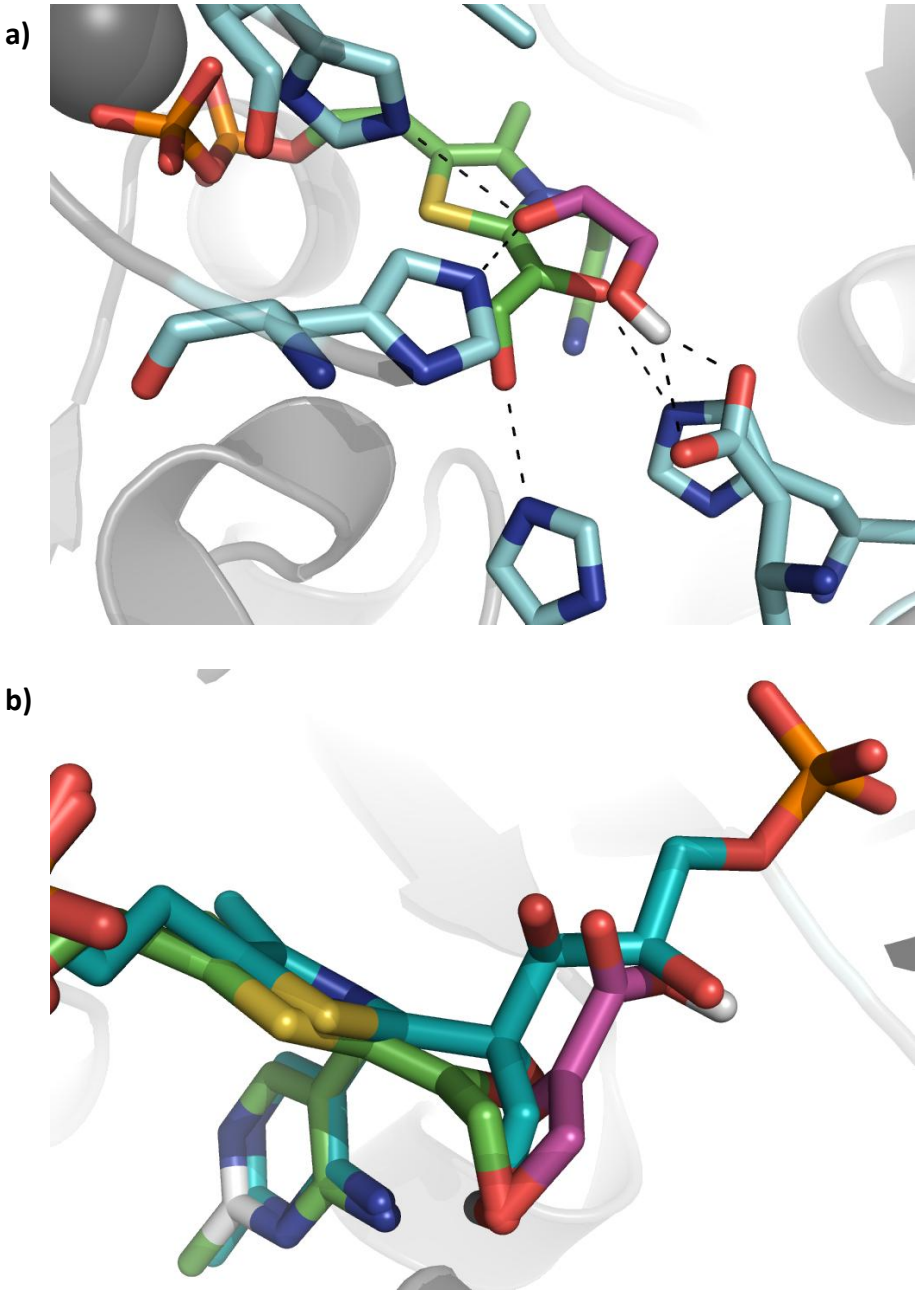

Figure 2.6 Docking of substrates into *E coli* TK for the reaction of hydroxypyruvate and glycolaldehyde. a) **Glycolaldehyde docked into *E. coli* TK in the presence of the modeled enamine.** b) **Transition from docked non-covalently bound HPA (magenta), via the covalently bound and strained tetrahedral intermediate with DX5P (blue - from crystal structure of Asztalos *et al* [21]), to the docked enamine (green).**

2.3.7 Comparison of docking for the ketol donors

Hydroxypyruvate (HPA) and D-xylulose-5-phosphate (DX5P) are both donor substrates for the TK catalysed reaction for which no structures of the non-covalent complexes have been obtained experimentally. Fluoropyruvate (FPA) is an analogue of HPA for which no measurable reaction is observed with TK. FPA and

HPA are both known competitive inhibitors of the pyruvate decarboxylase from *Zymomonas mobilis* [79] and preliminary data from our lab suggest that FPA can also inhibit the TK reaction when using HPA as the ketol donor (unpublished). Both of the ketol donor substrates and also FPA were found to dock in conformations that position the carbonyl within a reactive distance from the C2 carbon of the ThDP thiazolium ring (Figure 2.6 b). However, the DX5P docked conformation and position was found to be unusually different to all other substrates and the carbonyl was at an unfavourable orientation for reaction with the ThDP thiazolium ring (not shown). This dock was deemed to be suspect upon visual inspection, and indeed removal of DX5P from the plot of calculated and experimental log(Km) values in Figure 2.3 gave a slightly improved Pearson R2 correlation of 0.84 (not shown).

To examine the mechanism of binding for ketol donors, and their reaction with ThDP, the docking of HPA was compared to the covalently bound DX5P intermediate from an available crystal structure with *E. coli* TK [21], and also to the modelled ThDP-enamine intermediate (Figure 2.6 b). The most striking observation is that the reaction mechanism for HPA binding and subsequent covalent bond formation with ThDP (as observed by analogy in the DX5P complex), followed by the final enamine intermediate formation, involves a stepwise shortening of the emergent covalent bond between the C2 carbanion of ThDP and the substrate carbonyl, accompanied by an almost 90° rotation of the molecule. Throughout this reaction, the carbonyl O-atom and α-hydroxyl group in HPA remain in the same position, both maintaining hydrogen-bond interactions to His 473 and the amino

group on the pyrimidine ring of ThDP, and additionally between the carbonyl and His 100.

Hydrogen bonds from His 26 and His 261 to just one O-atom of the carboxyl group in HPA mirror those observed previously by crystallography in the covalently associated DX5P complex [21], where the two histidines interact with the C3 hydroxyl group (Figure 1.6). Asp 469 hydrogen bonds to the other carboxyl group O-atom in HPA which also mirrors an interaction with the C4 hydroxyl group in DX5P. However these interactions are all lost upon enamine formation by cleavage of the two-carbon ketol unit from HPA and DX5P.

Surprisingly, the Bergi-Dunitz angle for nucleophilic attack of the carbonyl of HPA by the ThDP carbanion is only 68°, which is a long way from the traditionally preferred 107° [80]. Such an unusual acute angle of attack is potentially made possible through a number of factors. First, the substrate is tightly anchored by interactions to the amino group on the pyrimidine ring of ThDP, His 100 and His 473, whereas Bergi-Dunitz angles of 107° are typically preferred in reactions between two unconstrained molecules. Second, the ThDP may attack in the carbene form, especially in the proximity of the negatively charged carboxyl group in HPA, which can take place from above a pi-system such as in a carbonyl. Finally, the conserved Asp 469 residue appears to be hydrogen bonded to one of the carboxyl group O-atoms in HPA (equivalent to the C1 hydroxyl group of DX5P). This may serve to lengthen the carbonyl bond in HPA giving it less double bond character, along with protonation of the carbonyl by the amino group on the pyrimidine ring of ThDP to

remove electron density from the O-atom, thus making an acute angle of attack more favourable.

FPA was found to dock in an identical manner to HPA with an RMSD of 0.75 Å suggesting that the fluorine atom can hydrogen bond with equivalent contacts to those found with HPA. FPA is less reactive than HPA as the high electronegativity of the fluorine atom decreases the polarity of the neighbouring carbonyl making it less reactive to the ThDP carbanion in TK. The identical binding of docked FPA and HPA indicates that FPA should provide a great opportunity for crystallographers to obtain a non-covalent complex of TK with an analogue of the ketol donor HPA.

The initial formation of a non-covalent ketol donor complex at an unusual angle of attack, through maximised substrate interactions, is consistent with the previous observation of strain in the subsequently formed tetrahedral intermediate [21]. This builds up a picture of the enzyme active site being poised catalytically such that the binding energetics allow the unusually constrained attack angle. The strain in the complex is released partially to form the out-of-plane covalent intermediate, and then released further upon formation of the enamine.

2.4 Conclusions

Although computational docking is not completely accurate, the most obvious errors can be eliminated by visual inspection as was the case for DX5P in this work. Furthermore, the lack of significant side-chain movements in the TK active site upon substrate binding eliminates errors that might otherwise have arisen by not modelling induced fit mechanisms. Computational docking in TK provided supportive evidence for understanding the enzyme mechanism where experimental structural studies have been difficult, and more importantly it has generated interesting hypotheses that can be tested in future experimental studies. The AutoDock algorithm used was able to determine binding conformations of several ketol donor and aldehyde acceptor substrates in the active site of *E. coli* TK with a good correlation between experimental and computationally derived K_m values. We were also able to model aldol acceptors into TK with the ThDP-enamine intermediate present as would be formed after reaction with the ketol donor substrate. The binding of aldol acceptors was found to be identical both in the presence and absence of the enamine intermediate indicating that the interactions made independently of the enamine are sufficient for binding in a reactive conformation. This has an important consequence for protein engineering attempts to alter the substrate specificity of a two-substrate reaction in which the interactions of the second substrate with the enzyme are partially overlapping with those made by the first.

An interesting potential mechanism for the ring opening of cyclic DR5P is suggested by comparison of a previous crystal structure to our docked acyclic DR5P. We have

identified potential general acid and general base residues for the ring opening, and also suggest how the molecule moved around a network of hydrogen bonding interactions to bring the linearised DR5P into place for reaction with the enamine intermediate.

Finally, a comparison of HPA docking to the modelled enamine and to a structurally determined covalent DX5P intermediate indicates a nucleophilic attack by the deprotonated ThDP cofactor with an acute Bergi-Dunitz angle of just 68°, rather than the typically preferred obtuse angle of 107°. A repeat of the HPA docking conformation but with that of the non-reactive analogue FPA suggests a possible method for testing this unusual hypothesis by crystallography.

3 Statistical Coupling Analysis of *Escherichia coli* transketolase

3.1 Introduction

Elucidation of the structure and mechanism of transketolase has led to the identification of several key residues involved in substrate recognition [18, 21], protonation of cofactor [23], transition state stabilisation [7], and deprotonation of substrate. Efforts to engineer the substrate specificity and enantioselectivity of TK have both utilised and built upon this knowledge of structure and mechanism.

Despite the detailed understanding of TK, work to date has focussed on the function of individual residues in isolation. Early experimental mechanistic work on yeast TK involved the site directed mutagenesis of individual residues [18, 19, 24], and engineering of *E. coli* TK has focussed on saturation mutagenesis targeted to individual residues [9-11, 47]. In addition to identifying individual residues with key functions, it is also desirable to identify key synergistic networks of residues. Identification of such networks will lead to a better understanding of function and aid in the engineering of TK.

Statistical coupling analysis (SCA) is a powerful tool for identifying co-evolved residues in protein multiple sequence alignments (MSA) [65, 66]. The co-evolution of residues indicates potential synergy between them that is driven by overall protein fitness or function. Various properties can impact on protein function; these include expression, folding, solubility, stability and allostery; synergistic relationships could be linked to any one of these properties. Here we have used the

SCA method to identify potentially synergistic networks of residues in *E. coli* TK. Other methods to measure co-evolution of residues include Explicit Likelihood of Subset Variation (ELSC), mutual information and correlation-based methods.

Statistical coupling analysis is based on two hypotheses, firstly that without evolutionary constraint, all amino acids at a specific position in a multiple sequence alignment will approach their mean distribution in all proteins. Secondly, that the epistatic coupling of two positions in a protein should mutually constrain their evolution [65]. In order to identify such coupled positions in a multiple sequence alignment, the distribution of amino acids at one site is altered (by removing a subset of sequences from the MSA) and other sites are monitored for concurrent changes in distribution of amino acids. Notably, identification of such relationships does not require that the level of conservation change at the second site, just that the distribution of amino acids be altered.

TK exists as a homodimer of two 680-residue chains, each consisting of three domains, the PP (pyrophosphate binding), the Pyr (pyrimidine binding), and the C-terminal domain. All TPP-dependent enzymes contain catalytic PP and Pyr domains which bind the ThDP cofactor, although different enzyme types have different domain architecture [81, 82]. Although the TPP-binding sites of these enzymes are very similar, each enzyme type has different substrate specificity. As the different enzyme types have diverged from a common ancestor, any synergistic networks of residues could be expected to create evolutionary constraints on the residues involved. Identification of such co-evolved networks could provide important

insights into substrate specificity and aid in the engineering of substrate specificity of *E. coli* TK.

The wild type *E. coli* TK enzyme has been engineered for improved substrate specificity towards the non-hydroxylated aldehyde acceptor substrate, propionaldehyde (PA) [10]. The D469T mutant was identified as giving the greatest improvement in activity on PA with a 5-fold increase in specific activity relative to wild type. A further mutant at site 469, D469Y, displayed the greatest substrate specificity with a 64-fold higher activity on PA relative to GA. Finally the D469E mutant displayed the greatest improvement in enantioselectivity with PA [10]. The repeated identification of Asp 469 variants among seventeen active site residues probed for three different selection criteria illustrates the importance of this residue. Identification of networks of synergistic residues involving Asp 469 could lead to further improvements in the engineering of *E. coli* TK.

Using SCA, we have identified residues that are statistically coupled to Asp 469. These include both a proximal connected network and a more distal and network distributed throughout the protein fold. Some of the residues had been previously identified as improving activity on non-natural substrates [9, 10] but the vast majority have not been investigated by mutagenesis before and represent new potential targets for rational design of expanded variant libraries.

In addition to measuring coupling between individual residues in an alignment, SCA allows global coupling analysis across all positions in the alignment that meet certain criteria. Two-dimensional hierarchical clustering, originally developed for microarray data analysis, can be used to identify networks of similarly coupled

residues throughout the protein sequence. For robust and conserved networks of residues, perturbations at network positions are expected to redundantly identify each other, clustering the coupling matrix allows the identification of such networks. We applied this method to identify inter- and intra-domain networks of coupled residues throughout the PP and Pyr domains of *E. coli* TK. Many of these networks were located in the interface between the two domains but we also identified interesting connected networks of residues in and around the active site.

3.2 Materials and Methods

3.2.1 Multiple sequence alignments

Costelloe *et al* carried out a phylogenetic analysis of seventeen different TPP dependant enzymes using sequence alignments of the conserved PP and PYR domains [82]. Transketolase (TK), D-xylulose-5-phosphate synthase (DXPS), dihydroxyacetone synthase (DHAS), phosphoketolase (PKL), 2-oxoisovalerate dehydrogenase (2OXO), pyruvate ferrodoxin reductase (PFRD), pyruvate decarboxylase (PDC), indolepyruvate decarboxylase (IPDC), phenylpyruvate decarboxylase (PhPDC), pyruvate oxidase (PO), acetolactone synthase (ALS), glyoxylate carboligase (GXC), benzoylformate decarboxylase (BFDC), benzyaldehyde lyase (BAL), oxalyl CoA decarboxylase (OCADC), sulfopyruvate decarboxylase (SPDC), and phosphopyruvate decarboxylase (PPDC) enzymes were included.

Costelloe *et al* identified TPP dependent enzyme sequences using BLASTP searches of the Swissprot and nr databases (Blosum62 matrix and default settings). Query sequences for each enzyme were selected from those with known structure or well defined biochemistry and homologous sequences were identified with >30% sequence identity. In total 382 sequences representing the 17 different enzymes were identified. Following removal of putative sequences these hits were aligned using ClustalW.

Alignments of the PP and PYR domains were generated separately. The PP domain was defined as residues 1-350 in *E. coli* TK and the PYR domain was defined as residues 323-528 in *Eco*TK. Crystal structures of *Eco*TK (1QGD.pdb), *P. putida* 2OXO

(2BP7.pdb), *D. africanus* PFRD (1B0P.pdb), *S. cerevisiae* PDC (1PVD.pdb), and *L. plantarum* PO (1POX.pdb) were used to refine the alignment of functionally important residues and secondary structural elements. Finally alignments were de-gapped to leave only residues found in *E. coli* TK.

3.2.2 Statistical coupling energy calculation

SCA Version 1.5 was used to calculate statistical coupling energies between sites in multiple sequence alignments (MSA's) of the PP and PYR domains. SCA Version 1.5 is a MATLAB implementation of the calculation described by Lockless et al, 1999 [65]. The calculation gives a quantitative measure of the change in amino acid distribution at site j given a perturbation at another position i. This is calculated as a statistical coupling energy ($\Delta\Delta G^{stat}_{j,i}$).

Briefly, each site in the MSA is described by a 20 element vector of binomial probabilities of individual amino acid frequencies given their frequencies in all proteins ($P_j = [P^{ala}_j, P^{cys}_j, P^{asp}_j,\ldots, P^{tyr}_j]$). P_j^x gives the probability of the observed number of x amino acids at position j, given its mean frequency in all proteins. The 20 element vector of P_j^x can then be converted into a vector of statistical energies that represents the evolutionary constraint at site j ($\Delta G^{stat}_j = [\Delta G^{ala}_j, \Delta G^{cys}_j, \Delta G^{asp}_j,\ldots, \Delta G^{tyr}_j]$). Each term in the vector is the value for amino acid x at site j and is given by $\Delta G^x_j = kT^* \ln(P_j^x/P_{MSA}^x)$, where kT* is an arbitrary energy unit and P_{MSA}^x represents a hypothetical site where all amino acids are observed at their mean frequencies in the MSA as a whole. This hypothetical site serves as a reference state for all sites and ΔG^x_j represents the statistical free energy separating site j from the

hypothetical site for amino acid x by the Boltzmann distribution. The magnitude of the ΔG^{stat}_j vector represents an evolutionary conservation parameter for site j.

To measure functional coupling between two positions j and i in the MSA, two statistical energy vectors are calculated, one from the full MSA (ΔG^{stat}_j) and one from a subalignment representing a perturbation of the amino acid frequencies at a second site i ($\Delta G^{stat}_{i|j}$). The magnitude of the difference in these two statistical energy vectors represents a quantitative measure of the degree to which the probability of individual amino acids at site j is dependent on the perturbation at i, $\Delta\Delta G^{stat}_{j,I} = \Delta G^{stat}_j - \Delta G^{stat}_{i|j}$. $\Delta\Delta G^{stat}_{j,I}$ is calculated for all sites j given a perturbation at position i.

3.2.3 Matrix assembly and cluster analysis

All acceptable perturbations, and their associated coupling energies to other positions in the sequence, are displayed as a matrix of statistical coupling energies. Each row in the matrix represents a position in the alignment and each column represents a specific perturbation.

Iterative clustering methods originally developed for microarray analysis are then used to identify co-evolving networks of positions. The process of iterative clustering involves sequential rounds of 2-dimensional clustering, after each round, sub-matrices representing areas of low signal are eliminated. The next round of clustering further refines the clusters focussing around positions and perturbations with significant statistical coupling. This process is repeated until the clusters converge and no further refinement is possible.

3.3 Results and Discussion

3.3.1 TPP-dependent multiple sequence alignment validation and perturbation of position 469

A 382 protein multiple sequence alignment (MSA) of the PP and PYR domains of TPP-dependent enzymes was converted into a matrix of residue frequencies and positions using SCA version 1.5. Calculation of evolutionary constraint at each site in the MSA reveals a diverse and well evolved collection of proteins. Figure 3.1 a illustrates graphically the evolutionary constraint at each position as measured by ΔG^{stat}. High values of ΔG^{stat} indicate a high degree of conservation or evolutionary constraint. Among the residues which display a very high degree of evolutionary constraint are Asp 155, Glu 411, and His 473. These three residues have important functions in the active site of TK. Asp 155 acts as a ligand for the metal ion CA^{2+} or Mg^{2+} [14], Glu 411 protonates the N_1' Nitrogen of the pyrimidine ring [23], and His 473 has a potential involvement in transition state stabilisation [7].

The MSA must be validated before carrying out SCA to ensure that it meets certain criteria. In order for functional constraints in the MSA to be exposed, the alignment should have diversified to the extent that frequencies of amino acids at un-conserved sites have relaxed near to their mean values in all natural proteins [65]. This is evident from the frequencies of residues at the un-conserved site 38 which are approaching the mean frequencies of residues in all proteins (Figure 3.1 b). This is in contrast to a conserved site such as 469 where the amino acid frequencies differ considerably from the mean values in all proteins (Figure 3.2 a).

Secondly, the MSA should be large enough that random elimination of sequences does not change the amino acid frequencies at un-conserved sites [65]. To validate the MSA for this criteria, the five least conserved positions that still represent at least 85% occupancy were identified (1QGD numbered positions: 38, 211, 363, 508, and 509) and average ΔG^{stat} values were determined across these five sites following elimination of different proportions of the MSA. Random elimination of large proportions of the MSA was possible without increasing the average ΔG^{stat} at these un-conserved positions (Figure 3.1 c). The alignment was therefore judged to have reached statistical equilibrium in sequence space, a necessary condition for applying Boltzmann statistics.

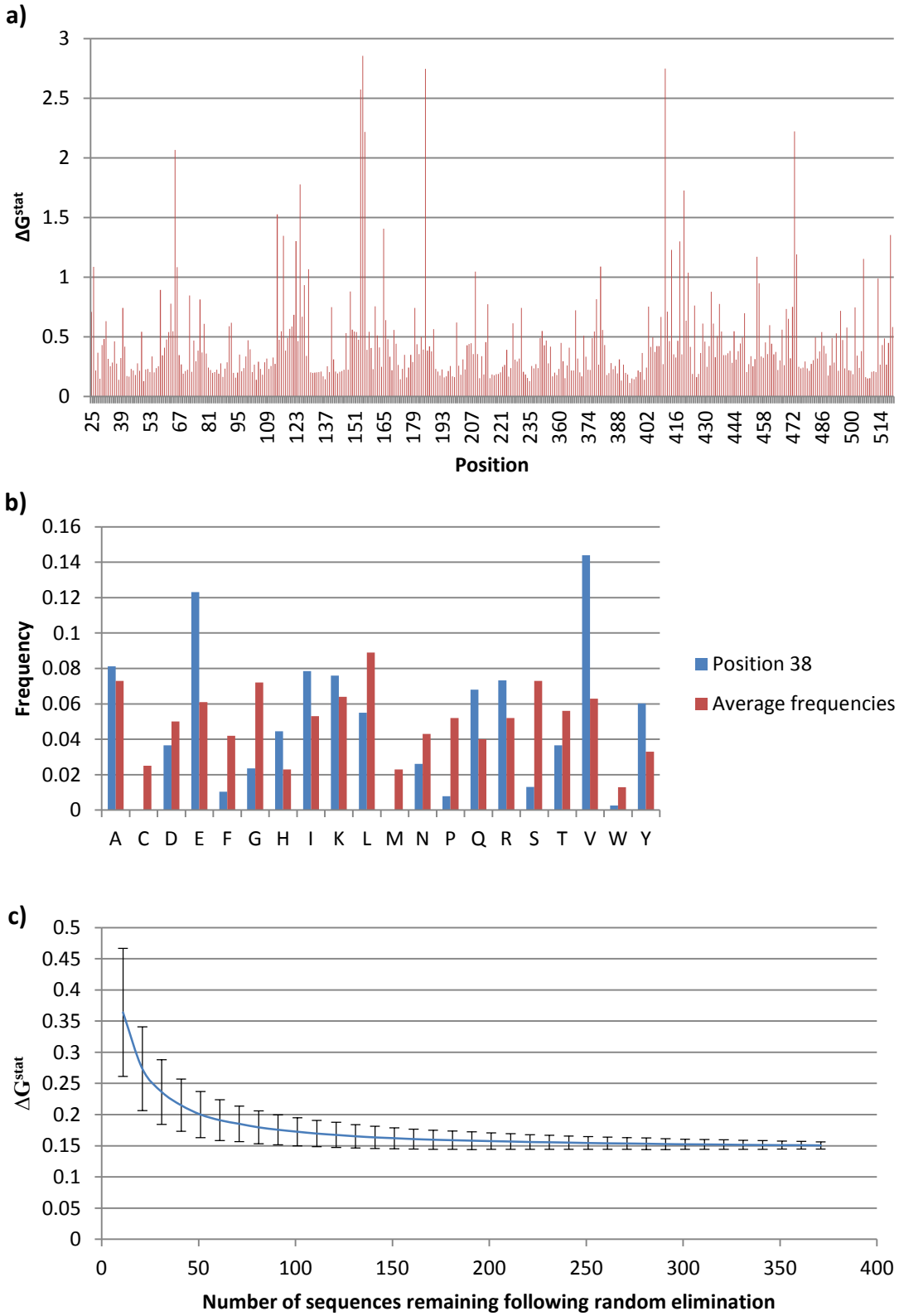

Figure 3.1 a Overall conservation across the MSA as measured by dGstat, an expression of divergence from the frequency of residues expected in all proteins. b Frequency of residues at position 38, the least conserved position in the MSA. c The 5 least conserved sites that retain at least 85% occupancy were selected and average dGstat at these 5 sites was evaluated following random elimination of increasing proportions of the MSA.

3.3.2 Identification of residues statistically coupled to Asp 469

Residue Asp 469 is known to be a functionally important residue in *E. coli* TK. Early studies identified the equivalent residue in yeast TK as having an important function in enantioselectivity [24] and recent work to engineer *E. coli* TK to accept non-natural substrates has identified several variants at this position that confer improved and desirable properties to the enzyme [9, 10]. Given the important function of this residue we used SCA to identify residues which display statistical coupling to Asp 469. Identification of such a network has important implications for the understanding of TK evolution and function but could also be applied to aid in the design variant libraries for engineering TK.

The residue Asp 469 is highly conserved in TK and in some of the other TPP-dependent enzymes (Figure 3.2 a). Using the SCA Toolbox we created a perturbation of the MSA to remove all sequences that do not contain an Asp at position 469, this perturbation resulted in a subalignment of 173 sequences. Statistical coupling to position 469 was then determined by calculation of the $\Delta\Delta G^{stat}$ values at all other positions in the alignment (Figure 3.2 b).

The statistical coupling energies between the 469D perturbation and other positions in the alignment are generally insignificant, however a relatively small number of positions display significant coupling to the 469D perturbation. Focusing on the seven sites displaying the highest levels of coupling to position 469 identifies an interesting cluster of residues surrounding the active site.

Mapping these sites onto the structure of *E. coli* TK reveals a network of connected residues within the protein core that display coupling with position 469.

Interestingly these are not restricted to residues in close proximity to position 469, coupling is also seen in distant residues and across the PP-PYR domain boundary (Figure 3.2 c).

Focusing on the active site of *E. coli* TK and the Asp 469 residue itself, four of the seven coupled residues form a connected cluster in and around the active site tunnel which is centred on Asp 469 (Figure 3.2 c). This cluster spans from residue Phe 437 to Thr 472 and then to Asp 469 of the PP domain. Asp 469 then forms a connecting bridge across the inter-domain barrier to His 26 which in turn interacts with His 66. Arg 520 is not physically in contact with this contiguous cluster but is relatively close to Asp 469 and reaches into the active site forming part of the entrance to the active site tunnel.

The two remaining residues, Tyr 72 and Pro 486, are more distant from the active site. Tyr 72 is located on the α-helix which leads towards His 66 of the active site and may therefore be responsible for positioning the loop containing His 66 to maintain the integrity of the active site. Pro 486 forms a hairpin loop at the opposite end of an α-helix which leads to residues Thr 472 and Asp 469. This residue may therefore have a similar function to Tyr 72 in maintaining tertiary structure and active site integrity.

Of the seven residues identified as coupling with Asp 469, two have been identified previously for their propensity to improve activity on non-natural substrates when mutated [9, 10]. Arg 520 was identified in screens for improved activity on both GA and PA and His 26 was identified in screens for improved activity on PA [10]. As Arg 520 is known to interact with the phosphate group of natural substrates, a rational

explanation for the increase in activity for non-phosphorylated substrates was a removal of the steric bulk around the entrance to the active site. The coupling between Arg 520 and Asp 469 suggests there may be a subtler synergistic explanation for the increased activity. Mutation of His 26 in *E. coli* TK led to variants with reversed enantioselectivity for PA [11]. This residue forms a pocket with Asp 469 which interacts with the α-hydroxyl group of natural substrates, coupling is not surprising for a residue with such a close functional and structural relationship with Asp 469.

Apart from Asp 469, His 26, and Arg 520, none of the remaining three active site residues in this network have been targeted for mutagenesis. The high hit-rate for obtaining improved mutants among these three sites indicates that similar success may be obtained at the other sites in the cluster. Identification of this network provides a good starting opportunity for creating targeted libraries of single and multiple mutants with potentially improved function on non-natural substrates.

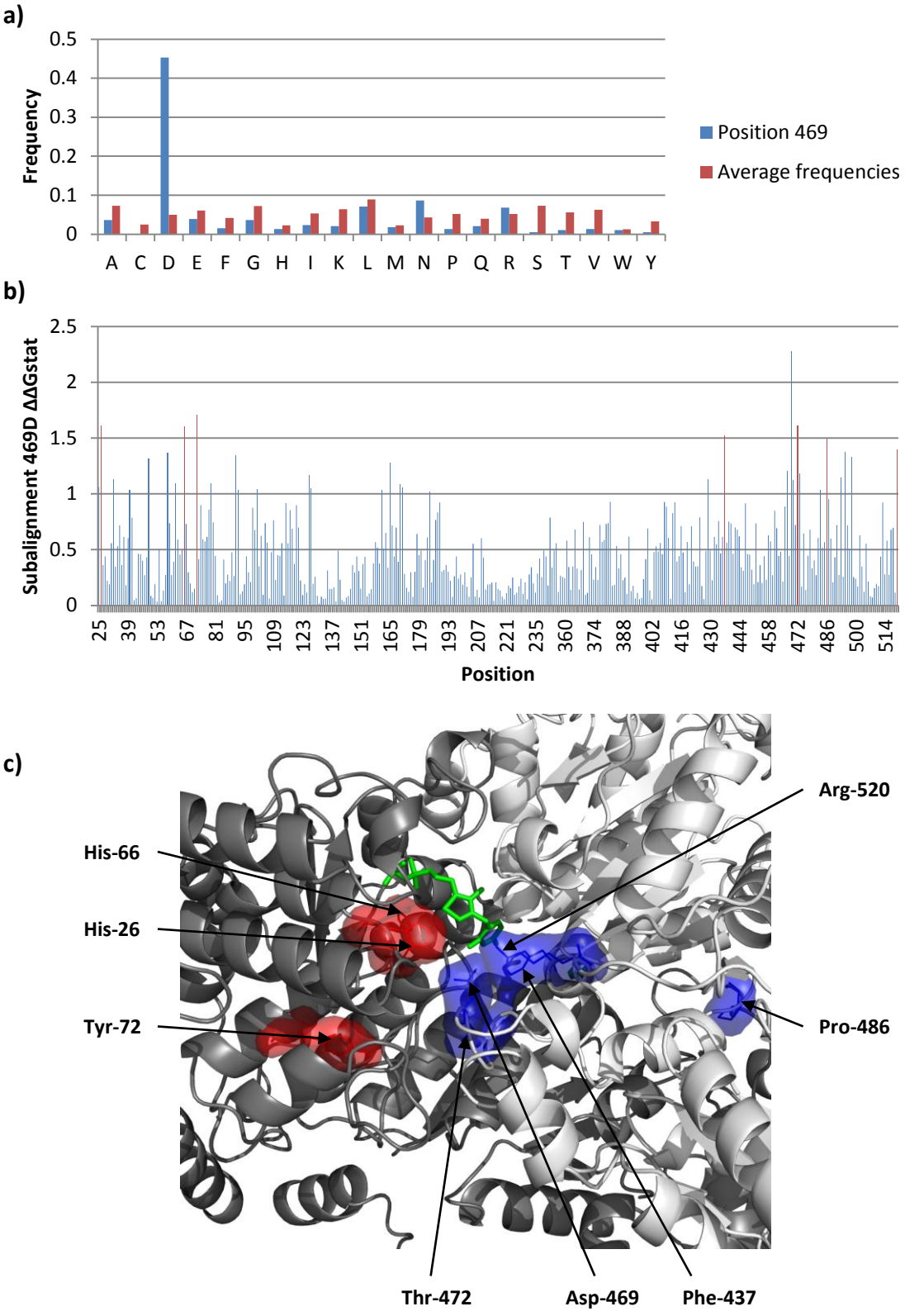

Figure 3.2 a Frequency of residues at position 469 in the MSA versus the expected frequency of residues in all proteins. b $\Delta\Delta G^{stat}$ values between the 469D perturbation and different positions in the MSA. The seven positions representing the highest coupling energies to position 469 are coloured red. c The seven positions coupled to 469 mapped onto the structure of *E. coli* TK (Asp 469 is also shown). Residues in Chain A are coloured red and in chain B are coloured blue. A structurally contiguous group of coupled residues spans the PYR domain of chain A and the PP domain of chain B around the active site tunnel.

3.3.3 Global SCA analysis of TPP-dependent enzymes

The results above demonstrate the ability of SCA to identify residues displaying evolutionary constraint to perturbations at residue Asp 469. Both proximal connected and distant unconnected residues were identified that express an evolutionary dependence on the identity of the residue at position 469. The residues identified as coupled to Asp 469 may be part of a larger interconnected network of coupled residues, not necessarily directly coupled to Asp 469. To identify such an extended network of interactions and to identify other networks that don't include Asp 469 we need to carry out a global SCA across the whole alignment.

To conduct a global SCA, each site in the MSA is subjected to perturbations to create subalignments. Perturbations are allowed that produce sub-alignments large enough to not represent global changes in conservation relative to the parent alignment [65]. To identify the cut off for sub-alignment size, the statistical coupling energy ($\Delta\Delta G^{stat}$) at un-conserved sites is monitored following random eliminations of different fractions of the MSA. The fraction of sequence elimination that begins to show coupling at un-conserved sites represents the limit of sequence elimination tolerated for the specific alignment. For the MSA of TPP dependent enzymes, un-conserved residues begin to display coupling where sub-alignments of less than 80 sequences are selected (Figure 3.3). Therefore for global SCA, perturbations were allowed that resulted in sub-alignments greater than 0.21 as a fraction of the total alignment size (382 sequences).

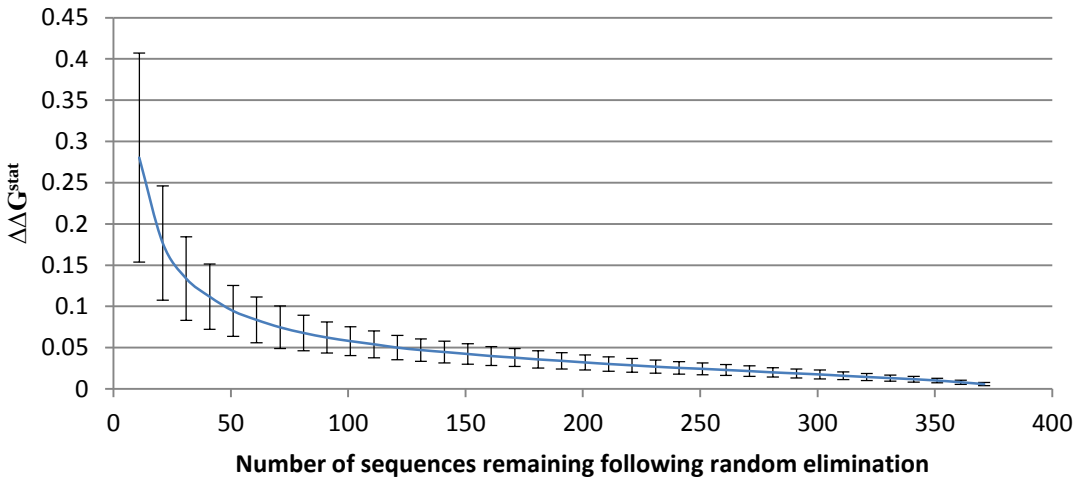

Figure 3.3 The 5 least conserved sites that retain at least 85% occupancy were selected and average $\Delta\Delta G^{stat}$ values were calculated at the 5 sites following random elimination of different proportions of the MSA.

Global SCA was carried out on the MSA in line with the criteria determined above and $\Delta\Delta G^{stat}$ values were determined for all positions in the alignment. Figure 3.4 shows the initial matrix with perturbations represented by columns and positions represented by rows. There is not a perturbation for each position in the alignment as some positions could not meet the cut-off for subalignment size. Therefore the matrix is naturally taller than it is wide. $\Delta\Delta G^{stat}$ values between residues are displayed as a linear colour scale from blue (0) to deep red (4). The highest level of coupling to position 469, identified following the Asp 469 perturbation, was Tyr72 with a $\Delta\Delta G^{stat}$ of 1.72. In contrast, many of the coupling interactions identified following global SCA are associated with coupling energies ($\Delta\Delta G^{stat}$) greater than 3 (Figure 3.4).

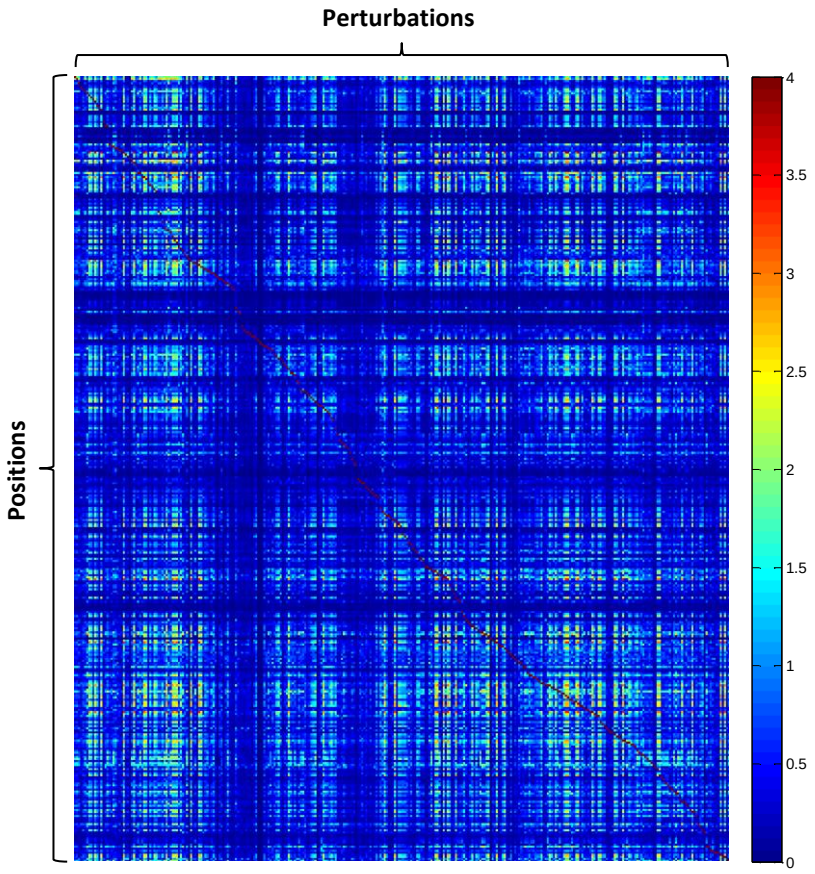

Figure 3.4 Matrix of $\Delta\Delta G^{stat}$ values following global statistical coupling analysis of TPP dependent enzymes. Columns represent specific perturbations of the MSA. Rows represent positions in the PP and PYR domains.

We carried out 2-dimensional hierarchical clustering to identify networks of coupled residues. Figure 3.5 shows the initial round of clustering. Large areas of the matrix are made up of low level coupling. Following clustering, large groups of perturbations or positions with low coupling energy were sequentially removed and the matrix was re-clustered to iteratively focus on the networks representing the highest statistical coupling.

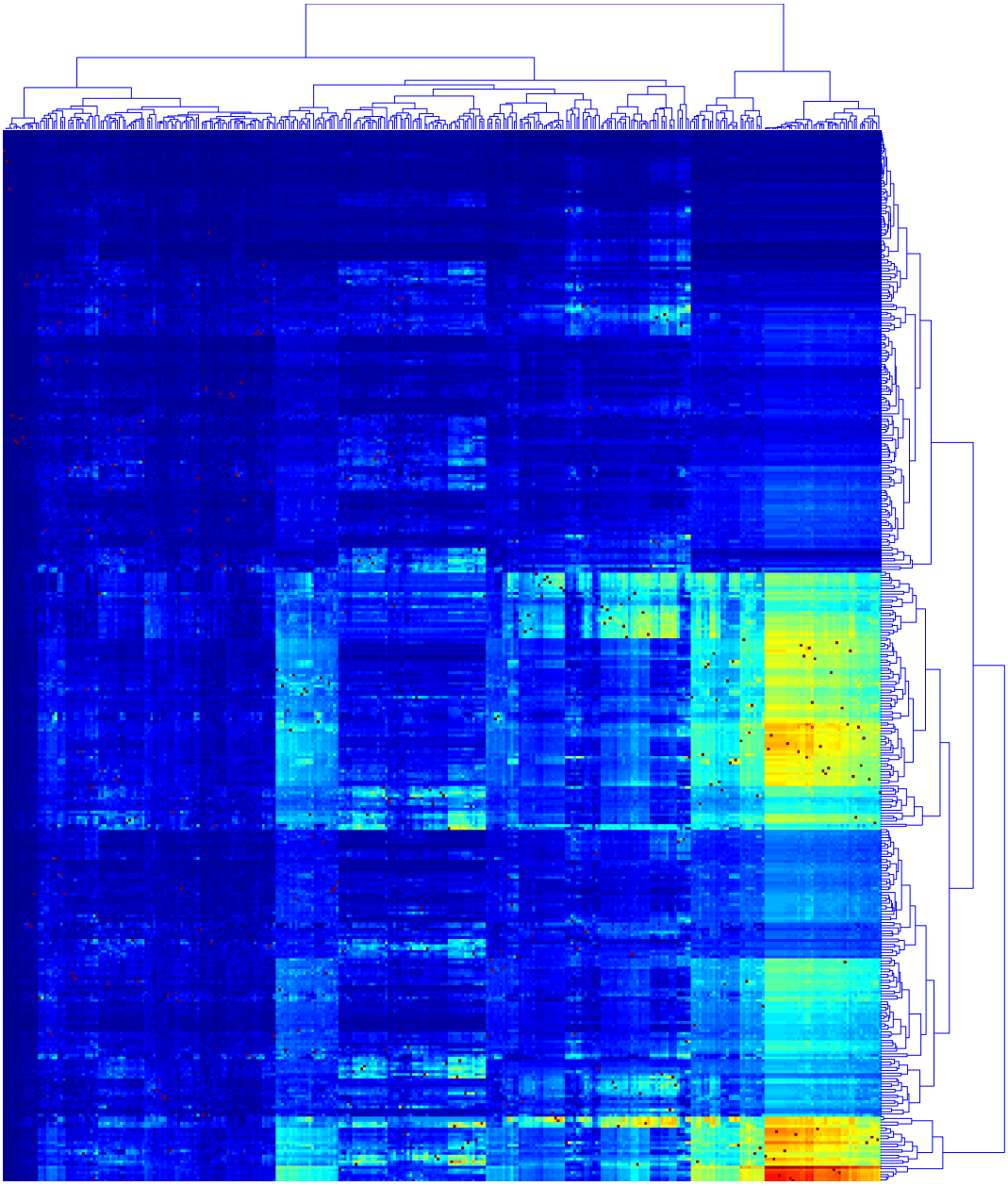

Figure 3.5 Initial clustered matrix of coupling energies following global perturbation analysis of PP and PYR domains.

Following five rounds of iterative clustering we identified a highly coupled network of 30 residues and 45 specific perturbations (Figure 3.6). Based on the clustering dendrogram, the 30 residues can be clustered into six groups of different sizes representing different coupling profiles. Six of the positions identified are known to have important functions in *E. coli* TK (Table 3.1). These include His 26 which forms a hydrogen bond with the α-hydroxyl group of natural acceptor substrates, His 66 which forms a hydrogen bond with the diphosphate group of ThDP and interacts

with the C1 hydroxyl group of donor substrates, Tyr 440 and Phe 434 which interact with the pyrimidine ring of ThDP, His 461 which binds the phosphate group of both donor and acceptor substrates, and Ile 187 which interacts with the divalent metal ion through its main chain oxygen. The identification of functionally defined residues demonstrates the robustness of SCA and indicates a potential application of the method where structure and functional information is lacking. Perhaps more interesting than the known residues are the residues for which we are unaware a function.

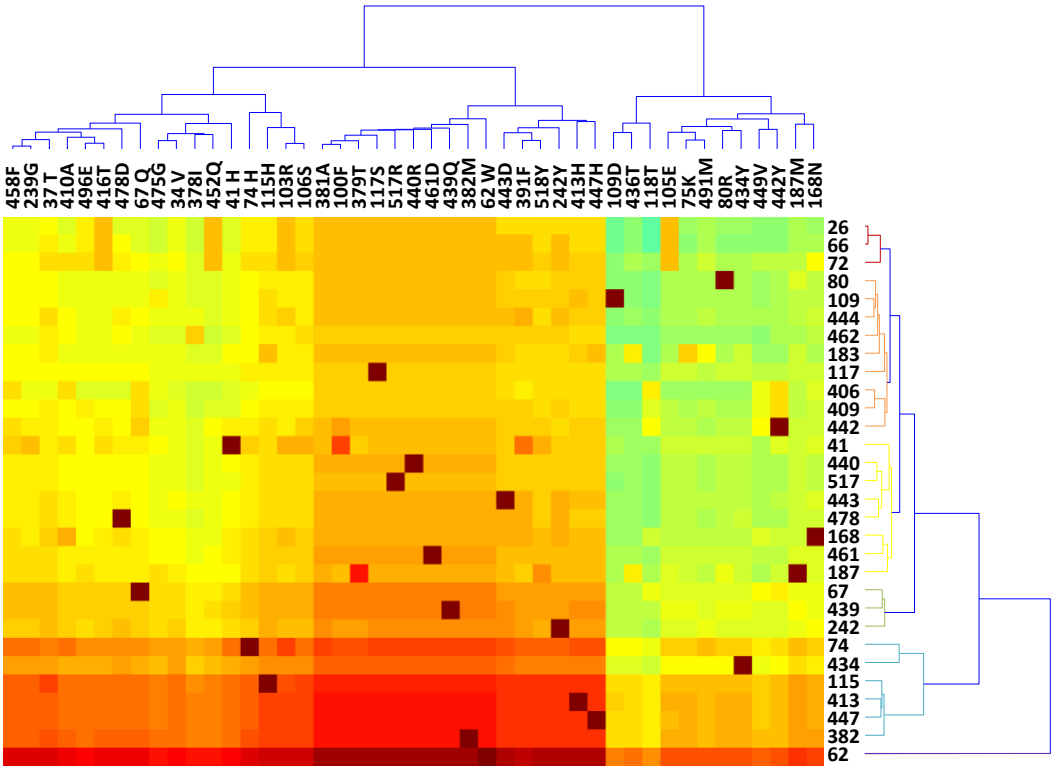

Figure 3.6 Final global SCA matrix following iterative focusing and reclustering around areas of high signal. As in previous figures, perturbations are represented by columns and positions by rows. The dendrogram of positions is coloured according to clusters.

The thirty residues identified with strong coupling interactions are not the most conserved residues in the alignment. This can be expected as highly conserved positions in an alignment are less likely to display changes in amino acid distribution

upon perturbation. Comparison of the thirty residues identified by SCA and the thirty most conserved residues in the alignment, as measured by evolutionary constraint (ΔG^{stat}), identifies only three residues present in both lists. These are His 26, His 66, and Gly 117. ΔG^{stat}, a measure of conservation, for the thirty highly coupled residues ranges from 0.27 to 1.35 with a mean of 0.51; for the thirty most conserved residues, ΔG^{stat} ranges from 0.88 to 2.86 with a mean of 1.50. Conservation is often used as the first tool to indicate potentially functional residues where structural and functional information is lacking, here we demonstrate an alternative approach to the identification of potentially functional residues which can complement the simple test of conservation.

Group	EcoTK Residue	Position	Known function
1	His 26	Active site surface	Catalysis/stereospecificity
	His 66	Active site surface	Substrate recognition
	Tyr 72	Internal	
2	Tyr 80	Internal	
	Val 109	Internal	
	Ala 444	Internal	
	Asp 462	Internal	
	Asp 183	Internal	
	Gly 117	Internal	
	His 406	Interdomain surface	
	Val 409	Interdomain surface	
	Arg 442	Interdomain surface	
3	Trp 41	Internal	
	Tyr 440	Interdomain surface	Forms hydrophobic pocket
	Ile 517	Internal	
	Asn 443	Interdomain surface	
	Gln 478	Internal	
	Ser 168	Interdomain surface	
	His 461	Interdomain surface	Phosphate binding
	Ile 187	Internal	Metal binding
4	Gly 67	Internal	
	Glu 439	Interdomain surface	
	Met 242	Internal	
5	Leu 74	Internal	
	Phe 434	Interdomain surface	Forms hydrophobic pocket
	Pro 115	Internal	
	Gly 413	Internal	
	Met 447	Interdomain surface	
	Leu 382	Interdomain surface	
6	Leu 62	Internal	

Table 3.1 Hierarchical clusters of coupled positions identified (Figure 3.6) together with their identities in *E. coli* TK and their function where known.

When mapped onto the surface of the *E. coli* TK enzyme, the thirty residues identified display an interesting pattern. Relatively few are exposed on the surface of the holoenzyme apart from in and around the active site (Figure 3.7 a). However, when the two chains of TK are separated (Figure 3.7 b) we see several of the coupled residues exposed on the subunit surface in a connected network which spans out from the active site itself. Rotating the two chains apart further displays the surface residues identified that make up the interface between the two

subunits (Figure 3.7 c). In total, fourteen of the thirty residues identified are located on the subunit surface in and around the active sites.

Some of the interface residues form the binding pocket for the ThDP cofactor, these include Asp 183, Ile 187, Val 409, Phe 434, and Tyr 440. Four residues that make up the active site entrance tunnel are also identified, Lue 382 and His 461 form one side of the active site tunnel and His 26 and His 66 make up the other side. The other five surface residues are located on the interface between the two subunits and are buried in the holoenzyme. These include His 406, Arg 442, Asn 443, Glu 439 and Met 447. Presence of coupled networks of residues on the interface between the two subunits of transketolase could be expected, as a change in the residue identity on one surface of the inter-subunit interface may require a corresponding change on the other face to avoid deleterious effects on subunit aggregation. This also holds true for residues on opposite sides of the active site or on opposite sides of the cofactor binding site.

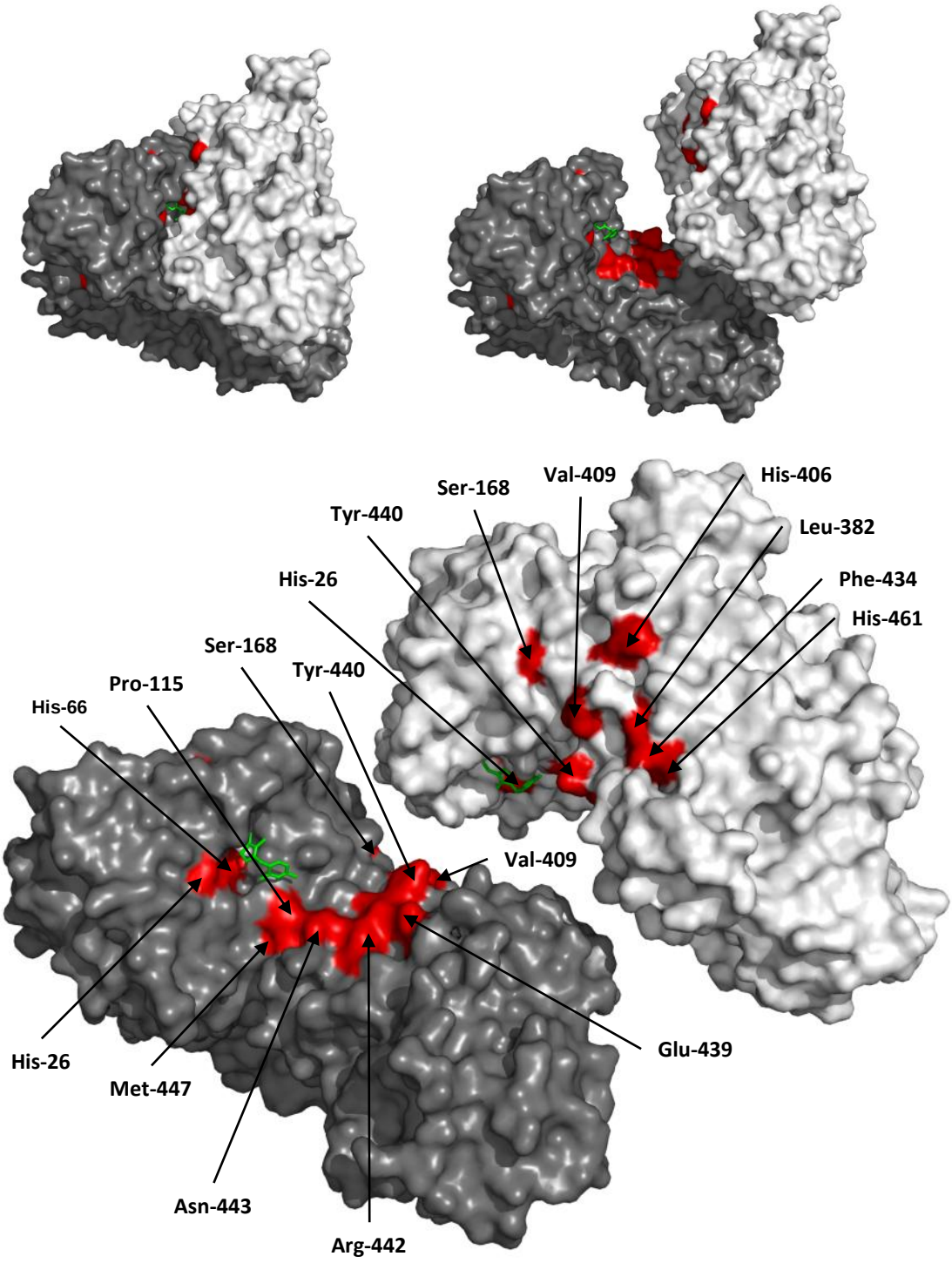

Figure 3.7 Surface rendering of TK showing two chains in different shades of gray and the coupled residues identified in red. a *E. coli* TK showing the active site tunnel with the TPP cofactor in green. b Separation of the two chains to expose the coupled residues that form the interaction face. c Rotation of the A chain by -45 degrees and the B chain by +45 degrees to expose the fourteen coupled residues in the interaction face and the active site.

In order to see the other sixteen coupled residues identified through SCA we need to look into the centre of the protein structure. In Figure 3.8 we see the same view

points but the individual clusters of coupled residues have been surface rendered and they are visualised with the cartoon secondary structure of the PP and PYR domains of chain B and coloured by hierarchical clustering. Although connected networks are apparent among the thirty residues, they are relatively widely distributed throughout the subunit. Examination of the residues in the structure indicates the presence of connected networks, but despite one or two exceptions, grouping of the residues by hierarchical clustering does not resolve all of these networks (Table 3.1). Several connected networks include residues from more than one clustering group. Despite the difficulty in resolving the individual networks, the majority of the residues identified are located on the subunit interface or one layer back from this interface, suggesting that the overriding pressure driving the coevolution of coupled networks in TK and other TPP-dependent enzymes is to support the interactions between the PP and Pyr domains which together form the active site.

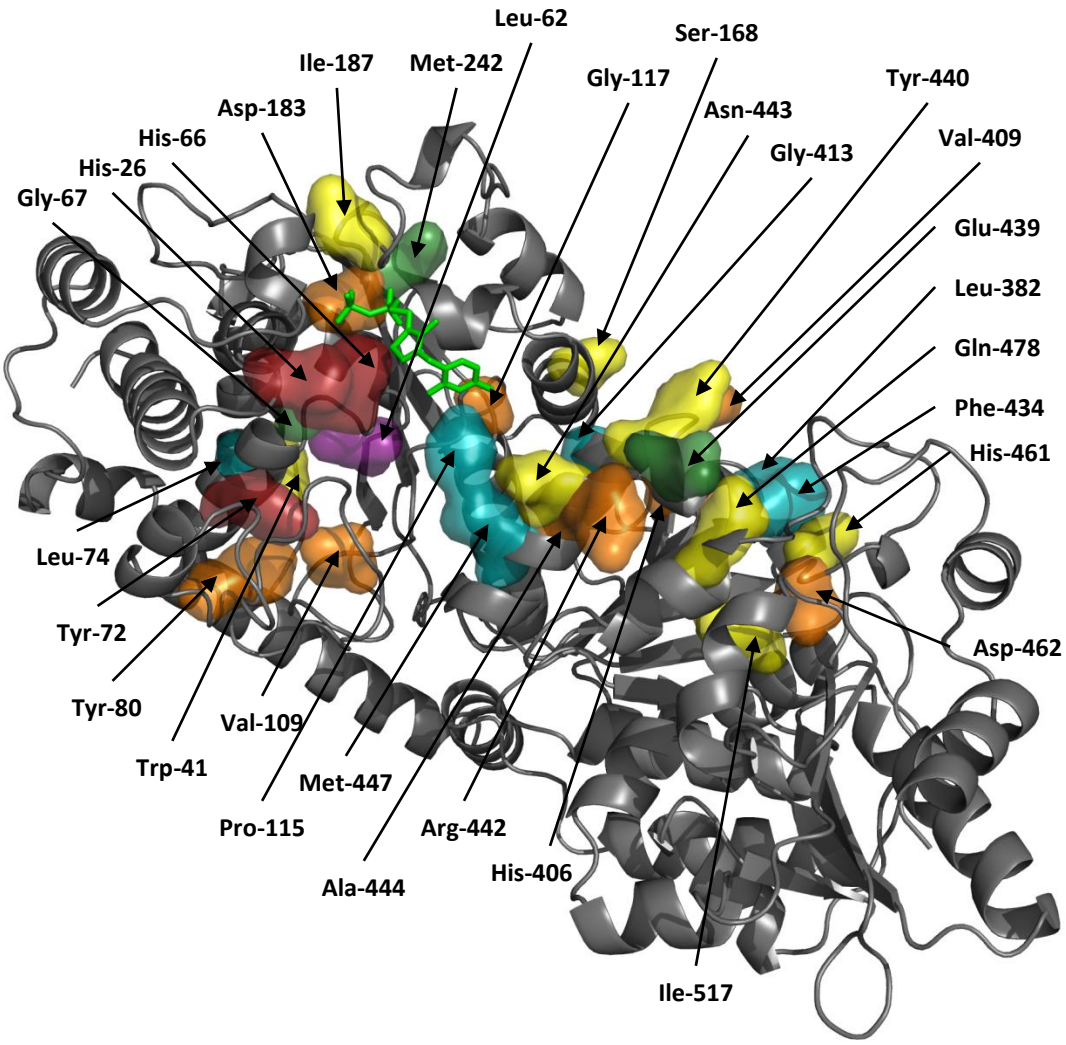

Figure 3.8 All residues identified following global SCA of PP and PYR domains. Residues are coloured by the cluster groupings in Figure 3.6 and mapped onto one subunit of *E. coli* TK.

Although Asp 469 was not identified by global SCA (Asp 469 displays relatively low coupling compared to the highly coupled residues identified), three of the seven residues that are coupled with Asp 469 were identified and these residues were clustered into an independent group by hierarchical clustering. These residues were His 26, His 66 and Tyr 72, the three PP residues identified for their coupling to Asp 469.

This group of residues has a distinct coupling pattern involving good coupling signals with the perturbations 416T, 452Q, 103R, and 105E (Figure 3.6). In contrast

to the vast majority of the coupled residues identified, this group did not co-select their perturbations in the final clustered matrix. This may be due to a distinct group of perturbations specific to the His 26 cluster being removed during the iterative clustering process. This further demonstrates the independence of this cluster from the other residues identified. The location of the three residues, in the active site (His 26 and His 66) and deep within the protein fold (Tyr 72) further suggests a co-evolutionary constraint on catalytic function as opposed to structural dimerization pressures which may explain the coupling of other residues.

The highly coupled but independent residue 62 is also located close to His 26 group. Residue 62 is not highly conserved but it exhibits the highest level of coupling of all the residues in the sequence and falls in a separate, independent cluster. We are unaware of the function of this residue but it displays particularly high coupling energies with other functionally defined residues and its function warrants further investigation.

3.3.4 Single PYR domain global SCA analysis

Position 469 did not display strong enough coupling to be selected in the network of highly coupled residues identified above, where the strongest coupling was seen in the interface between the two subunits of TK. The homodimer of holo-TK is formed through interaction of the PP domain of one subunit interacting with the Pyr domain of the other subunit. In order to identify subtler networks of coupled residues within the Pyr domain of TK we carried out global SCA on just the Pyr domain alignment. By focusing on the Pyr domain we hope to identify networks

containing the 469 position which could aid in the design of multiple mutant libraries with enhanced properties over the individual 469 variant libraries.

The MSA was divided to leave just the Pyr domains and global SCA was carried out as described above. Following initial clustering, a similar set of residues were identified with high coupling energies indicating that the coupling networks even if driven by inter-domain interactions can be identified within one domain in isolation. In addition to the high signal clusters, an interesting cluster of coupled residues was identified in a separate part of the matrix (red sections of dendrograms in Figure 3.9 a below). Upon closer examination this cluster was found to contain Asp 469.

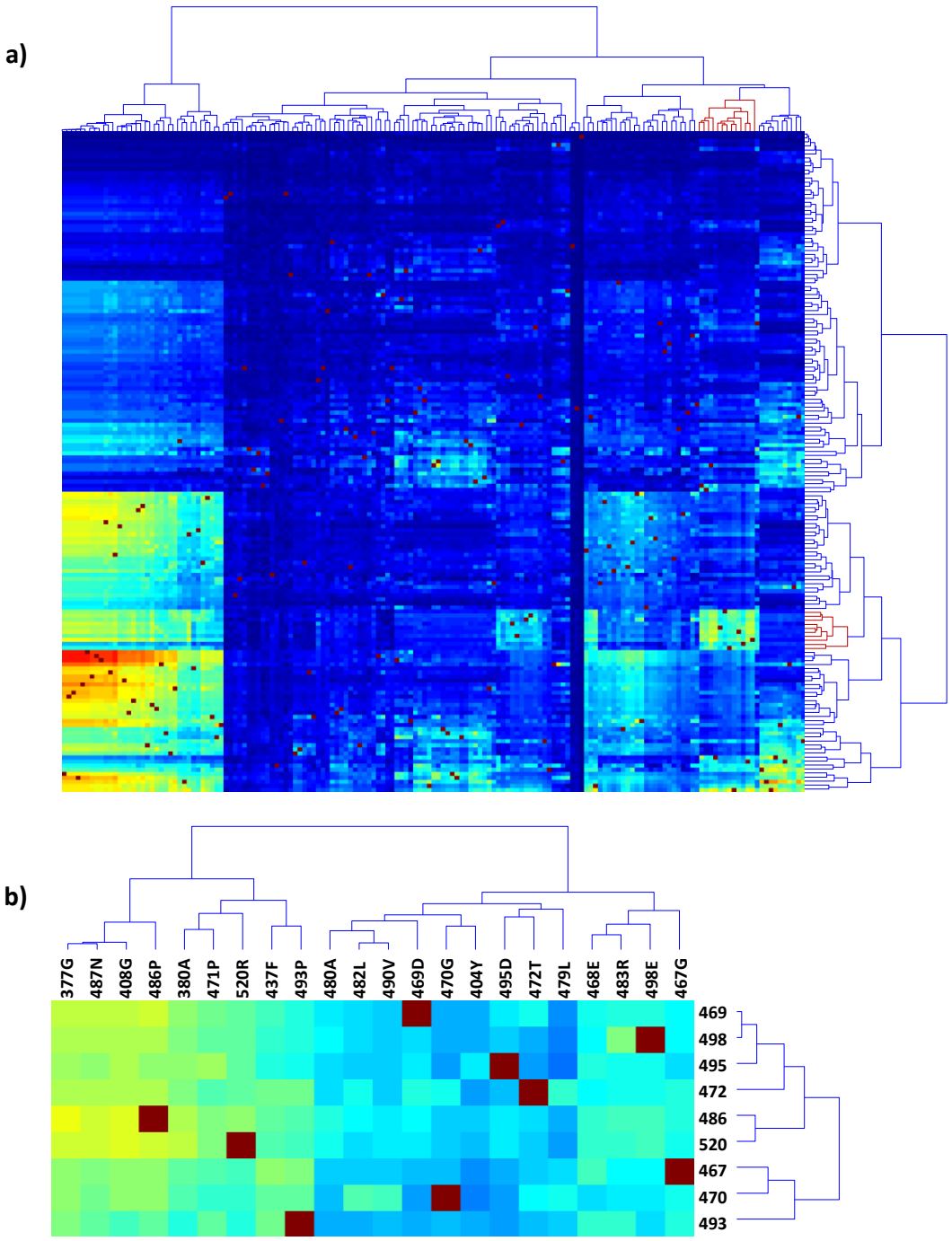

Figure 3.9 a Clustered matrix of $\Delta\Delta G^{stat}$ values following global SCA analysis of PYR domains. Interesting signal cluster containing position 469 identified by red colouring of dendrogram on perturbations and positions. b Matrix following iterative focusing and reclustering around interesting cluster identified in initial clustering

Iterative clustering to focus down to this cluster results in the final matrix seen in Figure 3.9 b. Nine positions are identified in this group including the 469 position. In contrast to the three position His 26 cluster identified following global SCA of the

PP and Pyr domains, this cluster shows self-consistency: the nine positions are also represented in the perturbations that identify them. Such self-consistency gives confidence in the robustness of the evolutionary coupled network.

The nine positions identified include Gly 467, Asp 469, Gly 470, Thr 472, Pro 486, Pro 493, Asp 495, Glu 498, and Arg 520. Three of these residues, Thr 472, Pro 486 and Arg 520, were previously identified by their coupling energy with Asp 469 but the remaining residues have not been identified before. When these positions are mapped onto the PYR domain, two connected networks are visualised, the first containing residues Asp 469, Gly 467, Gly 470, Thr 472, and Arg 520 and the second containing residues Pro 493, Asp 495, and Glu 498 (Figure 3.10 a). The ninth member of this conserved network, Pro 486, is located at a distant point relative to the other groups. However, in *E. coli* TK, Pro 486 forms a tight hairpin turn in the protein structure between an alpha helix and a beta sheet (Figure 3.10 b). This turn forms at a midway point between residues in the two groups described above. It seems likely that the coupling of Pro 486 to the other two groups is related to its function in maintaining the tertiary structure around these two groups of important residues.

By just selecting residues evolutionarily coupled to Asp 469 we identified part of the cluster above. By carrying out a global SCA of the Pyr domain we have identified other physically connected members of this network together with a second, distant group linked to the first via the Pro 486 hairpin turn.

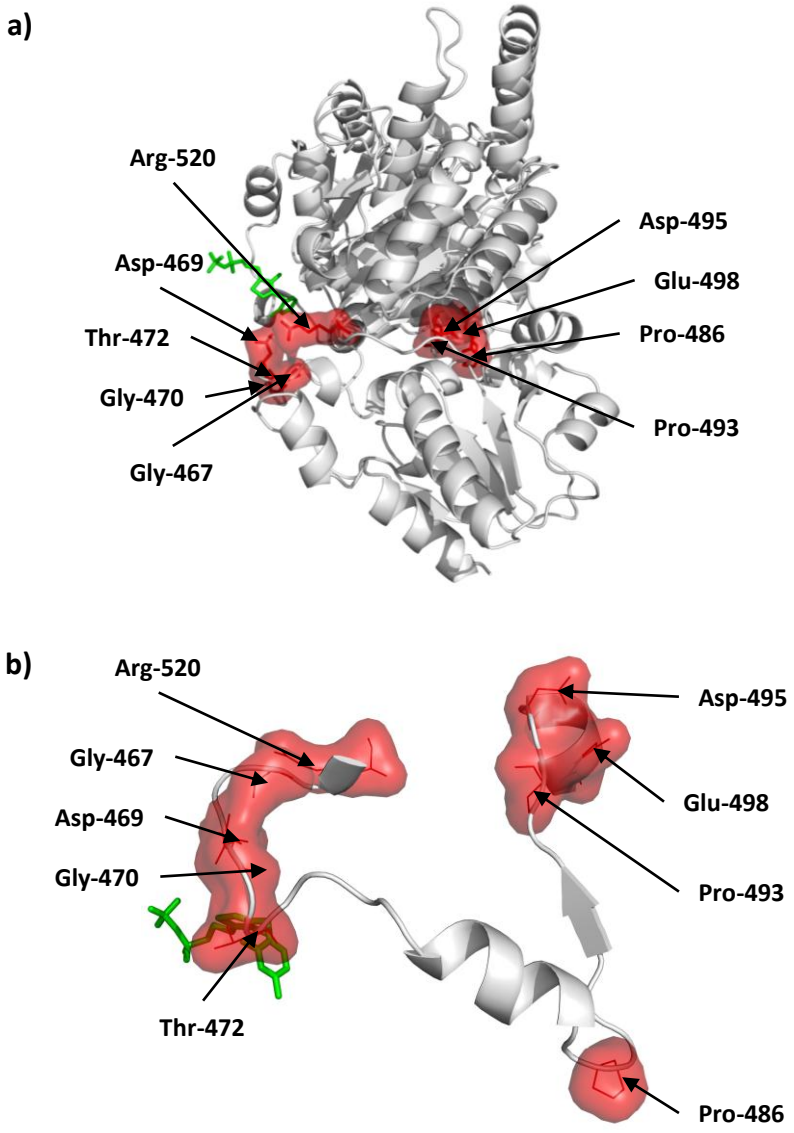

Figure 3.10 a Group of residues coupled to 469 when focusing on PYR domain. PYR domain of chain B displayed. b chain B is rotated away from view by 90 degrees in the X-plane to display relationship between the residues in the cluster. Secondary structure is only displayed for the region spanning residues 465 to 500 to emphasise the relationship between the residues

3.4 Conclusions

We initially investigated the evolutionary coupling between Asp 469 and other positions throughout the MSA of TPP-dependent enzymes. This approach identified seven residues which were either close in proximity to Asp 469 or more distant but with a potential to impact on the tertiary structure around Asp 469. In addition to residues in the same subunit of TK, Asp 469 appears to express evolutionary coupling to sites in the other subunit of the enzyme across the interface barrier.

Having identified residues coupled to Asp 469 we carried out global SCA on the whole MSA to identify further networks within the protein fold. Global SCA identified coupling energies far greater than those associated with Asp 469. Focusing on those high energy positions identified thirty residues dispersed across the two domains. The location of these residues in the interface between the two subunits of TK suggests that co-evolution of the networks identified is driven by structural requirements for dimerization to form the active site. Identification of such interaction surfaces indicates a potential new application for SCA in the identification of protein-protein interaction sites by combining the multiple sequence alignments of proteins known to interact.

Although the clustering of the highly coupled residues did not appear to resolve the detailed sub-networks between the thirty residues, one cluster of three residues did demonstrate structural connectivity and did not appear to be involved in interface interactions. The three residues in this group had previously been identified as the only PP domain residues coupled to Asp 469. The independent identification of this small network by global perturbation analysis suggests that

these residues form a strongly coupled sub-network within the network centred on Asp 469.

In order to identify networks of evolutionary coupling containing the Asp 469 residue we focused the global SCA on the Pyr domain of the MSA. As the subunit interactions are formed between the PP and the Pyr domains of opposite subunits it was hoped that this would filter out the strong coupling signals from the interface between the subunits. The networks of coupled interface residues appear to be so strong that they can be identified by perturbations of the Pyr domain alone. However, an interesting lower signal cluster was investigated and found to contain Asp 469.

The Asp 469 cluster identified some of the residues that had previously shown coupling to Asp 469, however, an additional five residues were newly identified. Eight of the nine residues in the cluster, are arranged in two distinct connected groups in the Pyr domain of TK. In between these two structures, the ninth residue in the group forms a hairpin loop that maintains the tertiary structure around the active site.

SCA is a powerful tool that has previously been applied to several different families of proteins to discover evolutionarily coupled networks of residues [66]. Here we have used the tool to investigate evolutionary coupling within the TPP-dependent enzymes, and specifically the networks of coupled residues in the *E. coli* TK enzyme. Focusing on a key active site residue that has been mutated to engineer improved TK activity on non-natural substrates, we have identified a further eleven residues that could be targeted either singly or in combination to engineer the properties of

E. coli TK. Nine of these residues have not been targeted for directed mutagenesis before.

4 Statistical coupling guided library design for enzyme engineering of Transketolase

4.1 Introduction

Through the reversible transfer of a two carbon ketol unit from D-xylulose-5-phosphate to either D-ribose-5-phosphate or D-erythrose-4-phosphate, transketolase bridges the non-oxidative pentose-phosphate pathway and glycolysis [1]. The substrate specificity of transketolase is relatively broad and the reaction can be made irreversible by replacing the ketol donor with β-hydroxypyruvate (HPA) [8, 27-29, 44, 67, 83]. These attributes make transketolase a very attractive biocatalyst for the stereoselective formation of carbon-carbon bonds in industrial synthesis. *Escherichia coli* transketolase has become the favoured enzyme for biocatalysis applications as it has a higher specific activity with HPA compared to yeast or spinach derived enzyme [1, 28, 30]. Bacterial transketolase is also easier and cheaper to produce in the high yields required for industrial applications [29].

Although transketolase has broad substrate specificity, activity is typically lower with non-phosphorylated aldehyde acceptors such as glycolaldehyde. Use of non-phosphorylated substrates is desirable as it removes the requirement of a de-phosphorylation step later on in synthesis. Various strategies have been applied to increase transketolase activity with non-phosphorylated substrates such as glycolaldehyde. In one example, saturation mutagenesis was targeted at residues in the active site identifying variants with up to 5-fold improvement in specific activity with non-posphorylated substrate relative to wild-type [9]. Transketolase activity is

lower still with non-hydroxylated aliphatic aldehydes [84] (typically 5-35% of those for α-hydroxylated substrates), however saturation mutagenesis targeted at the active site residues identified variants with up to 5-fold improvements in specific activity towards propionaldehyde, an aliphatic non-hydroxylated aldehyde [10].

The examples above demonstrate the potential for transketolase to be engineered to accept non-natural substrates, producing variants with beneficial activities relative to the wild type in industrial applications. Although specific activity has been improved up to 5-fold relative to wild-type for two different non-natural substrates, as we move further away from the natural substrates the ability to enhance activity with single changes to residues in the active site is expected to become more limited, with large increases in specific activity requiring multiple simultaneous mutations. The best mutations identified by saturation mutagenesis of *E. coli* transketolase have been recombined with the hope of achieving further improvements in activity on non-natural substrates. Unfortunately such improvements have proven elusive owing to the negative impact of multiple mutations on aspects of protein structure and function (unpublished data). New strategies are therefore required to identify multiple variants with the potential for enhanced activity towards non-natural substrates.

Different methods have been applied to identify residues which interact synergistically upon combined mutation to produce improvements that are greater than the sum of the respective single mutations. Synergistically interacting double mutants have been identified by targeting pairs of residues close in sequence [50, 85]. An alternative approach is to analyse the results of the first rounds of random

mutagenesis and recombine those predicted to be mutually beneficial [86, 87]. However, it is difficult to predict networks of synergistically acting residues not necessarily adjacent in sequence without prior experimental data on a considerable number of variants.

Statistical coupling analysis (SCA) is a powerful bioinformatics method for identifying co-evolved residues in aligned protein sequences. This technique has been applied to the transketolase enzyme and has identified potentially coupled networks of residues in and around the active site. The co-evolution of these residues may represent synergistic interactions for retained catalytic function, such synergy can be driven by various protein properties such as expression, folding, solubility, stability, activity or allostery.

Asp 469 has been identified as having a key role in substrate recognition and enantioselectivity in *E. coli* TK. Variants of Asp 469 were repeatedly identified from a large number of residues around the active site following directed evolution for improved catalytic activity on non-phosphorylated and non-α-hydroxylated substrates. Statistical coupling analysis of the TK enzyme also identified this residue among a cluster of co-evolving, potentially synergistic, residues. Individual or multiple variant libraries focused on these SCA identified residues could lead to further improvements in the activity of TK on non-natural substrates such as glycolaldehyde and propionaldehyde.

Following pre-incubation with HPA as a ketol donor, we have challenged both single and multiple SCA libraries for enhanced activity with the non-natural, non-hydroxylated substrate propionaldehyde. We used Asp 469 mutations known to

improve activity towards PA as a required initial perturbation and explored double and triple mutants using only the most frequently observed natural variant of six evolutionary coupled residues. This mutagenesis strategy successfully identified a triple mutant cluster which behaves synergistically, whereby the combination of all three mutations leads to greater activity than would be expected from the additive effects of each mutation in isolation. Further evaluation of the triple mutant cycle by kinetic analysis identified a double mutant with significantly improved k_{cat}. For the production of (3S) 1,3-dihydroxypentan-2-one (DHP), this is the highest k_{cat} obtained for any TK mutant to date. In industrial biocatalytic transformations the turnover constant k_{cat} is a very valuable property to improve. The identified variant therefore has considerable potential in the production of DHP.

4.2 Materials and methods

4.2.1 Materials

All chemicals were obtained from Sigma and used as supplied except β-hydroxypyruvate (HPA) which was prepared as the lithium salt as described in section 4.2.1.5.

4.2.1.1 Luria Bertani medium

Luria Bertani (LB) medium was prepared with 10 g L^{-1} tryptone, 10 g L^{-1} NaCl, and 5 g L^{-1} yeast extract in pure water. pH was adjusted to 7 using 4M sodium hydroxide solution and media was sterilised by autoclave (15 minutes, 2 bar, 124 ^{o}C).

4.2.1.2 LB agar plates

LB medium was prepared as described in section 4.2.1.1 above, with the addition of 20 g L^{-1} select agar. LB agar was sterilised by autoclave (15 minutes, 2 bar, 124 ^{o}C). After cooling, ampicillin was added to a final concentration of 150 mg L^{-1} before the solution was transferred to petri dishes to solidify.

4.2.1.3 NZYM broth

NXYM broth was prepared with 22 g L-1 NZYM broth in pure water. pH was adjusted to 7 using 4 M sodium hydroxide solution and broth was sterilised by autoclave (15 minutes, 2 bar, 124 ^{o}C).

4.2.1.4 Ampicillin

Ampicillin was prepared in pure water to a concentration of 150 g L^{-1}. 1ml stocks were sterilised by filtration and stored at -20 ^{o}C in 1.5 ml Eppendorf tubes.

4.2.1.5 β-Hydroxypyruvate

The lithium salt of β-hydroxypyruvate was prepared by modification of a previously described procedure [27]. A 0.06 M solution of bromopyruvic acid was prepared. Using a Metrohm autotitrator, 1 M LiOH was added to 100 ml bromopyruvic acid solution at 3 ml.min^{-1} to bring the pH to 7.0 (approximately 70 ml LiOH was required). LiOH flow rate was then reduced to 1 ml.min-1 and the pH was maintained at 9.0 until a total of 110 ml LiOH had been added. At the end of the reaction, the pH was immediately adjusted to pH 5 using glacial acetic acid and the solution was frozen at -20 ^{o}C (unless concentrated on the same day). The mixture was concentrated under low pressure (using a vacuum pump) to approximately 20 ml final volume. Concentrate was stored at 4 ^{o}C overnight before the crude product was filtered off and washed with ethanol. Crude product was suspended in 50 ml ethanol and 40 ^{o}C for 30 minutes using a rotavap with no vacuum. The white solid was then washed with further ethanol and dried under vacuum to give a white powder. This final product (approximately 2 g) was stored at 4 ^{o}C.

4.2.1.6 Stock co-factor solution

A 12x stock solution of co-factors was prepared with 28.8 mM TPP and 108 mM $MgCl_2$. 12x co-factors were aliquoted into 1.5 ml Eppendorfs and frozen immediately at -20 ^{o}C until required.

4.2.2 Standard procedures

4.2.2.1 Streaking agar plates

Cultures were streaked out on LB agar ampicillin plates with a sterilised wire loop. Plates were incubated at 37 ^{o}C for 16 hours and then stored at 4 ^{o}C.

4.2.2.2 Overnight cultures

Single colonies were picked with a sterilised wire loop from an agar plate into 10 ml LB medium with ampicillin (to a final concentration of 150 mg L^{-1}) in 50 ml Falcon tubes. Tubes were incubated for 16 hours at 37 ^{o}C with shaking at 200 rpm. 500 µl glycerol stocks were prepared (4.2.2.4) and the remaining culture was spun down at 4500 rpm for 10 minutes. Supernatent was discarded and the pellets were used immediately or stored at -20 ^{o}C.

4.2.2.3 100 ml fermentations

10 ml overnight culture was added to 90 ml LBamp and incubated at 37 ^{o}C with shaking at 200 rpm. 1 ml samples were taken each hour to determine biomass by spectrophotometry at OD_{600}. Fermentation was grown until stationary phase which was determined by biomass measurements (approximately 8 hours). At stationary phase 1 ml glycerol stocks were prepared (4.2.2.4) and the remaining fermentation was distributed to two 50 ml Falcon tubes and centrifuged at 4000 rpm for 10 minutes. Supernatent was discarded and pellets were frozen at -20 ^{o}C.

4.2.2.4 Glycerol stocks

Glycerol stocks of cultures were prepared by adding filter sterilised 40% glycerol to overnight culture in a 1:1 volume ratio to give a final glycerol concentration of 20%. Glycerol stocks were aliquoted into 1.5 ml Eppendorf tubes and stored at -80 ^{o}C.

4.2.2.5 Preparation of plasmid DNA

A Qiagen QIAprep Spin Miniprep Kit was used with a microcentrifuge to prepare plasmid DNA from pelleted overnight cultures. Plasmid DNA was eluted in 50 μl 10 mM Tris·Cl, pH 8.5. Concentration and purity were assessed by absorbance at OD_{260} and OD_{280} using a Thermo Scientific NanoDrop Spectropotometer. Final plasmid preparations were stored at -20 ^{o}C.

4.2.2.6 Quickchange™ site-directed mutagenesis

Polymerase chain reaction (PCR) mixture was prepared with 5 μl 10x reaction buffer (supplied by Stratagene), 2 μl pQR791 plasmid DNA (diluted to 10 ng/μl), 1.25 μl +ve primer (100 ng/μl), 1.25 μl -ve primer (100 ng/μl), 1 μl dNTP mix, 1 μl DMSO, 39.5 μl ddH2O (to total 50 μl), and 1 μl Pfu Turbo DNA Polymerase (2.5 U/μl). PCR was run with a 95 ^{o}C 30 second initialisation step followed by 16 cycles of PCR. Each cycle of PCR included a 95 ^{o}C 30 sec denaturing step, a 55 ^{o}C 1 min annealing step and a 68 ^{o}C 22 min elongation step (4 min/Kb). Finally, the plasmid mixture was digested by adding 1 μl Dpn1 and incubating at 37 °C for 2 hours.

4.2.2.7 XL10 Gold transformation

25μl of XL10 Gold cells (Stratagene Ltd.) were thawed on ice and aliquoted into prechilled falcon tubes. 1μl 2-mercaptoethanol was added and the mixture was incubated on ice for 10 minutes with gentle mixing by swirling every 2 minutes. 1μl of the dpn1 digest reaction was added and incubated on ice for 30 minutes. The mixture was heat pulsed at 42°C for 30 seconds then returned to ice for 2 minutes. 225μl NZYM broth (4.2.1.3) pre-heated to 42°C was added prior to incubation at 37°C for 1 hour with shaking at 225 rpm. The NZYM broth mixture was then plated out on LB agar plates and incubated overnight at 37 °C.

For Multi Site-Directed Mutagenesis 45 μl cells, 2 μl 2-mercaptoethanol, 1.5 μl Dpn1 treated multi-site DNA, and 0.5 ml NZYM broth were used.

4.2.2.8 Sequencing

LBamp plates were streaked out from glycerol stock and incubated for 16 hours at 37 °C. Single colonies were used to inoculate 10 ml overnight cultures. After 16 hour incubation at 37 °C, 250 μl was taken to create 20% glycerol stocks and the remaining culture was spun down at 4000 rpm for 10 minutes. Plasmid DNA was extracted from pellets using the standard Miniprep protocol (4.2.2.5). Plasmid DNA was quantified using a NanoDrop spectrophotometer. DNA was then diluted to 16 fmole/μl using ddH2O. Plasmid DNA (24 μl) was sent to Wolfson Institute Scientific Services for sequencing together with 12 μl sequencing primer (TKLibSeqS) per reaction (diluted 1:25).

4.2.2.9 His-tag protein purification

Binding buffer was prepared with 0.5 M NaCl, 20 mM Tris-HCl, and 40 mM Imidazole. Wash buffer was prepared with 0.5 M NaCl, 20 mM Tris-HCl, and 60 mM Imidazole. Elution buffer was prepared with 0.5 M NaCl, 20 mM Tris-HCl, and 0.5 M Imidazole.

Cell pellets from 100 ml fermentations were resuspended in 10 ml binding buffer on ice. Suspended cells were then lysed by 7 cycles of sonication (20 sec on, 20 sec off). The sonicate was centrifuged at 4000 rpm for 10 minutes at 4 ^{o}C. The supernatant was recovered and filtered using a Whatman Puradisc 25 AS 1.0 μm Polyethersulfone membrane followed by Minisart Sterile-EO, non-pyrogenic, Hydrophilic 0.20 μm filters. 0.5 ml samples were taken of sonicate, supernatant and filtrate for evaluation by SDS page gel electrophoresis.

Filtrate was loaded onto a Novagen His bind quick 900 cartridge which had been wetted and equilibrated with 6 ml binding buffer. The cartridge was then washed with 20 ml binding buffer followed by 10 ml wash buffer (provided by Novagen). Finally, protein was eluted with 4 ml elution buffer. Purified protein was dialysed overnight against 2 L 0.5 M NaCl 20 mM Tris (pH 7.0).

4.2.2.10 Protein concentration determination

Concentration of purified TK was determined using densitometry. The extinction coefficient of the TK dimer was calculated from the Escherichia coli TK1 sequence (P27302) [88]. The dimer of *E. coli* TK contains 1326 amino acids including 22 tryptophan residues, 46 tyrosine residues, and 10 cysteine residues. The molecular

weight of the TK dimer is 144405.4. The extinction coefficient (ε_{280}) calculated as described by Pace *et al* is 190790 $M^{-1}cm^{-1}$.

$$Concentration \ \ mg/ml \ = \frac{Abs_{280} \times Molecular\ weight}{\varepsilon_{280}}$$

Concentration of TK in total cell lysates was determined by densitometry of TK bands in coomassie stained SDS gels using the ImageJ program available from http://rsbweb.nih.gov/ij/. Concentrations were benchmarked against bands of purified TK for which concentration had been determined by spectrophotometry.

4.2.2.11 SDS PAGE gel electrophoresis

An 8% acrylamide:bisacrylamide resolving gel solution was prepared using 13.35 ml ProtoGel (supplied by National Diagnostics), 12.25 ml Resolving buffer, 23.6 ml ddH2O, 0.5 ml Ammonium persulfate (10% w/v), and 0.05 ml TEMED. The resolving gel was poured into a preassembled electrophoresis gel chamber and overlayed with ethanol. Stacking gel was prepared with 1.3 ml ProtoGel, 2.5 ml Stacking buffer, 6.1 ml ddH2O, 0.05 ml Ammonium persulfate (10% w/v) and 0.01 ml TEMED. Once the resolving gel had solidified, the ethanol was poured off and the stacking gel solution was poured into the chamber. Finally a Teflon comb was inserted to create the wells.

After polymerisation had completed, the gel was mounted in the SDS chamber. Tris-glycine electrophoresis buffer was used to fill the chamber and flush the wells prior to sample loading. Samples were prepared for SDS by mixing with 2x Laemmli Sample Buffer (Bio-Rad Laboratories) and heating at 100 ^{o}C for 2 minutes. 20 µl of

prepared samples were loaded per well. Gels were run at 80 V for 30 minutes followed by 120 V for an additional 50 minutes. Gels were stained with Coomasie Blue.

4.2.3 Mutant library construction

Single point mutations were introduced to the PQR791 plasmid template using Quickchange™ site directed mutagenesis as described in section 4.2.2.6. Primers for mutagenesis were designed according to the criteria defined by Stratagene and are listed in Table 4.1. Primers were sourced from Operon Biotechnologies. Following transformation of DPN1 digests, colonies were picked for overnight cultures. Pellets from overnight cultures were miniprepped and sequenced to verify mutation. Following sequence verification, a 96-well plate (Deep Square Well) containing 900 µl LBamp in each well was inoculated in triplicate with each variant.

Double mutant libraries were generated using pools of variant plasmids as templates and pools of primers to introduce the second mutation. A G467X/D495X library was created by pooling the four G467 variant plasmids (G467X plasmids) and the four D495 variant plasmids (D495X plasmids) separately. Primers were also pooled to give G467X(-), G467X(+), D495X(-), and D495X(+) primer pools. Two Quickchange™ site directed mutagenesis reactions were set up, one with G467X plasmid templates and D495X(-)/D495X(+) primers, and one with D495X plasmid templates and G467X(-)/G467X(+) primers. The dpn1 digest of both reactions were pooled to create a mixture of plasmids harbouring different combinations of G467X/D495X double mutations. The final pool of plasmid DNA was transformed into XL10 Gold cells and the transformation was plated out on an LBamp agar plate.

The mutagenesis strategy described above was repeated to create three further double mutant libraries, D469X/E498X, D469X/R520X and E498X/R520X. Following incubation at 37 ^{o}C overnight, a QPix robot was used to pick 90 colonies from each double mutant library into 96-well plates (Deep Square Well) containing 900 µl LBamp in each well.

A triple mutant library was created using double mutant libraries as templates. Entire library plates of D469X/E498X, D469X/R520X and E498X/R520X double mutants (each containing approximately 200 colonies) were used to inoculate three 10 ml overnight cultures. Pellets from overnight cultures were miniprepped to isolate plasmid template pools of the D469X/E498X, D469X/R520X and E498X/R520X libraries. A quickchange reaction was set up using D469X/E498X plasmid template together with R520X(-)/R520X(+) primers. Two further quickchange reactions were set up, one with D469X/R520X template and E498X(-)/E498X(+) primers, and one with E498X/R520X template and D469X(-)/D469X(+) primers. The dpn1 digestion products from all three reactions were pooled to create a D469X/E498X/R520X triple library. The plasmid library was transformed into XL10 Gold cells and plated out on six LBamp agar plates. Following incubation at 37 ^{o}C overnight, a QPix robot was used to pick 540 colonies from the six triple mutant library plates into six 96-well plates (Deep Square Well) containing 900 µl LBamp in each well.

The 96-well plates of single, double and triple libraries were incubated for 16 hours at 37 ^{o}C with shaking at 1000 rpm. Following incubation, each 96-well plate was split into six reaction plates (100 µl/well), four glycerol plates (50 µl culture per

well, 50 µl 40% glycerol per well), and one OD read plate (20 µl culture, 180 µl LB per well) using a Tecan high-throughput robot. Reaction and glycerol plates were frozen at -80 °C. Absorbance at 600 nm was measured from the OD read plate using the Tecan spectrophotometer.

Variant	(+) Primer sequence	(-) Primer sequence
G467D	ctccatcggtctggatgaagacgggccgac	gtcggcccgtcttcatccagaccgatggag
G467V	ctccatcggtctggtggaagacgggccgac	gtcggcccgtcttccaccagaccgatggag
G467S	ctccatcggtctgagcgaagacgggcc	ggcccgtcttcgctcagaccgatggag
G467A	tccatcggtctggcggaagacgggccga	tcggcccgtcttccgccagaccgatgga
D469A	ggtctgggcgaagcggggccgactcacc	ggtgagtcggccccgcttcgcccagacc
D469L	tccatcggtctgggcgaactggggccgactcac	gtgagtcggccccagttcgcccagaccgatgga
D469T	tccatcggtctgggcgaaaccgggccgact	agtcggcccggtttcgcccagaccgatgga
D469S	tccatcggtctgggcgaaagcgggccgact	agtcggcccgctttcgcccagaccgatgga
G470T	ggtctgggcgaagacaccccgactcaccagccg	cggctggtgagtcggggtgtcttcgcccagacc
G470N	ggtctgggcgaagacaacccgactcaccagccg	cggctggtgagtcgggttgtcttcgcccagacc
G470L	gtctgggcgaagacctgccgactcaccagc	gctggtgagtcggcaggtcttcgcccagac
G470I	ggtctgggcgaagacattccgactcaccagccg	cggctggtgagtcggaatgtcttcgcccagacc
T472S	gaagacgggccgagccaccagccggttg	caaccggctggtggctcggcccgtcttc
T472D	gcgaagacgggccggatcaccagccggttg	caaccggctggtgatccggcccgtcttcgc
T472A	cgaagacgggccggcgcaccagccggttg	caaccggctggtgcgccggcccgtcttcg
T472L	ggcgaagacgggccgctgcaccagccggttgag	ctcaaccggctggtgcagcggcccgtcttcgcc
D495E	tggcgtccgtgtgaacaggttgaatccgc	gcggattcaacctgttcacacggacgcca
D495N	acatgtctacatggcgtccgtgtaaccaggttgaat	attcaacctggttacacggacgccatgtagacatgt
D495Q	catggcgtccgtgtcagcaggttgaatccgc	gcggattcaacctgctgacacggacgccatg
D495L	tacatggcgtccgtgtctgcaggttgaatccgcgg	ccgcggattcaacctgcagacacggacgccatgta
E498I	tggcgtccgtgtgaccaggttatttccgcggtcgc	gcgaccgcggaaataacctggtcacacggacgcca
E498D	ccgtgtgaccaggttgattccgcggtc	gaccgcggaatcaacctggtcacacgg
E498A	gtgtgaccaggttgcgtccgcggtcgcgtg	cacgcgaccgcggacgcaacctggtcacac
E498V	gtgtgaccaggttgtgtccgcggtcgcgtg	cacgcgaccgcggacacaacctggtcacac
R520G	cactgatcctctccggccagaacctggcgca	tgcgccaggttctggccggagaggatcagtg
R520K	cgcactgatcctctccaaacagaacctggcgcagc	gctgcgccaggttctgtttggagaggatcagtgcg
R520Q	cactgatcctctcccagcagaacctggcgcag	ctgcgccaggttctgctgggagaggatcagtg
R520A	gcactgatcctctccgcgcagaacctggcgcag	ctgcgccaggttctgcgcggagaggatcagtgc

Table 4.1 Primers used to create site directed mutations in *E. coli* TK.

4.2.4 Colorimetric screening of libraries for activity

Biotransformations were prepared using reaction plates containing 100 µl of cell culture per well, lysed by a double freeze-thaw from -80 °C. Cell lysate was pre-incubated with co-factors (2.4 mM TPP, 9 mM $MgCl_2$ final concentration) for 20 minutes. After pre-incubation, Lithium Hydroxypyruvate (50 mM final concentration) followed by Propionaldehyde (50 mM final concentration) were

added to a total volume of 300 µl. All reagents were prepared in 50 mM Tris buffer at pH 7.0. Propionaldehyde was prepared fresh on the day of the biotransformation. The biotransformations were incubated for 48 hours at 21 ^{o}C.

Colorimetric screening was carried out on biotransformation reaction plates as described previously [89]. Fresh 96-well plates (Shallow Round Well) were prepared with 50 µl Tris buffer (50 mM, pH 7.0) and 20 mg MP-Carbonate Scavenger Resin (supplied by Biotage) in each well. Individual biotransformation reactions (50 µl) were then added to each well and incubated for 3 hours at 21 ^{o}C to quench any excess hydroxypyruvate. Following quenching, the reaction-resin mixture was diluted with 100 µL Tris buffer (50 mM, pH 7.0) and 100 µl of the reaction mixture was transferred to a new plate containing 20 µl 2,3,5-triphenyltetrazolium chloride solution (0.2% in methanol), leaving the resin beads in the first plate. A plate reader (Fluostar, BMG-labtech) fitted with an autoinjector was used to add 10 µl NaOH (3 M) to each well of the new plate. Following addition of NaOH, the plate was shaken for 10 seconds and left to stand for 1 minute before an OD measurement was taken for each of the wells at 485 nm (50 flashes per well).

4.2.4.1 Validation of colorimetric screen

The colorimetric screen was validated for its ability to identify positive variants relative to wild type level activity. Variants D469A, D469E, and D469T, known to demonstrate increased activity relative to wild type, were screened against wild type TK. In total, 93 positive controls and 93 wild type controls were screened (Figure 4.1). Results from the assay indicated twelve potential false positives in the

wild type group and five potential false negatives in the positive group. The colorimetric assay therefore displays good predictability of activity.

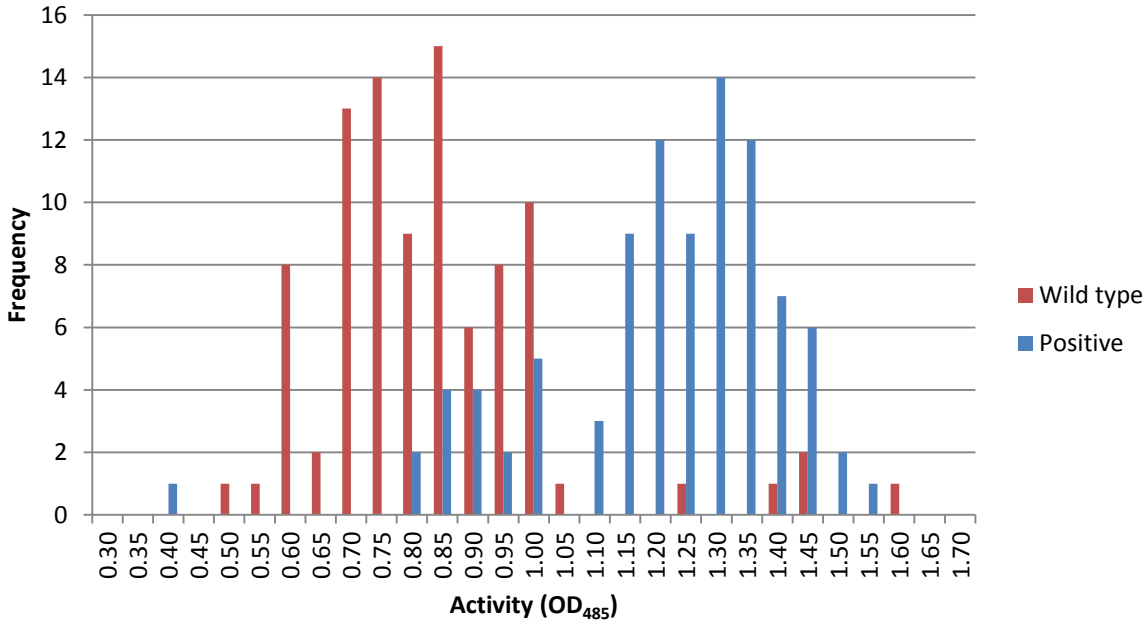

Figure 4.1 Validation of the colorimetric assay to distinguish between wild-type transketolase and improved variants on the PA reaction.

4.2.5 Solubilisation and refolding of insoluble variants

4.2.5.1 Solubilisation of transketolase variants

Pellets from 100 ml fermentations were resuspended in 40 ml binding buffer, sonicated (20 sec on, 20 sec off, 20 cycles), and spun down for 15 min at 5000 rpm. This wash step was repeated once more with 20 ml binding buffer. The final pellet was resuspended in 5 ml binding buffer with 3 M Guanidine HCl (concentration required to remove TK from insoluble fractions), sonicated and incubated overnight at 4 ^{o}C to solubilise the TK enzyme. The solubilised TK was spun down at 5000 rpm for 30 minutes and the supernatant was purified on an NiNTA column as described previously (4.2.2.9) but with 3 M Guanidine HCl in each buffer. Imidazole

concentration in the wash buffer was reduced to 20 mM to account for the Guanidine HCl.

4.2.5.2 Refolding by dialysis

Eluted TK was dialysed against decreasing concentrations of Guanidine HCl in 0.5 M NaCl, 20 mM Tris over a course of 20 hours. Dialysed samples in 0.5 M NaCl, 20 mM Tris were spun down at 5000 rpm for 30 minutes at 4 ^{o}C and analysed for protein concentration at $OD_{280\ nm}$.

4.2.5.3 Refolding by drip feeding

5 ml of eluted TK was drip fed into 45 ml 50 mM Tris HCl, 5 mM DTT over the course of 8 hours. Dilute solution of refolded protein was concentrated to 1 ml sequentially using 10,000 micron followed by 3,000 micron spin columns. Concentrated protein solution was dialysed against 20 mM Tris, 0.5 M NaCl.

4.2.6 Activity of purified enzymes

Wild-type and mutant transketolases were over-expressed and purified using His-tag affinity chromatography, and enzyme kinetics were determined using HPLC. 300 µl reactions were prepared in sealed glass vials using 150 µl purified protein. Purified protein was pre-incubated with co-factors (2.4 mM TPP, 9 mM $MgCl_2$ final concentration) for 20 minutes prior to the addition of Lithium Hydroxypyruvate (50 mM final concentration). Propionaldehyde was then added to varying final concentrations. Samples (20 µl) of reaction mixture were taken at twelve separate time points (at least one hour apart) and quenched with 180 µl 0.1% Trifluoroacetic acid (TFA). Quenching was carried out in a microplate which was stored at -20 ^{o}C in-

between time points. For each variant, reactions were prepared with seven different final concentrations of propionaldehyde, from 8 mM to 60 mM.

The reaction product was measured by HPLC using a 15 cm C18 column and a 15 min isocratic protocol of 0.1% TFA in 5% acetonitrile with a flow rate of 0.6 ml min^{-1}. Product was detected by UV at 200 nm. Standard curves were produced with 10-50 mM 1,3-dihydroxypentan-2-one and these were used to determine the product concentrations. New standard curves were produced for each microplate analysed.

4.2.7 Enantioselectivity of purified enzymes

The stereoselectivity of purified TK variants was established by gas chromatography as described previously [11]. Reactions were carried out to completion using purified TK with 50 mM LiHPA, 50 mM PA, 50 mM Tris-HCl, 2.4 mM TPP, 9 mM $MgCl_2$, 250 mM NaCl, pH 7.0 at 300 µl scale in sealed glass vials. Reaction mixture (100 µl) was transferred to vials containing 300 µl EtOAc. Vials were shaken and allowed to partition. The organic phase (100 µl) was transferred to fresh vials and pyridine (containing DMAP (10 mg/ml), 20 µl) was added to each vial. Following conversion of DHP to the diacetate, enantiomeric purity was assessed by gas chromatography on a Perkin-Elmer Autosystem XL Gas chromatograph with a β-Dex 225 chiral column (Supelco, 30 m x 0.25 mm). GC conditions: injection volume, 1 µl; carrier gas, He; carrier gas pressure, 15 psi; injector temperature, 250 ^{o}C; oven temperature, 60 ^{o}C then increased at 3 ^{o}C/min; detector temperature, 300 ^{o}C; detection, flame ionised detector (FID). Retention times: (3R)-pentan-2-one diacetate, 29.9 min; (3S)-pentan-2-one diacetate, 30.3 min.

4.3 Results and Discussion

4.3.1 Library design strategy

We described the use of SCA to identify co-evolving networks of residues in TPP-dependent enzymes. The identification of such networks enables the selection of residues for mutagenesis that are functionally linked to the active site and the rational design of multiple-mutant libraries with synergistic potential. We have identified a nine residue network within the Pyr domain of TPP-dependent enzymes that includes the functional Asp 469 residue in *E. coli* TK (Figure 4.2). This network was comprised of two structurally contiguous groups of residues with a proline residue forming a hairpin turn at a midway point between the two groups. Here we describe the creation of variant libraries by site directed mutagenesis focused on this nine residue network.

The nine positions identified in the Pyr cluster included Gly 467, Asp 469, Gly 470, Thr 472, Pro 486, Pro 493, Asp 495, Glu 498, and Arg 520. Of these nine residues, we selected seven to target for mutagenesis. The two proline residues, Pro 486 and Pro 493, were excluded as mutagenesis of these residues is likely to disrupt the tertiary structure of the TK enzyme limiting the potential to identify active variants. A second strategy adopted to avoid the introduction of destabilising mutants was to limit mutations to the most frequently observed natural variants in the TPP-dependent enzyme MSA (Table 4.2). The exceptions to this strategy included Asp 469 for which mutations were selected that were known to improve activity towards PA, and Gly 467 for which one of the common residues is a proline which was avoided for the stability issues discussed above.

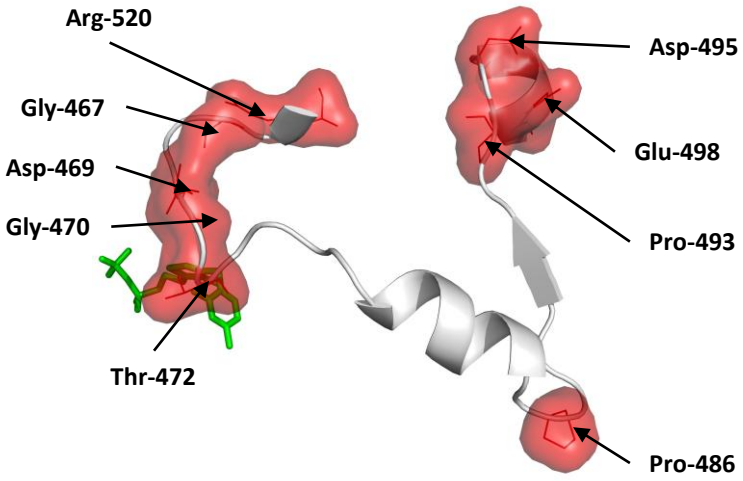

Figure 4.2 Cluster of co-evolving residues in *E. coli* TK identified by SCA of the PYR domain of TPP dependent enzymes. Two structurally contiguous groups of residues are linked by a proline residue (Pro 486) forming a hairpin turn in the tertiary structure. Arg 520, Gly 467, Asp 469, Gly 470, and Thr 472 make up the contiguous group proximal to the active site.

	Position							
Residue	467	469	470	472	495	498	520	Average in all proteins
A	**2.1**	**3.7**	2.1	**10.7**	3.7	**8.9**	**6.3**	7.3
C	0	0	0	0	0	0.5	2.6	2.5
D	**10.7**	***45.3***	2.9	**9.7**	***44.5***	**11.3**	1.0	5
E	1.8	3.9	0.3	0.5	**12.8**	***42.1***	1.8	6.1
F	0.3	1.6	0	1.8	2.4	1.0	2.6	4.2
G	***43.5***	3.7	***47.9***	0.5	0.5	1.0	**6.0**	7.2
H	1.3	1.3	0.3	0	0.3	0	0.3	2.3
I	1.0	2.4	**9.4**	0	1.0	6.0	3.9	5.3
K	0.5	2.1	2.6	0	0.3	1.0	**19.6**	6.4
L	0	**7.1**	**13.4**	**9.7**	**8.4**	4.5	0.3	8.9
M	0.3	1.8	2.6	0.3	0.8	1.8	1.0	2.3
N	0.3	8.6	4.2	0	**6.3**	0.5	2.1	4.3
P	3.4	1.3	0	1.8	0.8	0	0.3	5.2
Q	0	2.1	1.6	3.9	**6.5**	2.6	**6.8**	4
R	0	6.8	3.7	0.5	0.8	1.3	***39.3***	5.2
S	**2.9**	**0.5**	2.9	**5.8**	2.4	1.6	0.5	7.3
T	0	**1.0**	3.9	***47.4***	4.5	3.1	1.6	5.6
V	**2.4**	1.3	1.6	2.6	0.3	**11.3**	2.9	6.3
W	0	1.0	0	0	0	0.5	0.3	1.3
Y	0.3	0.5	0.3	4.2	0.3	0.5	0.5	3.3

Table 4.2 Frequency (%) of residues at selected positions within the TPP-dependent enzyme multiple sequence alignment. Chosen variants (bold), including the wild type residues (italic) were the most frequently occurring natural variants from an alignment of 382 homologous TPP-dependent enzymes. Exceptions (underlined) are G467P and D469E/N/R.

4.3.2 Construction and screening of SCA directed single mutant library

The twenty-eight single point mutations were introduced into *E. coli* TK by site directed mutagenesis and verified by sequencing. 96-well microplates were prepared as described in section 4.2.3 containing the single-point mutants of TK in triplicate. Measurement of cell density across microplates indicated successful growth with no positional effects on growth across the plate. Eight wells displayed unusually low cell density (Figure 4.3) but comparison with equivalent variants displaying high cell density demonstrated no correlation between activity of TK and cell density. Cell density does not therefore appear to correlate closely with the active enzyme concentration and cannot be used as a surrogate measure for protein concentration for the determination of specific activities.

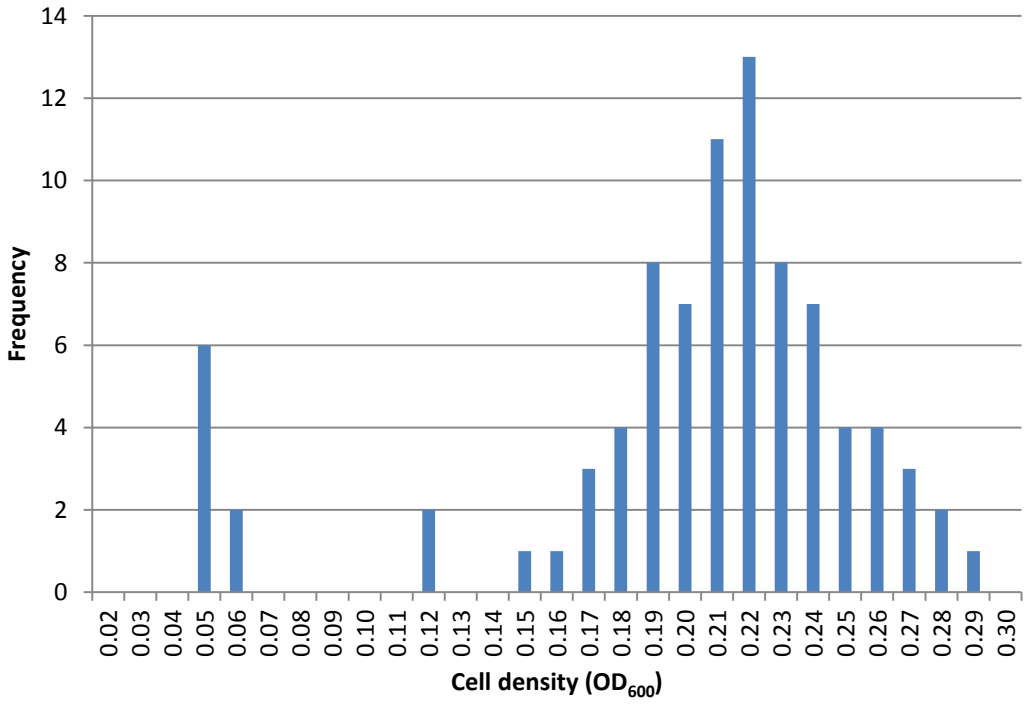

Figure 4.3 Distribution of cell growth across the microplate as measured by cell density (OD_{600}).

Activity of variants was determined for the TK catalysed conversion of propionaldehyde and HPA into DHP. The absolute activity of each variant was measured in triplicate using the colorimetric screen developed by Smith *et al* [89], relative activities were calculated using internal wild type standards (hextuplet). Good consistency was observed across the replicates giving confidence in the colorimetric screen to determine relative activities (Figure 4.4).

Variants with improved activities relative to wild type TK were identified for five of the seven residues in the SCA directed single mutant library, these sites included Gly 467, Asp 469, Gly 470, Tyr 472 and Arg 520 (Figure 4.4). Notably, these residues make up the structurally contiguous group of residues proximal to the active site (Figure 4.2). In contrast the two residues belonging to the more distant structural group failed to produce any variants with activity increases, all mutations at these positions resulted in seriously compromised TK enzyme with approximately 30% wild type activity (Figure 4.4).

As expected, all the Asp 469 variants displayed increased activity relative to the wild-type transketolase standards contained in the same plate (Figure 4.4). Asp 469 interacts with the α-hydroxyl group of natural aldehyde acceptors providing a possible explanation for the improved activity of variants at this position with non-α-hydroxylated substrates. Mutation of Arg 520 also produced a high proportion of variants with increased activity on PA relative to wild type TK. The Arg 520 variant R520V has previously been identified as improving TK activity on GA [9] and PA [10]. Arg 520 interacts with the phosphate group of natural TK substrates, it has been hypothesised that the reduction in steric bulk associated with variation of this

residue could explain the enhanced activity seen on non-phosphorylated substrates. Although R520G has been previously identified by directed evolution for enhanced activity on GA, R520K, R520Q and R520A have not.

The other three residues for which variants displayed improved activity- Gly 467, Gly 470, and Tyr 472- have not been previously targeted for saturation mutagenesis. The identification of variants at these positions with enhanced activity on PA demonstrates the potential of SCA to identify new positions which can be targeted for site directed mutagenesis. In this study only four variants were introduced at each site, the high frequency of improved variants despite the small sample size suggests that further improvements may be identified by full saturation mutagenesis of these SCA identified sites.

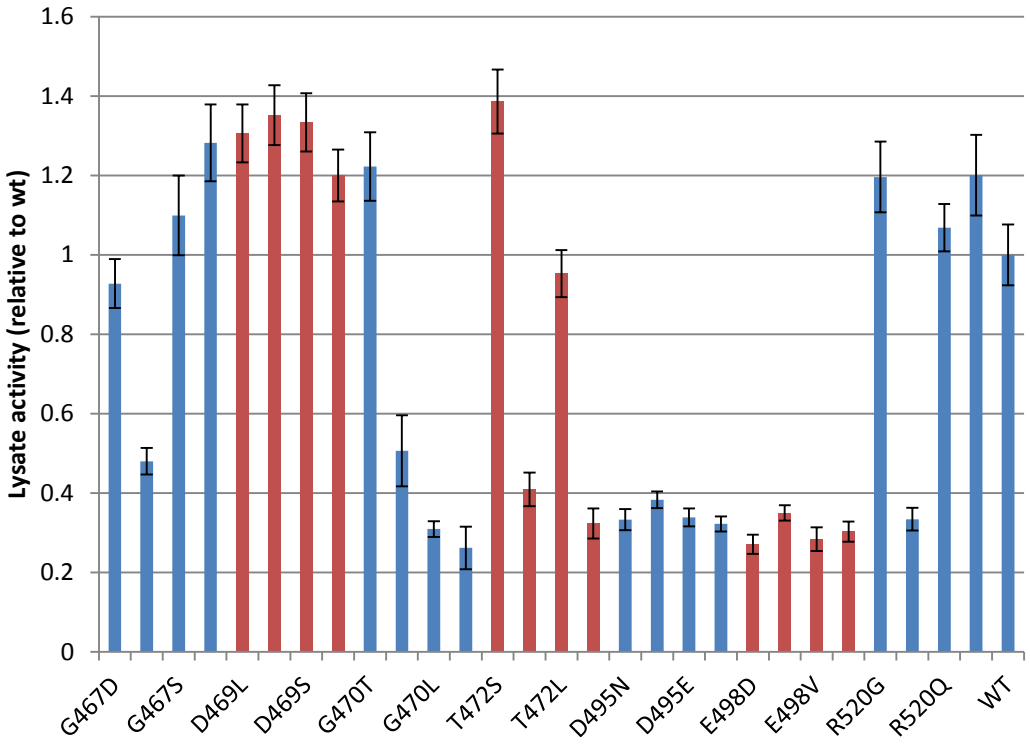

Figure 4.4 Relative lysate activities of single mutants relative to wild type on the reaction between HPA and propionaldehyde. Total activity determined using the high-throughput colorimetric assay with 50 mM LiHPA, 50 mM PA, and 50 mM Tris-HCl, 2.4 mM TPP, 9 mM $MgCl_2$, 250 mM NaCl, pH 7.0 to produce 1,3-dihydroxypentan-2-one (DHP).

4.3.3 Construction of SCA directed double and triple mutant libraries

Analysis of the single variant SCA directed library identified variants with both improved and impaired activity on PA relative to wild type TK. If the residues of this co-evolving cluster are synergistically coupled we could expect to see non-additive effects when the different mutations are combined in multiple mutants. Even with such a focussed and restricted library of tweny eight variants, the theoretical total number of mutant combinations at these seven sites would be 78,124. Libraries of this size are not out of the range of screening by high-throughput techniques but this is beyond the scope of the current study.

In order to test the hypothesis of synergy between the seven residues identified by SCA we have selected two groups of residues from which to produce smaller, more manageable multiple mutant libraries. Each of these groups includes residues from both the proximal contiguous cluster and the distal group of residues, for which no single variants with improved were identified.

The first group selected for combined mutagenesis includes residues Asp 469, Glu 498 and Arg 520. Variation at two of these residues has demonstrated improvements in activity on both GA and PA. In contrast, all four variants of Glu 498 resulted in severely impaired catalytic activity on PA. If synergistic relationships exist between these residues we could hope to see non-additive effects when the mutations are combined.

The second group selected for combined mutagenesis includes residues Gly 467 and Asp 495. Again this group includes positions from both contiguous structural clusters, one of which has produced improved variants (Gly 467), and one from which no improvements have been identified (Asp 495).

Following creation of the 540 variant triple mutant library (D469X/E498X/R520X) and the 90 variant double library (G467X/D495X), sample sequencing of ten wells from each was carried out to verify coverage of sequence space (Table 4.3). Full representation was established for the G467X/D495X library with all variants represented at each position. Although we did not attain full representation of variants across all the three sites of the D469X/E498X/R520X library, site D469 and E498 displayed three of the four possible variants, and at site R520 all four possible variants were observed. The diversity of the libraries therefore appeared very good, giving confidence that full coverage of the sequence space was attained. Notably, no wild type residues were identified in either library. In order to ensure that double as well as triple variants were captured for the D469X/E498X/R520X library, three further double mutant libraries were created for D469X/E498X, D469X/R520X, and E498X/R520X, each with 90 variants.

Sequencing sample	G467X/D495X Library	D469X/E498X/R520X Library
1	G467V/D495N	D469S/E498V/R520A
2	G467D/D495L	D469A/E498V/R520G
3	G467D/D495Q	D469A/E498I/R520K
4	G467D/D495N	D469T/E498D/R520A
5	G467A/D495E	D469T/E498D/R520A
6	G467D/D495E	Bad signal
7	G467S/D495N	D469S/E498V/R520Q
8	G467D/D495N	D469A/E498V/R520G
9	G467D/D495Stop	D469T/E498I/R520Q
10	Bad signal	D469T/E498V/R520Q

Table 4.3 Sample sequencing results of G467X/D495X and D469X/E498X/R520X libraries.

4.3.4 Double and triple mutant library colorimetric screen of activity

Libraries were screened in duplicate using the colorimetric screen developed by Smith *et al* [89]. For each plate, relative activity on the propionaldehyde HPA reaction was determined using internal wild type standards. The well-defined nature of the libraries produced (as determined by sample sequencing) presents an opportunity for analysis of variant libraries as a whole, comparing the average relative activities and the ranges of relative activities across libraries. The D469X/R520X library produced the highest mean relative activity. Average activities across the other four libraries were lower than wild type and the G467X/D495X library demonstrated the lowest average relative activity (Table 4.4).

	Experimental		Expected	
Library	Mean	Range	Mean	Range
G467X/D495X	0.73	0.42 – 1.04	0.33	0.15 – 0.49
D469X/E498X	0.68	0.36 – 0.95	0.39	0.33 – 0.47
D469X/R520X	1.07	0.64 – 1.49	1.23	0.40 – 1.62
E498X/R520X	0.92	0.65 – 1.16	0.29	0.09 – 0.42
D469X/E498X/R520X	0.90	0.25 – 1.91	0.37	0.11 – 0.57

Table 4.4 Mean relative activities and ranges of activities across libraries compared with that expected in unbiased libraries based on single variant relative activities. Total activity determined with 50 mM LiHPA, 50 mM PA, and 50 mM Tris-HCl, 2.4 mM TPP, 9 mM $MgCl_2$, 250 mM NaCl, pH 7.0 to produce 1,3-dihydroxypentan-2-one (DHP).

If we assume no bias in the libraries, we can calculate the expected mean activities based on the activities of single mutants. Comparing such expected mean relative activities with the experimental mean relative activities indicates generally higher than expected activity across the libraries. The exception to this is the D469X/R520X library which produced a lower experimental mean relative activity than that expected (Table 4.4).

Comparison of the ranges of expected and experimental activities alleviates the requirement for a lack of bias, assuming full coverage of variants has been attained. The experimental range of activities across the G467X/D495X library was 2.1- to 2.8-fold greater than expected. Relative activities at the low end of the range were as expected for the D469X/E498X library but activities at the high end were 2.0-fold greater than expected. The range of activities for the D469X/R520X library was as expected although the experimental range was slightly tighter than the expected range. The experimental ranges for both the E498X/R520X and D469X/E498X/R520X were markedly higher than expected. For the E498X/R520X library this was most apparent at the low end with 7.2-fold greater activity than expected, and for the D469X/E498X/R520X library the biggest increase was at the high end with a 3.4-fold increase over that expected.

These data suggest potential synergy between the mutations in the multiple mutant libraries. General synergy is apparent between Gly 467 and Asp 495 variants with higher than expected activities. Variants of residue Glu 498 display potential synergy with both the Asp 469 (D469X/E498X library) and the Arg 520 variants (E498X/R520X library). However, no double variants have been identified in either

library with superior activity to the single variants of Asp 469 or Arg 520. This suggests that the synergistic relationships in both combinations are acting to alleviate the negative impact of variants at Glu 498. In the triple library, D469X/E498X/R520X, variants have been identified that display a synergistic increase in activity over and above the activity seen with any single variant. Although no synergy is apparent between Asp 469 and Arg 520 variants in the D469X/R520X library, these residues may have a more complex synergistic relationship incorporating the third variant, Glu 498.

The most active variant following the primary colorimetric screen was found in the triple mutant library D469X/E498X/R520X which displayed a relative activity of 1.91. Sequencing identified this variant as D469S/E498D/R520Q. Such a triple variant is of particular interest because the E498D mutation results in an inactive enzyme in isolation. In order to explore the synergistic relationships between these residues further, a mutant cycle of this triple variant was created and purified for further detailed analysis.

4.3.5 Total lysate activities of the triple mutant cycle D469S/E498D/R520Q

In order to produce a full triple mutant cycle, constructs were created by site directed mutagenesis for the double variants D469S/E498D, D469S/R520Q, and E498D/R520Q. Single variants had been produced previously by site directed mutagenesis. Following production and verification of the triple cycle, total lysate relative activities were determined for the triple mutant cycle using the colorimetric assay (Figure 4.5).

The D469S mutation and the R520Q mutation independently alleviate the negative impact of E498D, producing higher relative activities than expected with the D469S/E498D and the E498D/R520Q combinations. When all three mutations are combined, a triple variant is produced with considerably higher relative activity than could be expected taking each of the variants in isolation. These results suggest significant synergy between the three variants. However, in the absence of the E498D mutation, no synergy is apparent between D469S and R520Q based on this analysis.

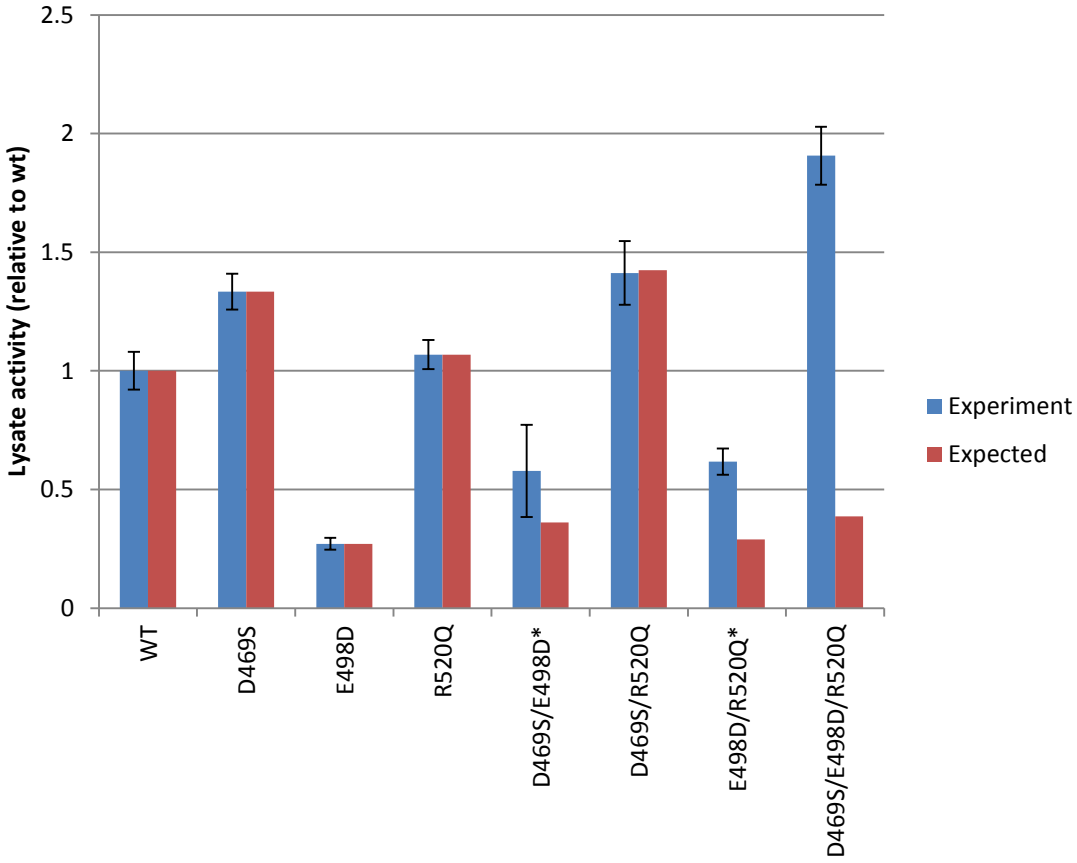

Figure 4.5 Experimental and expected total lysate activities of Transketolase variants in the triple mutant cycle of D469S/E498D/R520Q. Total activity determined with 50 mM LiHPA, 50 mM PA, and 50 mM Tris-HCl, 2.4 mM TPP, 9 mM $MgCl_2$, 250 mM NaCl, pH 7.0 to produce 1,3-dihydroxypentan-2-one (DHP).

4.3.6 Purification of the triple mutant cycle D469S/E498D/R520Q

Lab scale fermentations of the selected triple mutant cycle variants were carried out and variants were purified on Ni-NTA columns as described in section 4.2.2.9. Expression and solubility profiles of the different variants provide information on the potential origin of synergy between these three positions.

Expression of the single variant D469S was marginally decreased relative to wild type TK, in contrast the expression of the R520Q variant was increased by 40%. However, introduction of the E498D variant reduced expression to less than 40% that of wild type TK (Figure 4.6). All of the codons introduced by site directed mutagenesis were the optimal for expression in *E. coli* TK so the decrease in expression with E498D is likely to be due to a loss of protein stability or solubility.

The combination of the two variants in the double mutant E498D/R520Q recovers the total protein expression of TK but the protein remains insoluble as determined from the concentration of TK in the soluble fraction. The double mutant D469S/E498D fails to improve total protein expression but does marginally improve the solubility relative to the E498D mutation in isolation. The triple mutant D469S/E498D/R520Q increases the total protein expression relative to E498D but no increase in the soluble fraction of TK is observed (Figure 4.6).

Based on the results above the enhanced activity of the triple mutant cannot be explained by an increase in expression or stability relative to wild type TK. Instead, the improvement appears to be due to enhanced specific activity or better folding of the soluble fraction to the active native state.

For all variants, a similar percentage of soluble protein was His-tag purified using His affinity resin. In all variants containing the E498D variant, the yield was too low to carry out further analysis on purified enzyme.

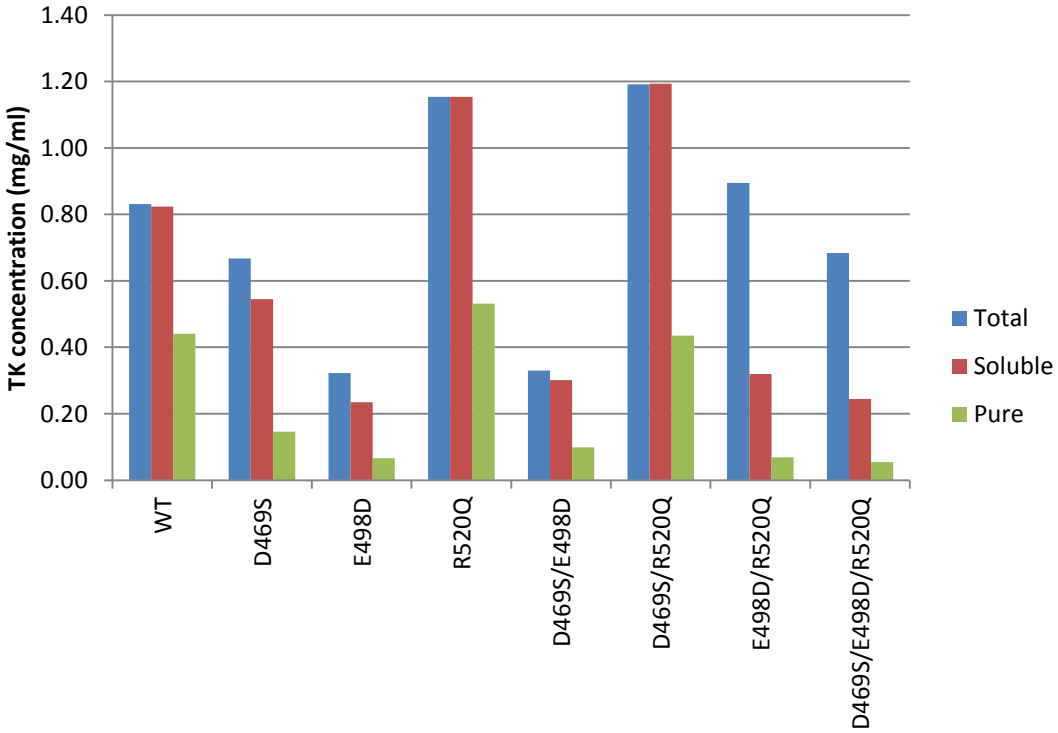

Figure 4.6 Total, soluble and pure concentrations of TK variants.

4.3.7 Solubilisation and refolding of E498D containing variants

In order to obtain kinetic data on the full triple mutant cycle of D469S/E498D/R520Q, efforts were made to obtain purified variants in suitable quantities for the three members of the cycle containing the E498D variant. New 100 ml fermentations were produced for each variant and prior to purification, TK was solubilised with Guanidine HCl as described in section 4.2.5.1. Following purification, refolding was attempted by both dialysis and drip-feeding. Unfortunately neither technique resulted in active protein as determined by HPLC

kinetic analysis. Further analysis of purified variants has therefore been limited to those variants that did not contain the E498D mutation.

4.3.8 Enzyme kinetics of purified variants

The enzyme kinetics of His-tag purified wild type TK and variants D469S, R520Q, and D469S/R520Q were established by HPLC with 50 mM HPA over a range of propionaldehyde concentrations (8 mM-60 mM) (Table 4.6 and Figure 4.7). At 50 mM, the concentration of HPA used here is approximately 10 times the K_m of wild type TK.

The single mutation D469S produced a variant of TK with a 60% increase in k_{cat} (57 min^{-1} vs 35 min^{-1}) and a 40% decrease in K_m (71 mM vs 181 mM) relative to wild type. The combined effect of these changes was a 4-fold increase in the corresponding k_{cat}/K_m (0.81 min^{-1} mM^{-1} vs 0.19 min^{-1} mM^{-1}) relative to wild type. The R520Q variant resulted in a similar k_{cat} to wild type TK (31 min^{-1} vs 35 min^{-1}). However, the K_m for this variant almost doubled relative to wild type (329 mM vs 181 mM) resulting in a k_{cat}/K_m approximately half that of the wild type enzyme (0.10 min^{-1} mM^{-1} vs 0.19 min^{-1} mM^{-1}).

The most dramatic changes in kinetic parameters were observed with the double mutant D469S/R520Q. This variant displayed a 20-fold increase in k_{cat} (700 min^{-1} vs 35 min^{-1}) which more than compensated for a 3.5-fold increase in K_m (628 mM vs 181 mM). The resulting k_{cat}/K_m was 6-fold higher than that of wild type (1.11 min^{-1} mM^{-1} vs 0.19 min^{-1} mM^{-1}), representing the highest turnover constant determined for the production of DHP with any TK variant to date (Figure 4.7).

Although the high K_m of D469S/R520Q indicates poor substrate affinity for PA, the concentration of PA used in screens (50 mM) is at the lower end of the spectrum of what is used in cost-effective industrial biocatalytic transformations. Such low substrate affinity would be acceptable in industrial biocatalysis as long as substrate concentration could be increased sufficiently to achieve reasonable saturation of the active site. It is also important that enantioselectivity is not negatively impacted by a reduction in the number, or strength, of enzyme substrate interactions.

Previous kinetic analysis of purified wild type TK with propionaldehyde determined the K_m to be 140±50 mM [10]. The K_m determined here is higher than that previously determined but is within the calculated error. The source of this discrepancy could also be the reaction conditions. In the current study, reactions were carried out in a salt concentration of 250 mM NaCl which was included to aid in the purification of the enzyme. Hibbert *et al* carried out their kinetic analysis in the absence of NaCl. The salt concentration used here was the same for each variant so we do not expect this discrepancy to adversely impact on our analysis of relative kinetic parameters.

	Initial Velocities (mM min^{-1})						
Enzyme	[PA] 8mM	[PA] 16mM	[PA] 24mM	[PA] 32mM	[PA] 40mM	[PA] 48mM	[PA] 60mM
WT	0.005	0.008	0.014	0.018	0.017	0.021	0.034
D469S	0.006	0.011	0.015	0.020	0.020	0.022	0.028
R520Q	0.003	0.006	0.007	0.012	0.011	0.016	-[a]
D469S/R520Q	0.027	0.051	0.077	0.120	0.099	0.153	0.236

Table 4.5 Initial velocities of a triple mutant cycle of TK mutants at varying propionaldehyde (PA) concentrations. Initial velocities were determined from the concentration of DHP using HPLC and purified protein. Activity determined with 50 mM LiHPA, and 50 mM Tris-HCl, 2.4 mM TPP, 9 mM $MgCl_2$, 250 mM NaCl, pH 7.0 to produce 1,3-dihydroxypentan-2-one (DHP). [a]Not available.

Enzyme	Lysate activity relative to wt	[Protein] [b] (mg/ml)	k_{cat} (min^{-1})	K_m (mM)	k_{cat}/K_m (min^{-1} mM^{-1})	e.e.[c]
Wt[a]	1.00 ± 0.08	0.44	35	181	0.19	57.1
D469S	1.33 ± 0.08	0.15	57	71	0.81	64.9
E498D	0.27 ± 0.02	0.07	n.a.[d]	n.a.	n.a.	n.a.
R520Q	1.07 ± 0.06	0.53	31	330	0.10	57.8
D469S/E498D	0.58 ± 0.19	0.10	n.a.	n.a.	n.a.	n.a.
D469S/R520Q	1.41 ± 0.13	0.44	700	628	1.11	67.4
E498D/R520Q	0.62 ± 0.06	0.07	n.a.	n.a.	n.a.	n.a.
D469S/E498D/R520Q	1.91 ± 0.12	0.05	n.a.	n.a.	n.a.	n.a.

Table 4.6 Kinetic parameters and enantioselectivities of a triple mutant cycle of TK mutants for the propionaldehyde (PA) substrate. Lysate activities were determined using a colorimetric assay; kinetic parameters were determined using HPLC and purified protein. Total activity determined with 50 mM LiHPA, 50 mM PA, and 50 mM Tris-HCl, 2.4 mM TPP, 9 mM $MgCl_2$, 250 mM NaCl, pH 7.0 to produce 1,3-dihydroxypentan-2-one (DHP). [a]Wild-type specific activity is 0.029 ± 0.001 µmol/mg/min [10]. [b]Obtained after purification. [c]Enantiomeric excess of the *S*-isomer. [d]Not available.

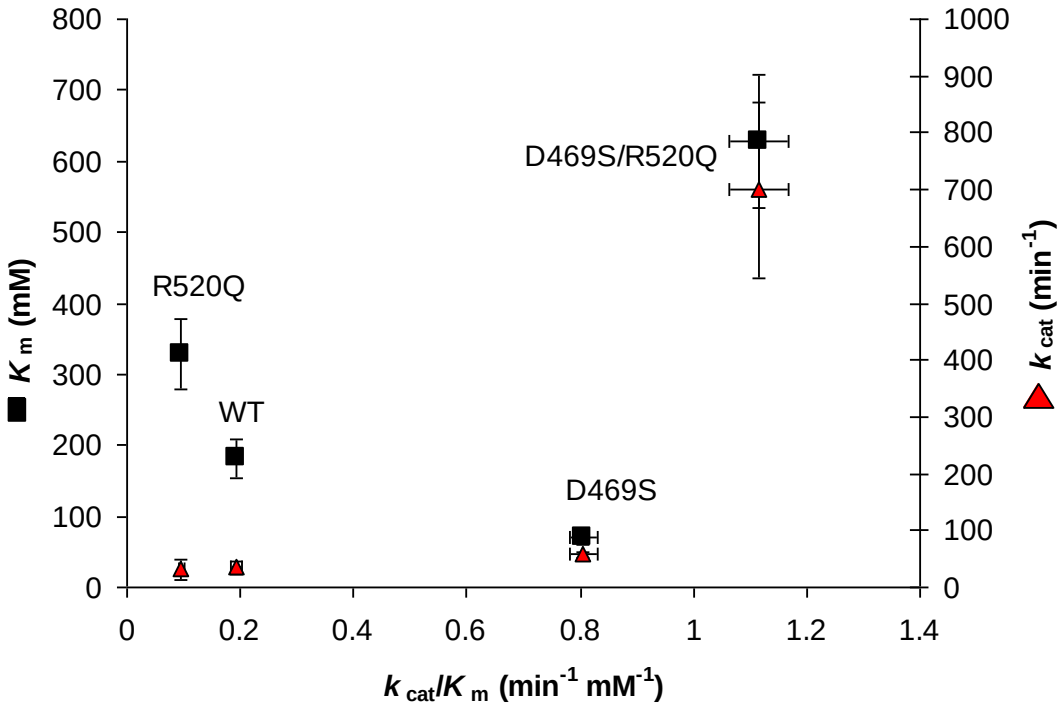

Figure 4.7 Comparison of k_{cat}, K_m and k_{cat}/K_m for the double mutant cycle of D469S and R520Q.

4.3.9 Enantioselectivity of variants compared to wild type

In addition to potential synergistic effects on turnover rate and substrate affinity, the synergy between co-evolving residues may also be associated with effects on enantioselectivity. Mutants of TK have been identified in previous work that have both improved and reversed enantioselectivity [11], evaluation of such changes in

the SCA directed variants may indicate further synergistic associations between the residues. It is also important to ascertain whether the reduced substrate affinity of the double mutant D469S/R520Q has negatively impacted on the enantioselectivity of the enzyme.

Gas chromatography was used to determine the stereospecificity of wild type TK and the three purified TK variants (Table 4.6). Wild type TK catalysed the production of S-DHP in 57% enantiomeric excess, this correlates closely with previous results for wild type TK [11]. The D469S variant demonstrated improved enantioselectivity relative to wild type, producing S-DHP in 65% enantiomeric excess, this is similar to the increase observed with another variant, D469T [11]. In contrast, the R520Q variant appeared to have no effect on enantioselectivity (S-DHP 58% ee). When the two variations were combined in the double mutant D469S/R520Q, enantioselectivity was increased to the same extent observed with D469S in isolation (S-DHP 67% ee).

These results suggest that the co-evolutionary pressures on Asp 469 and Arg 520 are more likely to be associated with turnover rate and substrate affinity rather than enantioselectivity. However, these particular variants were selected based on increased activity on the PA substrate. Full evaluation of the enantioselective pressures on co-evolution would require the enantiomeric evaluation of many more variants. Importantly for the use of the D469S/R520Q variant in industrial biocatalytic transformations, we have demonstrated that the potential decrease in substrate affinity has not negatively impacted on enantioselectivity and in fact the enantioselectivity has been improved relative to wild type TK.

4.4 Conclusions

We have produced libraries of single, double and triple TK variants based around a cluster of co-evolving residues identified by SCA. The cluster of residues comprised of two structurally contiguous groups of residues and although only a small number of variants were introduced at each position, single variants with improved activity on the non-natural substrate propionaldehyde were identified for each of the positions in the structural group proximal to the active site. This demonstrates the potential of the SCA technique to identify new residues to target for site directed mutagenesis in directed evolution experiments.

Although the distal residues did not confer enhanced activity in isolation, the co-evolution of such residues suggests potential synergistic relationships between these and the proximal residues. We sought to identify evidence of such synergistic relationships by producing targeted double and triple variant libraries. The positions selected for combination were chosen such that negatively impacting variants would be combined with positively impacting variants. Synergistic relationships are expected to be more easily identifiable for such combinations.

Across the double and triple libraries, one variant was identified as significantly increasing activity on PA. This variant was D469S/E498D/R520Q and a triple mutant cycle was created to further investigate the synergistic relationships between each mutation. Analysis of the total lysate activities of the members of this triple mutant cycle indicates a lack of synergy between D469S and R520Q, however, both of these mutations alleviate the negative impact of the E498D mutation and when all three mutations are present together, activity is increased considerably. Analysis of the

total concentration and soluble fraction for each member of the cycle suggested that the combined effect of these mutations on activity cannot be explained by synergistic effects on protein expression or solubility. Instead, synergy is likely to be related to specific activity or better folding of the soluble fraction to the active native state.

Although negative effects on expression and solubility meant that no E498D containing variants could be purified for further kinetic analysis, the kinetic analysis of the other members of the triple mutant cycle has revealed some interesting relationships between the residues. Both the D469S and the R520Q mutations have a relatively small impact on enzyme kinetic parameters in isolation. However, when these two mutations are combined in D469S/R520Q, the turnover constant is increased by 20-fold relative to wild type TK. The K_m is also increased relative to wild type for the double mutant, suggesting a decrease in substrate affinity, but the combined effects of these changes still resulted in a 5.8-fold increase in k_{cat}/ K_m.

In contrast with earlier results based on total lysate relative activity, enzyme kinetic analysis indicates significant synergy between the two mutations D469S and R520Q. However, total lysate relative activities were determined at the low PA concentration of 50 mM. This is 12.6-fold lower than the K_m of D469S/R520Q and as such, any synergistic increase in turnover constant could be masked by the concurrent increase in K_m. The synergy between these residues may have been apparent in earlier screens had a higher concentration of propionaldehyde been adopted.

Without the enzyme kinetics for the triple mutant D469S/E498D/R520Q it is difficult to explain why combination of all three mutations had such a beneficial effect in earlier screens. However, we can hypothesis that by altering the conformation of the active site, the E498D mutation may have alleviated the increase in K_m, thereby unmasking the synergistic increase in turnover constant at the lower substrate concentration used in the screen.

Interestingly, the D469S/R520Q double mutant of TK obtained by this approach is not found in any of the natural 382 TPP-dependent enzyme sequences used to perform the SCA. For the naturally occurring R520Q mutation, the equivalent to Asp 469 in TK is found to be Lys in various PDC and PPDC enzymes, Tyr in one TK and Asp in several ALS enzymes, but not Ser. When D469S occurs, the equivalent to Arg 520 in TK is found to be Glu or Arg. However, as the natural variants have been selected during their evolution for a particular range of functions useful to the cell, it is not necessarily expected that precisely the same natural combinations would be found when selecting for a new property such as altered substrate specificity.

In D469S/R520Q we have identified a multiple variant of TK that has a higher turnover constant for the PA reaction than any other TK variant discovered to date. Although the K_m was also increased, this does not pose a problem as long as substrate concentration can be increased sufficiently and the lower substrate affinity doesn't negatively impact on enantioselectivity. We have shown that enantioselectivity is actually increased with PA relative to wild type. The D469S/R520Q mutant is therefore very promising for the synthesis of chiral aliphatic keto diols, particularly (3S)-1,3-dihydroxy pentan-2-one.

5 General Discussion

5.1 Overall summary of thesis

The aim of this thesis was to utilise computational and bioinformatics tools to further our understanding of the transketolase enzyme and to aid in our efforts to engineer transketolase for biocatalytic applications.

Initially we sought to increase our mechanistic understanding by modelling substrate binding in the active site of *E. coli* transketolase and the results presented in chapter 2 add to the growing body of structural information on this enzyme. Computational docking allowed us to model transient, reactive structures that would be very difficult or impossible to determine experimentally. Of particular interest was the docked conformation of the ketol donor HPA, which indicates an interesting angle of nucleophilic attack, which although unusual, is supported by recently published structural data.

In chapter 3 we have used a powerful bioinformatics approach termed Statistical Coupling Analysis to identify networks of co-evolving residues across the TPP-dependent enzymes. Statistical Coupling Analysis or SCA, provides an opportunity to delve deeper than the structure of proteins, uncovering networks of residues within the protein fold that have acted together through evolution to maintain or improve fitness. The identification of such networks in transketolase has important implications for enzyme engineering, suggesting combinations of residues to target simultaneously and identifying distant residues that are functionally coupled to key residues within the active site.

In chapter 4 we used the results of statistical coupling analysis to guide the design of multiple transketolase mutants with improved activity on non-natural substrates. Small targeted mutagenesis libraries were produced based on one of the co-evolving networks and simultaneous mutation of multiple residues within this cluster displayed synergistic effects on enzyme activity that would not have been anticipated from the effects of each mutation in isolation. Notably, we have identified a double mutant with a 20-fold improvement in turnover-rate using the non-natural substrate propionaldehyde. This is greater than any improvement identified to date from single variant libraries.

In these three results chapters we have achieved the main aims of this thesis. However, many questions have been raised in the course of this work and considerable additional work is required to test and expand on the conclusions presented here. In the following discussion we will review the conclusions presented and propose further work which we hope will develop these conclusions further.

5.2 Computational automated docking in transketolase

Computational automated docking is a powerful technique that can help to rationalise experimental observations from enzyme kinetics, identify potential transient structures along an enzyme reaction pathway that are difficult to obtain by experimental structure determination, and generate hypotheses to test further by experiment. Although computational docking is not completely accurate, the most obvious errors can be eliminated by visual inspection, as was the case with DX5P in this work. Transketolase is a particularly good model for this approach as

the lack of induced-fit side chain movements within the enzyme eliminates the requirement to model side chain flexibility and the potential errors this can introduce.

We used the AutoDock algorithm to reproduce the structures of known substrate-protein complexes as an initial benchmark for using the docking technique in other transketolase complexes. AutoDock was able to accurately reproduce the complex of DE4P bound in yeast TK within 1.65 Å RMSD of the crystal structure. Although AutoDock appears to struggle with explicitly charged groups, resulting in a slight shift of DE4P towards the phosphate interacting residues, the hydrogen bond network of the docked substrate was predicted accurately. Docking DE4P in *E. coli* TK demonstrated a near identical binding conformation to that for yeast TK. This is an important finding as it allows us to confidently apply the knowledge gained from studies of yeast TK to *E. coli* TK and *visa versa*.

Having demonstrated the accuracy of AutoDock we docked a series of known ketol donor and aldehyde acceptor substrates into the active site of *E. coli* TK and calculated their K_m values from AutiDock reported binding energies. Comparison with experimentally determined K_m values demonstrated good correlation, further validating the approach. Although AutoDock appears to systemically underestimate K_m values, this is not of concern for the use of the binding energy calculation to select minimal energy docked conformations.

Examination of the structures of TK-substrate complexes reveals a common binding conformation, similar to that of DE4P. Phosphorylated substrates all bound with the phosphate group interacting with a conserved group of residues near the entrance

to the active site. This strong interaction leads to low experimental and calculated K_m values, and the phosphate groups anchoring effects result in an inversely proportional relationship between substrate chain length and the distance of docked substrate to the ThDP cofactor. Both phosphorylated and non-phosphorylated aldol acceptor substrates bound with the Re-face of the aldehyde carbonyl exposed to nucleophilic attack by the α-carbon of the enamine to give S-enantiomer products.

Two of the aldehyde acceptors, glycolaldehyde and DE4P were docked both in the presence and absence of the reactive ThDP-enamine intermediate. Such structures would be difficult or impossible to determine experimentally given their reactive nature. Binding of the two substrates was found to be identical in the presence and absence of the enamine, indicating that formation of the enamine is not a pre-requisite for binding in a reactive conformation.

Comparison of docked acyclic DR5P with the recently published structure of the bound cyclic form suggests a potential mechanism for the ring opening of the substrate. A series of C-C bond rotations and hydrogen bond exchanges has been proposed that collectively unwind the DR5P molecule and orientate the newly acyclic form in readiness for nucleophilic attack by the enamine.

We have also docked ketol donors HPA and DX5P in the active site of *E. coli* TK. Unfortunately the docked conformation of DX5P was orientated unfavourably relative to the ThDP thiazolium ring; however, examination of the docked conformation of HPA has produced some of the most interesting findings of the computational docking work. HPA was docked in such a conformation that the

angle of nucleophillic attack by the deprotonated ThDP cofactor is 68^{o} rather than the favoured Bergi-Dunitz angle of 107^{o}. This unusual result correlates well with the observed strain in the covalent ThDP-DX5P intermediate and supports the growing picture of a catalytically poised active site in which substrate interaction energies are converted into the strained high-energy intermediate. The identical docking conformation of unreactive FPA provides an opportunity to test this conclusion experimentally.

5.3 Statistical coupling analysis of transketolase

Computational modelling of substrate binding in the active site of TK has provided evidence supporting our previous assumptions that substrate binding is equivalent between *E. coli* and yeast TK, and that many of the natural substrate interactions are maintained with non-natural substrates. This work gives us confidence in using such assumptions and has also increased our mechanistic understanding of TK. However, we have not identified any new residue functions that could lead to the improved engineering of TK for biocatalytic applications. This is perhaps unsurprising given the extensive mutagenesis and enzyme engineering work which has focussed on the residues around the active site.

When it comes to engineering TK, and enzyme engineering as a whole, the main gaps in our experience relate to multiple mutation of residues and the identification of target residues distant to the active site. These types of interactions are governed by complex relationships that are difficult to tease apart with structural data alone. The relatively new technique of statistical coupling analysis (SCA) has the potential to guide our search for beneficial multiple and distant mutations and

the following results describe the application of this technique to the transketolase enzyme.

Using a multiple sequence alignment of the PP and Pyr domains of TPP-dependent enzymes we initially used SCA to identify residues evolutionarily coupled to the important functional residue Asp 469. Seven residues were identified, five of which made up a structurally contiguous group around the active site. The other two residues were more distant; however, both were positioned on elements of secondary structure leading directly to the active site and may play a role in fine adjustment of the tertiary structure. Two of the five identified active site residues, Arg 520 and His 26, had been previously identified in enzyme engineering for modified substrate specificity. The improved activity of Arg 520 variants on non-natural substrates has been rationalised by the role of Arg 520 in phosphate binding. Evolutionary coupling between Arg 520 and Asp 469 suggests there may be a subtler synergistic explanation for the increased activity of these variants.

In order to expand our analyses of evolutionary coupling we carried out global SCA on the whole PP and Pyr domain MSA. Focusing on areas of high coupling energy we identified thirty highly coupled residues, six of which have a known function in TK. Evolutionary conservation is often used to determine potentially functional residues; SCA offers an alternative approach to the identification of functional residues. Notably, only three of the thirty SCA identified residues would also have been identified in a cut of the thirty most conserved residues. Two of these residues, His 26 and His 66, are well characterised but the third, Gly 117, would

make an interesting target for saturation mutagenesis given its redundant identification by both approaches.

Residues identified by global SCA were dominated by those located at the subunit interface between the PP and Pyr domains; this is not unexpected as changes on one side are likely to require changes on the other side to maintain interactions. However, one small sub-cluster did stand out among the thirty residues, this sub-cluster included residues His 26, His 66 and Tyr 72. This group of residues displayed a distinct coupling pattern and was also identified among the residues coupled to Asp 469. Leu 62 was also of interest, displaying the highest levels of coupling in the whole alignment and clustered independently of the other twenty-nine residues.

In order to identify subtler networks of coupled residues that may have been masked by strong subunit interaction networks, SCA global analysis was repeated with just the Pyr domains. This strategy identified an interesting network of nine coupled residues which included Asp 469. When mapped onto the structure of TK, this cluster forms two structurally contiguous groups of residues linked midway by the ninth residue which forms a hairpin turn. Confidence in this cluster is enhanced by its self-consistency and its structurally contiguous nature.

The identification of co-evolving networks of residues in the TPP-dependent enzymes demonstrates the power of this technique. The co-dependence of variation through evolution is likely to mirror co-dependency between newly introduced mutations. As such, the networks identified provide a new recourse of residues to target both in isolation and in combination for the engineering of *E. coli* TK. The secondary finding of this work, that many coupling interactions are located

on the interface between interacting subunits, suggests a new application of the SCA technique. Determination of the sites of protein-protein interaction in multi-protein complexes is an experimentally intensive process. Multiple sequence alignments of two proteins known to interact could be concatenated prior to statistical coupling analysis, providing a new method for the prediction of protein-protein interaction sites.

5.4 SCA guided library design for engineering transketolase activity

Based on the networks of evolutionarily coupled residues identified by SCA, we sought to engineer the activity of transketolase by targeting multiple residues for combined mutagenesis. As a high-throughput colorimetric screen had been developed in the lab for activity on the propionaldehyde substrate, improved activity on this reaction was selected as an engineering goal. We chose the nine residue Pyr domain cluster of co-evolving residues to target for mutagenesis as it displays self-consistency, is structurally contiguous, and contains the Asp 469 residue (mutation of which has improved activity on PA).

Single point mutation of seven of the nine cluster residues to common variants in the multiple sequence alignment produced interesting results, with all residues proximal to the active site producing improvements in activity on PA. In contrast, mutation of the two residues making up the structural group distal to the active site did not confer any improvement in activity, in fact activity was severely impaired. The identification of improved activity in a relatively small library of single variants demonstrates the potential of SCA to select residues for mutagenesis. Full

saturation mutagenesis at all the sites identified by SCA could be a productive strategy in the future directed evolution of TK.

The potential for SCA to identify combinations of residues for multiple mutation was investigated by selecting two groups of residues from the cluster for combined mutagenesis. Average relative activities and ranges of relative activities across these libraries indicated synergy between the residues. This synergy was also displayed in a triple mutant cycle of a particularly active triple mutant, D469S/E498D/R520Q. Although these results support our assumption of synergistic relationships between co-evolving residues, we have not investigated whether any synergy is present between non-co-evolving residues. Such an experiment would represent an important negative control for further work.

Detailed kinetic analysis of a subset of the triple mutant cycle demonstrated that the double mutant D469S/R520Q increases turnover rate of TK on the PA reaction by 20-fold. Although K_m was also increased for this variant, the combined effect of these changes was a 5.8-fold increase in k_{cat}/K_m. The apparent synergy between these mutations contradicts earlier results which suggested the requirement of a third mutation at Glu 498 to unlock the synergistic relationships at these sites. However, it is likely that the increase in K_m, combined with the relatively low PA concentration used in earlier analyses, masked the synergistic increase in turnover rate of this double mutant.

Using SCA to guide the selection of multiple variants we have identified a double variant in D469S/R520Q that has a higher turnover rate for the production of DHP than any other TK variant discovered to date. These residues were known

previously for their propensity to improve activity on the PA reaction following mutagenesis. Based on this prior knowledge it could be argued that combination of such variants would be expected to give further improvements in activity. However, the improvements demonstrated here are greater than could be expected based on the effects of each mutation in isolation and earlier work to combine beneficial mutations in *E. coli* TK has failed to produce any improvements in activity.

Given the promising results obtained from targeting the nine residue Pyr domain cluster, further work should be carried out to investigate the potential of the other SCA clusters for mutagenesis. Of particular interest would be the small PP domain cluster of His 26, His 66 and Tyr 72, which demonstrated very robust clustering in our analysis. Many other residues were identified by SCA that have not been targeted for mutagenesis to date. The results presented here suggest that the creation of saturation mutagenesis libraries of these positions could be a very promising strategy for the future engineering of TK.

6 References

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7 Appendix

7.1 Example Autodock input files

7.1.1 DPF example file format

```
outlev 1                              # diagnostic output level
intelec                               # calculate internal electrostatics
seed pid time                         # seeds for random generator
ligand_types C HD OA                  # atoms types in ligand
fld 1QGD.maps.fld                     # grid_data_file
map 1QGD.C.map                        # atom-specific affinity map
map 1QGD.HD.map                       # atom-specific affinity map
map 1QGD.OA.map                       # atom-specific affinity map
elecmap 1QGD.e.map                    # electrostatics map
desolvmap 1QGD.d.map                  # desolvation map
move HPA.pdbqt                        # small molecule
about 909.9433 895.6123 902.4398      # small molecule center
tran0 random                          # initial coordinates/A or random
quat0 random                          # initial quaternion
ndihe 4                               # number of active torsions
dihe0 random                          # initial dihedrals (relative) or random
tstep 2.0                             # translation step/A
qstep 50.0                            # quaternion step/deg
dstep 50.0                            # torsion step/deg
torsdof 2 0.274000                    # torsional degrees of freedom and coefficient
rmstol 0.5                            # cluster_tolerance/A
extnrg 1000.0                         # external grid energy
e0max 0.0 10000                       # max initial energy; max number of retries
ga_pop_size 150                       # number of individuals in population
ga_num_evals 50000000                   # maximum number of energy evaluations
ga_num_generations 50000              # maximum number of generations
ga_elitism 1                          # number of top individuals to survive to next generation
ga_mutation_rate 0.02                 # rate of gene mutation
ga_crossover_rate 0.8                 # rate of crossover
ga_window_size 10                     #
ga_cauchy_alpha 0.0                   # Alpha parameter of Cauchy distribution
ga_cauchy_beta 1.0                    # Beta parameter Cauchy distribution
set_ga                                # set the above parameters for GA or LGA
sw_max_its 300                        # iterations of Solis & Wets local search
sw_max_succ 4                         # consecutive successes before changing rho
sw_max_fail 4                         # consecutive failures before changing rho
sw_rho 1.0                            # size of local search space to sample
sw_lb_rho 0.01                        # lower bound on rho
ls_search_freq 0.06                   # probability of performing local search on individual
set_sw1                               # set the above Solis & Wets parameters
compute_unbound_extended              # compute extended ligand energy
ga_run 50                             # do this many hybrid GA-LS runs
analysis                              # perform a ranked cluster analysis
```

7.1.2 GPF example file format

```
npts 64 64 64                         # num.grid points in xyz
gridfld 1QGD.maps.fld                 # grid_data_file
spacing 0.202777777778                # spacing(A)
receptor_types A C HD N OA P SA       # receptor atom types
ligand_types C HD OA                  # ligand atom types
receptor 1QGD.pdbqt                   # macromolecule
gridcenter -11.806 24.875 37.708      # xyz-coordinates or auto
smooth 0.5                            # store minimum energy w/in rad(A)
map 1QGD.C.map                        # atom-specific affinity map
map 1QGD.HD.map                       # atom-specific affinity map
map 1QGD.OA.map                       # atom-specific affinity map
elecmap 1QGD.e.map                    # electrostatic potential map
dsolvmap 1QGD.d.map                 # desolvation potential map
dielectric -0.1465                    # <0, AD4 distance-dep.diel;>0, constant
```

7.1.3 PDBQT 1QGD file input

```
REMARK   4 XXXX COMPLIES WITH FORMAT V. 2.0
ATOM      1  N   SER A   2     -20.614  26.561   2.838  1.00 40.61    -0.064 N
ATOM      2  HN1 SER A   2     -20.435  27.122   2.005  1.00  0.00     0.275 HD
ATOM      3  HN2 SER A   2     -21.375  25.896   2.700  1.00  0.00     0.275 HD
ATOM      4  HN3 SER A   2     -19.868  25.890   3.021  1.00  0.00     0.275 HD
ATOM      5  CA  SER A   2     -20.857  27.468   4.000  1.00 41.29     0.297 C
ATOM      7  C   SER A   2     -19.695  28.413   4.244  1.00 36.15     0.251 C
ATOM      8  O   SER A   2     -18.548  28.052   3.949  1.00 40.50    -0.271 OA
ATOM      9  CB  SER A   2     -21.127  26.624   5.254  1.00 37.74     0.206 C
ATOM     12  OG  SER A   2     -22.251  25.785   5.015  1.00 50.58    -0.398 OA
ATOM     13  HG  SER A   2     -22.418  25.263   5.791  1.00  0.00     0.209 HD
ATOM     14  N   SER A   3     -19.983  29.605   4.754  1.00 31.54    -0.344 N
ATOM     15  HN  SER A   3     -20.954  29.884   4.892  1.00  0.00     0.163 HD
ATOM     16  CA  SER A   3     -18.897  30.515   5.117  1.00 28.90     0.200 C
ATOM     18  C   SER A   3     -18.118  29.888   6.289  1.00 24.09     0.243 C
ATOM     19  O   SER A   3     -18.650  29.043   7.027  1.00 22.26    -0.271 OA
ATOM     20  CB  SER A   3     -19.424  31.872   5.573  1.00 28.08     0.199 C
ATOM     23  OG  SER A   3     -20.260  31.729   6.723  1.00 28.69    -0.398 OA
ATOM     24  HG  SER A   3     -20.588  32.574   7.007  1.00  0.00     0.209 HD
ATOM     25  N   ARG A   4     -16.925  30.428   6.498  1.00 23.06    -0.346 N
ATOM     26  HN  ARG A   4     -16.577  31.140   5.856  1.00  0.00     0.163 HD
ATOM     27  CA  ARG A   4     -16.098  30.017   7.639  1.00 21.92     0.176 C
ATOM     29  C   ARG A   4     -16.850  30.305   8.917  1.00 22.03     0.241 C
ATOM     30  O   ARG A   4     -16.830  29.457   9.812  1.00 22.94    -0.271 OA
ATOM     31  CB  ARG A   4     -14.735  30.712   7.632  1.00 22.03     0.036 C
ATOM     34  CG  ARG A   4     -13.929  30.273   6.420  1.00 22.16     0.023 C
ATOM     37  CD  ARG A   4     -12.451  30.521   6.582  1.00 25.62     0.138 C
ATOM     40  NE  ARG A   4     -11.829  29.397   7.276  1.00 31.17    -0.227 N
ATOM     41  HE  ARG A   4     -12.270  29.073   8.137  1.00  0.00     0.177 HD
ATOM     42  CZ  ARG A   4     -10.739  28.768   6.874  1.00 24.97     0.665 C
ATOM     43  NH1 ARG A   4     -10.121  29.133   5.752  1.00 29.86    -0.235 N
ATOM     44 1HH1 ARG A   4      -9.279  28.647   5.442  1.00  0.00     0.174 HD
ATOM     45 2HH1 ARG A   4     -10.449  29.914   5.184  1.00  0.00     0.174 HD
ATOM     46  NH2 ARG A   4     -10.316  27.760   7.607  1.00 34.82    -0.235 N
ATOM     47 1HH2 ARG A   4      -9.474  27.274   7.297  1.00  0.00     0.174 HD
ATOM     48 2HH2 ARG A   4     -10.789  27.480   8.466  1.00  0.00     0.174 HD
ATOM     49  N   LYS A   5     -17.539  31.451   8.998  1.00 19.31    -0.346 N
ATOM     50  HN  LYS A   5     -17.552  32.106   8.216  1.00  0.00     0.163 HD
ATOM     51  CA  LYS A   5     -18.272  31.745  10.229  1.00 19.34     0.176 C
ATOM     53  C   LYS A   5     -19.350  30.740  10.537  1.00 18.28     0.241 C
ATOM     54  O   LYS A   5     -19.581  30.418  11.708  1.00 15.31    -0.271 OA
ATOM     55  CB  LYS A   5     -18.926  33.157  10.213  1.00 25.44     0.035 C
ATOM     58  CG  LYS A   5     -17.810  34.179  10.373  1.00 39.34     0.004 C
ATOM     61  CD  LYS A   5     -18.308  35.562  10.737  1.00 50.52     0.027 C
ATOM     64  CE  LYS A   5     -17.391  36.650  10.186  1.00 58.53     0.229 C
ATOM     67  NZ  LYS A   5     -18.180  37.877   9.865  1.00 66.78    -0.079 N
ATOM     68  HZ1 LYS A   5     -17.567  38.604   9.497  1.00  0.00     0.274 HD
ATOM     69  HZ2 LYS A   5     -18.719  38.204  10.667  1.00  0.00     0.274 HD
ATOM     70  HZ3 LYS A   5     -18.956  37.677   9.233  1.00  0.00     0.274 HD
ATOM     71  N   GLU A   6     -20.077  30.251   9.524  1.00 18.06    -0.346 N
ATOM     72  HN  GLU A   6     -19.908  30.563   8.568  1.00  0.00     0.163 HD
ATOM     73  CA  GLU A   6     -21.114  29.266   9.810  1.00 16.83     0.177 C
ATOM     75  C   GLU A   6     -20.499  27.956  10.283  1.00 15.27     0.241 C
ATOM     76  O   GLU A   6     -21.078  27.321  11.179  1.00 17.44    -0.271 OA
ATOM     77  CB  GLU A   6     -21.921  28.946   8.519  1.00 33.90     0.045 C
ATOM     80  CG  GLU A   6     -23.396  28.818   8.839  1.00 55.63     0.116 C
ATOM     83  CD  GLU A   6     -24.232  27.829   8.070  1.00 75.67     0.172 C
ATOM     84  OE1 GLU A   6     -23.806  27.388   6.979  1.00 65.99    -0.648 OA
ATOM     85  OE2 GLU A   6     -25.343  27.492   8.560  1.00 61.69    -0.648 OA
ATOM     86  N   LEU A   7     -19.329  27.598   9.706  1.00 14.23    -0.346 N
ATOM     87  HN  LEU A   7     -18.918  28.165   8.964  1.00  0.00     0.163 HD
ATOM     88  CA  LEU A   7     -18.669  26.383  10.169  1.00 16.12     0.177 C
ATOM     90  C   LEU A   7     -18.213  26.543  11.619  1.00 15.90     0.241 C
ATOM     91  O   LEU A   7     -18.395  25.623  12.395  1.00 16.21    -0.271 OA
ATOM     92  CB  LEU A   7     -17.443  26.031   9.288  1.00 12.40     0.038 C
ATOM     95  CG  LEU A   7     -17.889  25.706   7.832  1.00 15.18    -0.020 C
ATOM     97  CD1 LEU A   7     -16.660  25.489   6.977  1.00 18.92     0.009 C
ATOM    101  CD2 LEU A   7     -18.868  24.538   7.849  1.00 17.59     0.009 C
ATOM    105  N   ALA A   8     -17.667  27.702  11.980  1.00 14.64    -0.346 N
ATOM    106  HN  ALA A   8     -17.543  28.436  11.282  1.00  0.00     0.163 HD
ATOM    107  CA  ALA A   8     -17.241  27.944  13.361  1.00 17.03     0.172 C
ATOM    109  C   ALA A   8     -18.425  27.999  14.298  1.00 17.03     0.240 C
ATOM    110  O   ALA A   8     -18.399  27.557  15.471  1.00 14.80    -0.271 OA
ATOM    111  CB  ALA A   8     -16.415  29.263  13.406  1.00 11.08     0.042 C
ATOM    115  N   ASN A   9     -19.595  28.483  13.823  1.00 15.31    -0.346 N
ATOM    116  HN  ASN A   9     -19.645  28.837  12.868  1.00  0.00     0.163 HD
ATOM    117  CA  ASN A   9     -20.791  28.503  14.668  1.00 14.90     0.185 C
ATOM    119  C   ASN A   9     -21.314  27.123  15.058  1.00 15.44     0.241 C
ATOM    120  O   ASN A   9     -21.992  26.975  16.106  1.00 17.34    -0.271 OA
ATOM    121  CB  ASN A   9     -21.949  29.334  14.079  1.00 16.96     0.137 C
ATOM    124  CG  ASN A   9     -21.640  30.809  14.053  1.00 22.48     0.217 C
ATOM    125  ND2 ASN A   9     -22.302  31.618  13.221  1.00 19.99    -0.370 N
ATOM    126 1HD2 ASN A   9     -22.093  32.616  13.203  1.00  0.00     0.159 HD
ATOM    127 2HD2 ASN A   9     -23.040  31.242  12.626  1.00  0.00     0.159 HD
ATOM    128  OD1 ASN A   9     -20.747  31.264  14.712  1.00 19.85    -0.272 OA
ATOM    129  N   ALA A  10     -20.983  26.095  14.317  1.00 15.19    -0.346 N
ATOM    130  HN  ALA A  10     -20.462  26.263  13.457  1.00  0.00     0.163 HD
ATOM    131  CA  ALA A  10     -21.325  24.723  14.665  1.00 17.57     0.172 C
ATOM    133  C   ALA A  10     -20.699  24.377  16.027  1.00 16.07     0.240 C
ATOM    134  O   ALA A  10     -21.378  23.787  16.866  1.00 16.07    -0.271 OA
ATOM    135  CB  ALA A  10     -20.844  23.743  13.627  1.00 15.95     0.042 C
ATOM    139  N   ILE A  11     -19.454  24.786  16.268  1.00 14.61    -0.346 N
ATOM    140  HN  ILE A  11     -18.934  25.258  15.528  1.00  0.00     0.163 HD
ATOM    141  CA  ILE A  11     -18.809  24.573  17.577  1.00 11.15     0.180 C
ATOM    143  C   ILE A  11     -19.557  25.292  18.681  1.00 15.40     0.241 C
ATOM    144  O   ILE A  11     -19.772  24.795  19.812  1.00 13.22    -0.271 OA
ATOM    145  CB  ILE A  11     -17.354  25.114  17.496  1.00 15.56     0.013 C
ATOM    147  CG1 ILE A  11     -16.596  24.389  16.393  1.00 15.89     0.002 C
ATOM    150  CG2 ILE A  11     -16.660  24.997  18.881  1.00 11.38     0.012 C
ATOM    154  CD1 ILE A  11     -15.164  24.882  16.196  1.00 15.79     0.005 C
ATOM    158  N   ARG A  12     -19.923  26.556  18.388  1.00 13.56    -0.346 N
ATOM    159  HN  ARG A  12     -19.670  26.952  17.487  1.00  0.00     0.163 HD
ATOM    160  CA  ARG A  12     -20.673  27.370  19.339  1.00 14.39     0.176 C
ATOM    162  C   ARG A  12     -22.003  26.743  19.739  1.00 20.53     0.241 C
ATOM    163  O   ARG A  12     -22.302  26.662  20.934  1.00 16.62    -0.271 OA
ATOM    164  CB  ARG A  12     -20.930  28.781  18.814  1.00 13.97     0.036 C
ATOM    167  CG  ARG A  12     -19.607  29.535  18.545  1.00 11.65     0.023 C
ATOM    170  CD  ARG A  12     -19.948  31.034  18.306  1.00 14.61     0.138 C
ATOM    173  NE  ARG A  12     -18.647  31.703  18.324  1.00 18.83    -0.227 N
ATOM    174 HE  ARG A  12     -18.274  31.929  19.246  1.00  0.00     0.177 HD
ATOM    175  CZ  ARG A  12     -17.900  32.049  17.301  1.00 15.74     0.665 C
ATOM    176  NH1 ARG A  12     -18.309  31.913  16.031  1.00 19.82    -0.235 N
ATOM    177 1HH1 ARG A  12     -17.729  32.182  15.236  1.00  0.00     0.174 HD
ATOM    178 2HH1 ARG A  12     -19.224  31.522  15.806  1.00  0.00     0.174 HD
ATOM    179  NH2 ARG A  12     -16.727  32.550  17.590  1.00 13.53    -0.235 N
ATOM    180 1HH2 ARG A  12     -16.147  32.819  16.795  1.00  0.00     0.174 HD
ATOM    181 2HH2 ARG A  12     -16.416  32.653  18.556  1.00  0.00     0.174 HD
ATOM    182  N   ALA A  13     -22.756  26.256  18.745  1.00 21.78    -0.346 N
ATOM    183  HN  ALA A  13     -22.423  26.308  17.782  1.00  0.00     0.163 HD
ATOM    184  CA  ALA A  13     -24.057  25.649  19.036  1.00 15.49     0.172 C
ATOM    186  C   ALA A  13     -23.907  24.377  19.853  1.00 14.54     0.240 C
ATOM    187  O   ALA A  13     -24.542  24.217  20.903  1.00 14.76    -0.271 OA
ATOM    188  CB  ALA A  13     -24.740  25.275  17.697  1.00 19.58     0.042 C
ATOM    192  N   LEU A  14     -23.058  23.454  19.397  1.00 14.53    -0.346 N
ATOM    193  HN  LEU A  14     -22.564  23.593  18.515  1.00  0.00     0.163 HD
ATOM    194  CA  LEU A  14     -22.846  22.228  20.191  1.00 14.49     0.177 C
ATOM    196  C   LEU A  14     -22.380  22.526  21.610  1.00 14.32     0.241 C
ATOM    197  O   LEU A  14     -22.840  21.919  22.577  1.00 15.05    -0.271 OA
ATOM    198  CB  LEU A  14     -21.759  21.382  19.519  1.00 13.61     0.038 C
ATOM    201  CG  LEU A  14     -22.244  20.732  18.206  1.00 16.46    -0.020 C
ATOM    203  CD1 LEU A  14     -21.047  20.090  17.523  1.00 18.85     0.009 C
ATOM    207  CD2 LEU A  14     -23.396  19.754  18.466  1.00 19.36     0.009 C
ATOM    211  N   SER A  15     -21.472  23.476  21.779  1.00 17.40    -0.344 N
ATOM    212  HN  SER A  15     -21.128  23.986  20.966  1.00  0.00     0.163 HD
ATOM    213  CA  SER A  15     -20.948  23.813  23.114  1.00 16.52     0.200 C
ATOM    215  C   SER A  15     -22.014  24.409  24.013  1.00 22.08     0.243 C
ATOM    216  O   SER A  15     -22.127  23.978  25.152  1.00 15.25    -0.271 OA
ATOM    217  CB  SER A  15     -19.782  24.801  23.046  1.00 18.59     0.199 C
ATOM    220  OG  SER A  15     -18.732  24.319  22.221  1.00 31.33    -0.398 OA
ATOM    221  HG  SER A  15     -18.008  24.933  22.179  1.00  0.00     0.209 HD
ATOM    222  N   MET A  16     -22.773  25.414  23.522  1.00 17.95    -0.346 N
ATOM    223  HN  MET A  16     -22.663  25.763  22.570  1.00  0.00     0.163 HD
ATOM    224  CA  MET A  16     -23.773  25.973  24.456  1.00 16.68     0.177 C
ATOM    226  C   MET A  16     -24.896  24.991  24.734  1.00 17.17     0.241 C
ATOM    227  O   MET A  16     -25.390  24.916  25.884  1.00 15.59    -0.271 OA
ATOM    228  CB  MET A  16     -24.292  27.323  23.963  1.00 17.71     0.045 C
ATOM    231  CG  MET A  16     -25.168  27.234  22.706  1.00 20.91     0.076 C
ATOM    234  SD  MET A  16     -25.524  28.917  22.066  1.00 26.35    -0.173 SA
ATOM    235  CE  MET A  16     -26.318  28.472  20.513  1.00 28.02     0.089 C
ATOM    239  N   ASP A  17     -25.285  24.179  23.739  1.00 17.53    -0.346 N
ATOM    240  HN  ASP A  17     -24.831  24.224  22.827  1.00  0.00     0.163 HD
ATOM    241  CA  ASP A  17     -26.369  23.230  23.982  1.00 19.04     0.186 C
ATOM    243  C   ASP A  17     -25.920  22.097  24.899  1.00 20.33     0.241 C
ATOM    244  O   ASP A  17     -26.735  21.657  25.716  1.00 21.46    -0.271 OA
ATOM    245  CB  ASP A  17     -26.894  22.613  22.681  1.00 20.65     0.147 C
ATOM    248  CG  ASP A  17     -27.608  23.643  21.804  1.00 23.17     0.175 C
ATOM    249  OD1 ASP A  17     -28.178  24.638  22.277  1.00 21.95    -0.648 OA
ATOM    250  OD2 ASP A  17     -27.620  23.472  20.565  1.00 20.05    -0.648 OA
ATOM    251  N   ALA A  18     -24.681  21.611  24.756  1.00 16.83    -0.346 N
ATOM    252  HN  ALA A  18     -24.050  21.991  24.050  1.00  0.00     0.163 HD
ATOM    253  CA  ALA A  18     -24.249  20.515  25.640  1.00 18.07     0.172 C
ATOM    255  C   ALA A  18     -24.117  20.986  27.091  1.00 14.48     0.240 C
ATOM    256  O   ALA A  18     -24.500  20.293  28.041  1.00 17.49    -0.271 OA
ATOM    257  CB  ALA A  18     -22.949  19.934  25.128  1.00 18.68     0.042 C
ATOM    261  N   VAL A  19     -23.616  22.198  27.288  1.00 12.87    -0.346 N
ATOM    262  HN  VAL A  19     -23.287  22.739  26.488  1.00  0.00     0.163 HD
ATOM    263  CA  VAL A  19     -23.525  22.777  28.633  1.00 16.35     0.180 C
ATOM    265  C   VAL A  19     -24.931  22.940  29.192  1.00 21.26     0.241 C
ATOM    266  O   VAL A  19     -25.193  22.646  30.355  1.00 15.91    -0.271 OA
ATOM    267  CB  VAL A  19     -22.795  24.113  28.580  1.00 18.25     0.009 C
ATOM    269  CG1 VAL A  19     -22.907  24.938  29.855  1.00 20.14     0.012 C
ATOM    273  CG2 VAL A  19     -21.299  23.849  28.319  1.00 16.63     0.012 C
ATOM    277  N   GLN A  20     -25.856  23.381  28.326  1.00 20.23    -0.346 N
ATOM    278  HN  GLN A  20     -25.605  23.565  27.355  1.00  0.00     0.163 HD
ATOM    279  CA  GLN A  20     -27.225  23.596  28.786  1.00 20.24     0.177 C
ATOM    281  C   GLN A  20     -27.868  22.283  29.223  1.00 18.69     0.241 C
ATOM    282  O   GLN A  20     -28.478  22.242  30.295  1.00 23.10    -0.271 OA
ATOM    283  CB  GLN A  20     -28.062  24.287  27.687  1.00 20.82     0.044 C
ATOM    286  CG  GLN A  20     -29.350  24.882  28.245  1.00 23.98     0.105 C
ATOM    289  CD  GLN A  20     -29.121  25.873  29.379  1.00 26.40     0.215 C
ATOM    290  NE2 GLN A  20     -29.897  25.720  30.463  1.00 25.96    -0.370 N
ATOM    291 1HE2 GLN A  20     -29.744  26.384  31.222  1.00  0.00     0.159 HD
ATOM    292 2HE2 GLN A  20     -30.608  24.993  30.538  1.00  0.00     0.159 HD
ATOM    293  OE1 GLN A  20     -28.259  26.755  29.288  1.00 31.11    -0.274 OA
ATOM    294  N   LYS A  21     -27.715  21.213  28.464  1.00 17.01    -0.346 N
ATOM    295  HN  LYS A  21     -27.191  21.302  27.593  1.00  0.00     0.163 HD
ATOM    296  CA  LYS A  21     -28.262  19.915  28.818  1.00 18.90     0.176 C
ATOM    298  C   LYS A  21     -27.702  19.350  30.112  1.00 20.38     0.241 C
ATOM    299  O   LYS A  21     -28.434  18.802  30.957  1.00 19.71    -0.271 OA
ATOM    300  CB  LYS A  21     -27.992  18.892  27.676  1.00 16.45     0.035 C
ATOM    303  CG  LYS A  21     -28.870  17.655  27.953  1.00 21.55     0.004 C
ATOM    306  CD  LYS A  21     -28.980  16.806  26.687  1.00 35.45     0.027 C
ATOM    309  CE  LYS A  21     -29.730  15.515  26.981  1.00 33.64     0.229 C
ATOM    312  NZ  LYS A  21     -28.874  14.462  27.598  1.00 36.33    -0.079 N
ATOM    313  HZ1 LYS A  21     -29.377  13.597  27.795  1.00  0.00     0.274 HD
ATOM    314  HZ2 LYS A  21     -28.416  14.814  28.439  1.00  0.00     0.274 HD
ATOM    315  HZ3 LYS A  21     -28.052  14.280  27.022  1.00  0.00     0.274 HD
ATOM    316  N   ALA A  22     -26.383  19.504  30.319  1.00 17.28    -0.346 N
ATOM    317  HN  ALA A  22     -25.813  19.986  29.624  1.00  0.00     0.163 HD
ATOM    318  CA  ALA A  22     -25.759  18.982  31.540  1.00 16.17     0.172 C
ATOM    320  C   ALA A  22     -26.101  19.852  32.733  1.00 21.57     0.240 C
ATOM    321  O   ALA A  22     -25.888  19.452  33.890  1.00 19.42    -0.271 OA
ATOM    322  CB  ALA A  22     -24.230  18.978  31.361  1.00 16.65     0.042 C
ATOM    326  N   LYS A  23     -26.387  21.116  32.426  1.00 21.06    -0.346 N
ATOM    327  HN  LYS A  23     -26.465  21.359  31.439  1.00  0.00     0.163 HD
ATOM    328  CA  LYS A  23     -26.596  22.172  33.402  1.00 20.53     0.176 C
ATOM    330  C   LYS A  23     -25.312  22.390  34.202  1.00 23.88     0.241 C
ATOM    331  O   LYS A  23     -25.329  22.629  35.407  1.00 21.98    -0.271 OA
ATOM    332  CB  LYS A  23     -27.749  21.888  34.366  1.00 34.52     0.035 C
ATOM    335  CG  LYS A  23     -29.099  22.254  33.745  1.00 50.97     0.004 C
ATOM    338  CD  LYS A  23     -30.186  21.305  34.220  1.00 73.40     0.027 C
ATOM    341  CE  LYS A  23     -31.265  21.108  33.168  1.00 83.35     0.229 C
ATOM    344  NZ  LYS A  23     -32.045  19.861  33.394  1.00 88.89    -0.079 N
ATOM    345  HZ1 LYS A  23     -32.769  19.729  32.688  1.00  0.00     0.274 HD
ATOM    346  HZ2 LYS A  23     -32.437  19.836  34.335  1.00  0.00     0.274 HD
ATOM    347  HZ3 LYS A  23     -31.433  19.047  33.453  1.00  0.00     0.274 HD
ATOM    348  N   SER A  24     -24.175  22.282  33.519  1.00 17.91    -0.344 N
ATOM    349  HN  SER A  24     -24.205  22.121  32.512  1.00  0.00     0.163 HD
ATOM    350  CA  SER A  24     -22.882  22.391  34.195  1.00 18.48     0.200 C
ATOM    352  C   SER A  24     -21.828  22.606  33.125  1.00 15.27     0.242 C
ATOM    353  O   SER A  24     -22.058  22.032  32.037  1.00 17.08    -0.271 OA
ATOM    354  CB  SER A  24     -22.605  21.061  34.940  1.00 17.14     0.199 C
ATOM    357  OG  SER A  24     -21.289  21.051  35.505  1.00 19.18    -0.398 OA
ATOM    358  HG  SER A  24     -21.119  20.236  35.962  1.00  0.00     0.209 HD
ATOM    359  N   GLY A  25     -20.732  23.321  33.400  1.00 15.81    -0.350 N
ATOM    360  HN  GLY A  25     -20.591  23.773  34.303  1.00  0.00     0.163 HD
ATOM    361  CA  GLY A  25     -19.737  23.414  32.307  1.00 15.97     0.225 C
ATOM    364  C   GLY A  25     -19.539  24.877  31.964  1.00 20.32     0.236 C
ATOM    365  O   GLY A  25     -20.090  25.790  32.591  1.00 19.20    -0.272 OA
ATOM    366  N   HIS A  26     -18.668  25.084  30.964  1.00 15.02    -0.346 N
ATOM    367  HN  HIS A  26     -18.358  24.285  30.410  1.00  0.00     0.163 HD
ATOM    368  CA  HIS A  26     -18.149  26.404  30.640  1.00 16.39     0.182 C
ATOM    370  C   HIS A  26     -18.317  26.717  29.159  1.00 18.63     0.243 C
ATOM    371  O   HIS A  26     -17.562  26.218  28.340  1.00 17.32    -0.271 OA
ATOM    372  CB  HIS A  26     -16.627  26.397  30.908  1.00 14.48     0.093 C
ATOM    375  CG  HIS A  26     -16.250  26.061  32.319  1.00 17.68     0.028 A
ATOM    376  CD2 HIS A  26     -15.780  26.836  33.332  1.00 19.52     0.114 A
ATOM    378  ND1 HIS A  26     -16.359  24.771  32.824  1.00 20.30    -0.354 N
ATOM    379  HD1 HIS A  26     -16.673  23.950  32.306  1.00  0.00     0.166 HD
ATOM    380  CE1 HIS A  26     -15.984  24.791  34.097  1.00 26.27     0.180 A
ATOM    382  NE2 HIS A  26     -15.620  26.035  34.428  1.00 20.57    -0.360 N
ATOM    383  HE2 HIS A  26     -15.281  26.335  35.342  1.00  0.00     0.166 HD
ATOM    384  N   PRO A  27     -19.311  27.525  28.840  1.00 17.60    -0.337 N
ATOM    385  CA  PRO A  27     -19.569  27.872  27.463  1.00 16.46     0.179 C
ATOM    387  C   PRO A  27     -18.716  29.029  26.960  1.00 20.18     0.241 C
ATOM    388  O   PRO A  27     -18.633  29.203  25.739  1.00 17.56    -0.271 OA
ATOM    389  CB  PRO A  27     -21.036  28.273  27.511  1.00 18.25     0.037 C
ATOM    392  CG  PRO A  27     -21.181  28.925  28.846  1.00 20.95     0.022 C
ATOM    395  CD  PRO A  27     -20.327  28.097  29.785  1.00 16.67     0.127 C
ATOM    398  N   GLY A  28     -18.160  29.852  27.847  1.00 18.93    -0.351 N
ATOM    399  HN  GLY A  28     -18.225  29.632  28.841  1.00  0.00     0.163 HD
ATOM    400  CA  GLY A  28     -17.462  31.059  27.429  1.00 18.06     0.225 C
ATOM    403  C   GLY A  28     -16.308  30.909  26.476  1.00 18.65     0.236 C
ATOM    404  O   GLY A  28     -16.279  31.481  25.371  1.00 17.98    -0.272 OA
ATOM    405  N   ALA A  29     -15.304  30.137  26.866  1.00 14.46    -0.347 N
ATOM    406  HN  ALA A  29     -15.376  29.652  27.761  1.00  0.00     0.163 HD
ATOM    407  CA  ALA A  29     -14.102  29.955  26.064  1.00 15.13     0.172 C
ATOM    409  C   ALA A  29     -14.352  29.293  24.730  1.00 15.69     0.243 C
ATOM    410  O   ALA A  29     -13.839  29.674  23.685  1.00 16.24    -0.271 OA
ATOM    411  CB  ALA A  29     -13.013  29.256  26.865  1.00 16.50     0.042 C
ATOM    415  N   PRO A  30     -15.154  28.228  24.698  1.00 17.74    -0.337 N
ATOM    416  CA  PRO A  30     -15.489  27.555  23.452  1.00 15.63     0.179 C
ATOM    418  C   PRO A  30     -16.160  28.534  22.498  1.00 16.53     0.241 C
ATOM    419  O   PRO A  30     -15.839  28.554  21.313  1.00 16.46    -0.271 OA
ATOM    420  CB  PRO A  30     -16.414  26.401  23.922  1.00 17.27     0.037 C
ATOM    423  CG  PRO A  30     -15.764  26.113  25.253  1.00 20.41     0.022 C
ATOM    426  CD  PRO A  30     -15.749  27.514  25.872  1.00 18.42     0.127 C
ATOM    429  N   MET A  31     -17.058  29.419  22.930  1.00 13.41    -0.346 N
ATOM    430  HN  MET A  31     -17.323  29.408  23.915  1.00  0.00     0.163 HD
ATOM    431  CA  MET A  31     -17.680  30.408  22.044  1.00 14.61     0.177 C
ATOM    433  C   MET A  31     -16.703  31.482  21.600  1.00 14.80     0.240 C
ATOM    434  O   MET A  31     -16.695  31.975  20.473  1.00 14.63    -0.271 OA
ATOM    435  CB  MET A  31     -18.890  31.021  22.756  1.00 12.65     0.045 C
ATOM    438  CG  MET A  31     -19.980  29.950  22.931  1.00 17.09     0.076 C
ATOM    441  SD  MET A  31     -21.322  30.565  23.965  1.00 23.81    -0.173 SA
ATOM    442  CE  MET A  31     -22.156  31.633  22.751  1.00 26.44    -0.089 C
ATOM    446  N   GLY A  32     -15.784  31.849  22.499  1.00 16.12    -0.351 N
ATOM    447  HN  GLY A  32     -15.813  31.433  23.430  1.00  0.00     0.163 HD
ATOM    448  CA  GLY A  32     -14.743  32.821  22.198  1.00 13.72     0.225 C
ATOM    451  C   GLY A  32     -13.689  32.342  21.197  1.00 15.23     0.236 C
ATOM    452  O   GLY A  32     -13.230  33.120  20.366  1.00 14.27    -0.272 OA
ATOM    453  N   MET A  33     -13.301  31.066  21.258  1.00  8.49    -0.346 N
ATOM    454  HN  MET A  33     -13.781  30.440  21.905  1.00  0.00     0.163 HD
ATOM    455  CA  MET A  33     -12.231  30.533  20.447  1.00  8.85     0.177 C
ATOM    457  C   MET A  33     -12.702  29.737  19.229  1.00 12.57     0.241 C
ATOM    458  O   MET A  33     -11.818  29.306  18.503  1.00 10.39    -0.271 OA
ATOM    459  CB  MET A  33     -11.360  29.544  21.319  1.00 12.16     0.045 C
ATOM    462  CG  MET A  33     -10.700  30.377  22.466  1.00 16.88     0.076 C
ATOM    465  SD  MET A  33      -9.268  29.475  23.125  1.00 19.64    -0.173 SA
ATOM    466  CE  MET A  33      -7.964  30.030  22.017  1.00 19.49     0.089 C
ATOM    470  N   ALA A  34     -14.000  29.688  18.917  1.00 11.14    -0.346 N
ATOM    471  HN  ALA A  34     -14.682  30.213  19.465  1.00  0.00     0.163 HD
ATOM    472  CA  ALA A  34     -14.437  28.869  17.775  1.00 12.63     0.172 C
ATOM    474  C   ALA A  34     -13.814  29.235  16.442  1.00  8.49     0.240 C
ATOM    475  O   ALA A  34     -13.480  28.363  15.589  1.00 11.87    -0.271 OA
ATOM    476  CB  ALA A  34     -15.967  28.860  17.734  1.00 11.45     0.042 C
ATOM    480  N   ASP A  35     -13.695  30.531  16.126  1.00  9.41    -0.346 N
ATOM    481  HN  ASP A  35     -13.994  31.230  16.805  1.00  0.00     0.163 HD
ATOM    482  CA  ASP A  35     -13.161  30.976  14.865  1.00 12.89     0.186 C
ATOM    484  C   ASP A  35     -11.685  30.635  14.737  1.00 13.75     0.241 C
ATOM    485  O   ASP A  35     -11.237  30.276  13.641  1.00 11.87    -0.271 OA
ATOM    486  CB  ASP A  35     -13.339  32.506  14.622  1.00 13.08     0.147 C
ATOM    489  CG  ASP A  35     -14.793  32.914  14.795  1.00 20.67     0.175 C
ATOM    490  OD1 ASP A  35     -15.647  32.340  14.098  1.00 14.39    -0.648 OA
ATOM    491  OD2 ASP A  35     -15.105  33.776  15.626  1.00 17.28    -0.648 OA
ATOM    492  N   ILE A  36     -10.899  30.691  15.817  1.00 11.58    -0.346 N
ATOM    493  HN  ILE A  36     -11.296  30.983  16.710  1.00  0.00     0.163 HD
ATOM    494  CA  ILE A  36      -9.472  30.339  15.742  1.00 12.13     0.180 C
ATOM    496  C   ILE A  36      -9.328  28.826  15.495  1.00 10.01     0.241 C
ATOM    497  O   ILE A  36      -8.517  28.355  14.691  1.00 12.12    -0.271 OA
ATOM    498  CB  ILE A  36      -8.763  30.727  17.067  1.00 13.13     0.013 C
ATOM    500  CG1 ILE A  36      -8.945  32.250  17.298  1.00 11.87     0.002 C
ATOM    503  CG2 ILE A  36      -7.288  30.342  17.077  1.00 11.19     0.012 C
ATOM    507  CD1 ILE A  36      -8.769  32.582  18.807  1.00 15.98     0.005 C
ATOM    511  N   ALA A  37     -10.126  28.057  16.184  1.00 10.43    -0.346 N
ATOM    512  HN  ALA A  37     -10.790  28.487  16.828  1.00  0.00     0.163 HD
ATOM    513  CA  ALA A  37     -10.101  26.585  16.064  1.00 13.54     0.172 C
ATOM    515  C   ALA A  37     -10.488  26.169  14.652  1.00 14.54     0.240 C
ATOM    516  O   ALA A  37      -9.842  25.278  14.081  1.00 13.72    -0.271 OA
ATOM    517  CB  ALA A  37     -10.999  25.772  16.993  1.00  8.66     0.042 C
ATOM    521  N   GLU A  38     -11.483  26.849  14.075  1.00 11.87    -0.346 N
ATOM    522  HN  GLU A  38     -11.951  27.600  14.582  1.00  0.00     0.163 HD
ATOM    523  CA  GLU A  38     -11.908  26.507  12.688  1.00 12.12     0.177 C
ATOM    525  C   GLU A  38     -10.771  26.627  11.721  1.00 14.20     0.241 C
ATOM    526  O   GLU A  38     -10.478  25.722  10.916  1.00 11.75    -0.271 OA
ATOM    527  CB  GLU A  38     -13.144  27.348  12.308  1.00 11.76     0.045 C
ATOM    530  CG  GLU A  38     -13.795  26.823  11.009  1.00 11.75     0.116 C
ATOM    533  CD  GLU A  38     -13.178  27.449   9.786  1.00 15.69     0.172 C
ATOM    534  OE1 GLU A  38     -12.629  28.577   9.776  1.00 17.44    -0.648 OA
ATOM    535  OE2 GLU A  38     -13.217  26.775   8.726  1.00 20.84    -0.648 OA
ATOM    536  N   VAL A  39     -10.054  27.775  11.759  1.00 12.15    -0.346 N
ATOM    537  HN  VAL A  39     -10.316  28.520  12.405  1.00  0.00     0.163 HD
ATOM    538  CA  VAL A  39      -8.900  27.945  10.869  1.00 11.40     0.180 C
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ATOM    540  C   VAL A  39      -7.818  26.900  11.134  1.00 12.19      0.241 C
ATOM    541  O   VAL A  39      -7.211  26.267  10.254  1.00 12.00     -0.271 OA
ATOM    542  CB  VAL A  39      -8.300  29.360  11.033  1.00 15.21      0.009 C
ATOM    544  CG1 VAL A  39      -6.965  29.509  10.316  1.00 12.73      0.012 C
ATOM    548  CG2 VAL A  39      -9.284  30.422  10.519  1.00 12.12      0.012 C
ATOM    552  N   LEU A  40      -7.450  26.764  12.415  1.00 10.84     -0.346 N
ATOM    553  HN  LEU A  40      -7.926  27.277  13.157  1.00  0.00      0.163 HD
ATOM    554  CA  LEU A  40      -6.334  25.847  12.717  1.00 12.73      0.177 C
ATOM    556  C   LEU A  40      -6.631  24.416  12.245  1.00 10.31      0.241 C
ATOM    557  O   LEU A  40      -5.802  23.764  11.603  1.00 11.29     -0.271 OA
ATOM    558  CB  LEU A  40      -6.064  25.851  14.239  1.00 12.52      0.038 C
ATOM    561  CG  LEU A  40      -5.041  24.788  14.701  1.00 15.11     -0.020 C
ATOM    563  CD1 LEU A  40      -3.701  25.040  14.043  1.00 13.43      0.009 C
ATOM    567  CD2 LEU A  40      -4.863  24.795  16.229  1.00 14.98      0.009 C
ATOM    571  N   TRP A  41      -7.793  23.896  12.681  1.00  9.86     -0.346 N
ATOM    572  HN  TRP A  41      -8.460  24.478  13.188  1.00  0.00      0.163 HD
ATOM    573  CA  TRP A  41      -8.088  22.494  12.421  1.00  9.46      0.181 C
ATOM    575  C   TRP A  41      -8.437  22.241  10.951  1.00 12.76      0.241 C
ATOM    576  O   TRP A  41      -7.979  21.228  10.441  1.00 14.33     -0.271 OA
ATOM    577  CB  TRP A  41      -9.274  22.023  13.299  1.00 10.69      0.075 C
ATOM    580  CG  TRP A  41      -8.799  21.653  14.681  1.00 12.27     -0.028 A
ATOM    581  CD1 TRP A  41      -8.185  22.493  15.574  1.00  8.73      0.008 A
ATOM    583  CD2 TRP A  41      -8.857  20.370  15.306  1.00 11.27     -0.002 A
ATOM    584  CE2 TRP A  41      -8.295  20.495  16.586  1.00  9.35      0.042 A
ATOM    585  CE3 TRP A  41      -9.349  19.125  14.883  1.00 14.55      0.014 A
ATOM    587  NE1 TRP A  41      -7.873  21.798  16.737  1.00 11.96     -0.365 N
ATOM    588  HE1 TRP A  41      -7.411  22.186  17.560  1.00  0.00      0.165 HD
ATOM    589  CZ2 TRP A  41      -8.185  19.403  17.458  1.00 15.48      0.030 A
ATOM    591  CZ3 TRP A  41      -9.249  18.049  15.760  1.00 18.23      0.001 A
ATOM    593  CH2 TRP A  41      -8.678  18.195  17.043  1.00 16.09      0.002 A
ATOM    595  N   ARG A  42      -9.156  23.155  10.305  1.00 11.74     -0.346 N
ATOM    596  HN  ARG A  42      -9.474  24.015  10.752  1.00  0.00      0.163 HD
ATOM    597  CA  ARG A  42      -9.464  22.836   8.883  1.00 12.96      0.176 C
ATOM    599  C   ARG A  42      -8.328  23.131   7.943  1.00 17.14      0.241 C
ATOM    600  O   ARG A  42      -8.147  22.394   6.952  1.00 15.58     -0.271 OA
ATOM    601  CB  ARG A  42     -10.764  23.549   8.450  1.00 11.69      0.036 C
ATOM    604  CG  ARG A  42     -11.964  23.020   9.205  1.00  9.88      0.023 C
ATOM    607  CD  ARG A  42     -13.315  23.594   8.759  1.00 20.64      0.138 C
ATOM    610  NE  ARG A  42     -13.485  23.315   7.355  1.00 27.01     -0.227 N
ATOM    611  HE  ARG A  42     -13.686  22.339   7.137  1.00  0.00      0.177 HD
ATOM    612  CZ  ARG A  42     -13.424  24.111   6.307  1.00 28.86      0.665 C
ATOM    613  NH1 ARG A  42     -13.199  25.409   6.333  1.00 21.29     -0.235 N
ATOM    614  1HH1 ARG A  42     -13.152  26.025   5.522  1.00  0.00      0.174 HD
ATOM    615  2HH1 ARG A  42     -13.070  25.834   7.251  1.00  0.00      0.174 HD
ATOM    616  NH2 ARG A  42     -13.592  23.556   5.108  1.00 21.95     -0.235 N
ATOM    617  1HH2 ARG A  42     -13.545  24.172   4.297  1.00  0.00      0.174 HD
ATOM    618  2HH2 ARG A  42     -13.766  22.551   5.088  1.00  0.00      0.174 HD
ATOM    619  N   ASP A  43      -7.527  24.170   8.172  1.00 14.09     -0.346 N
ATOM    620  HN  ASP A  43      -7.642  24.724   9.021  1.00  0.00      0.163 HD
ATOM    621  CA  ASP A  43      -6.496  24.513   7.220  1.00 16.29      0.186 C
ATOM    623  C   ASP A  43      -5.089  24.069   7.572  1.00 18.44      0.241 C
ATOM    624  O   ASP A  43      -4.298  24.049   6.627  1.00 15.14     -0.271 OA
ATOM    625  CB  ASP A  43      -6.401  26.031   6.998  1.00 15.39      0.147 C
ATOM    628  CG  ASP A  43      -7.587  26.610   6.240  1.00 25.46      0.175 C
ATOM    629  OD1 ASP A  43      -8.662  26.027   6.079  1.00 25.52     -0.648 OA
ATOM    630  OD2 ASP A  43      -7.463  27.775   5.853  1.00 30.01     -0.648 OA
ATOM    631  N   PHE A  44      -4.729  23.760   8.812  1.00 11.35     -0.346 N
ATOM    632  HN  PHE A  44      -5.423  23.725   9.558  1.00  0.00      0.163 HD
ATOM    633  CA  PHE A  44      -3.339  23.474   9.090  1.00  9.86      0.180 C
ATOM    635  C   PHE A  44      -3.101  22.124   9.783  1.00 14.56      0.241 C
ATOM    636  O   PHE A  44      -2.059  21.526   9.531  1.00 14.75     -0.271 OA
ATOM    637  CB  PHE A  44      -2.761  24.562  10.050  1.00  9.51      0.073 C
ATOM    640  CG  PHE A  44      -2.713  25.903   9.337  1.00 11.66     -0.056 A
ATOM    641  CD1 PHE A  44      -1.686  26.131   8.422  1.00 14.86      0.007 A
ATOM    643  CD2 PHE A  44      -3.733  26.829   9.512  1.00 10.16      0.007 A
ATOM    645  CE1 PHE A  44      -1.653  27.359   7.739  1.00 19.74      0.001 A
ATOM    647  CE2 PHE A  44      -3.710  28.038   8.822  1.00 11.54      0.001 A
ATOM    649  CZ  PHE A  44      -2.665  28.276   7.929  1.00 14.01      0.000 A
ATOM    651  N   LEU A  45      -4.012  21.732  10.662  1.00  8.62     -0.346 N
ATOM    652  HN  LEU A  45      -4.905  22.208  10.786  1.00  0.00      0.163 HD
ATOM    653  CA  LEU A  45      -3.615  20.537  11.450  1.00 10.36      0.177 C
ATOM    655  C   LEU A  45      -3.438  19.302  10.605  1.00 11.33      0.241 C
ATOM    656  O   LEU A  45      -4.317  18.902   9.806  1.00 12.53     -0.271 OA
ATOM    657  CB  LEU A  45      -4.635  20.369  12.568  1.00  9.60      0.038 C
ATOM    660  CG  LEU A  45      -4.332  19.348  13.676  1.00 13.24     -0.020 C
ATOM    662  CD1 LEU A  45      -3.343  19.958  14.657  1.00 13.78      0.009 C
ATOM    666  CD2 LEU A  45      -5.639  19.014  14.398  1.00 14.26      0.009 C
ATOM    670  N   LYS A  46      -2.356  18.587  10.919  1.00 11.39     -0.346 N
ATOM    671  HN  LYS A  46      -1.712  18.893  11.648  1.00  0.00      0.163 HD
ATOM    672  CA  LYS A  46      -2.123  17.312  10.156  1.00 10.46      0.176 C
ATOM    674  C   LYS A  46      -2.523  16.173  11.089  1.00 11.89      0.241 C
ATOM    675  O   LYS A  46      -1.798  15.952  12.069  1.00 11.51     -0.271 OA
ATOM    676  CB  LYS A  46      -0.650  17.214   9.822  1.00 10.22      0.035 C
ATOM    679  CG  LYS A  46      -0.251  15.965   9.040  1.00 12.57      0.004 C
ATOM    682  CD  LYS A  46       1.242  15.945   8.727  1.00 18.12      0.027 C
ATOM    685  CE  LYS A  46       2.046  15.477   9.932  1.00 20.62      0.229 C
ATOM    688  NZ  LYS A  46       3.488  15.342   9.551  1.00 14.72     -0.079 N
ATOM    689  HZ1 LYS A  46       4.027  15.028  10.358  1.00  0.00      0.274 HD
ATOM    690  HZ2 LYS A  46       3.862  16.202   9.149  1.00  0.00      0.274 HD
ATOM    691  HZ3 LYS A  46       3.617  14.734   8.742  1.00  0.00      0.274 HD
ATOM    692  N   HIS A  47      -3.617  15.478  10.815  1.00 12.22     -0.346 N
ATOM    693  HN  HIS A  47      -4.142  15.666   9.961  1.00  0.00      0.163 HD
ATOM    694  CA  HIS A  47      -4.070  14.437  11.743  1.00 10.85      0.182 C
ATOM    696  C   HIS A  47      -4.953  13.460  10.946  1.00 11.16      0.241 C
ATOM    697  O   HIS A  47      -5.327  13.768   9.802  1.00 11.54     -0.271 OA
ATOM    698  CB  HIS A  47      -4.904  15.013  12.901  1.00 14.97      0.093 C
ATOM    701  CG  HIS A  47      -6.159  15.697  12.460  1.00 11.91      0.028 A
ATOM    702  CD2 HIS A  47      -6.357  16.669  11.526  1.00 10.87      0.114 A
ATOM    704  ND1 HIS A  47      -7.412  15.396  12.967  1.00 11.92     -0.354 N
ATOM    705  HD1 HIS A  47      -7.598  14.683  13.672  1.00  0.00      0.166 HD
ATOM    706  CE1 HIS A  47      -8.336  16.166  12.407  1.00 10.88      0.180 A
ATOM    708  NE2 HIS A  47      -7.710  16.950  11.515  1.00 13.34     -0.360 N
ATOM    709  HE2 HIS A  47      -8.163  17.645  10.921  1.00  0.00      0.166 HD
ATOM    710  N   ASN A  48      -5.150  12.300  11.524  1.00 10.52     -0.346 N
ATOM    711  HN  ASN A  48      -4.695  12.090  12.413  1.00  0.00      0.163 HD
ATOM    712  CA  ASN A  48      -6.029  11.297  10.891  1.00 13.33      0.185 C
ATOM    714  C   ASN A  48      -6.990  10.850  11.966  1.00 12.07      0.243 C
ATOM    715  O   ASN A  48      -6.654  10.083  12.879  1.00 12.53     -0.271 OA
ATOM    716  CB  ASN A  48      -5.205  10.118  10.358  1.00 13.02      0.137 C
ATOM    719  CG  ASN A  48      -6.086   9.043   9.733  1.00 13.41      0.217 C
ATOM    720  ND2 ASN A  48      -5.528   7.871   9.445  1.00 10.80     -0.370 N
ATOM    721  1HD2 ASN A  48      -4.542   7.665   9.603  1.00  0.00      0.159 HD
ATOM    722  2HD2 ASN A  48      -6.118   7.151   9.027  1.00  0.00      0.159 HD
ATOM    723  OD1 ASN A  48      -7.282   9.293   9.541  1.00 10.30     -0.274 OA
ATOM    724  N   PRO A  49      -8.270  11.217  11.829  1.00 13.12     -0.337 N
ATOM    725  CA  PRO A  49      -9.313  10.860  12.781  1.00 13.42      0.179 C
ATOM    727  C   PRO A  49      -9.505   9.365  12.915  1.00 15.36      0.241 C
ATOM    728  O   PRO A  49      -9.935   8.884  13.983  1.00 16.57     -0.271 OA
ATOM    729  CB  PRO A  49     -10.606  11.513  12.235  1.00 15.84      0.037 C
ATOM    732  CG  PRO A  49     -10.145  12.514  11.256  1.00 16.70      0.022 C
ATOM    735  CD  PRO A  49      -8.791  12.083  10.751  1.00 11.63      0.127 C
ATOM    738  N   GLN A  50      -9.153   8.635  11.867  1.00 13.08     -0.346 N
ATOM    739  HN  GLN A  50      -8.807   9.092  11.023  1.00  0.00      0.163 HD
ATOM    740  CA  GLN A  50      -9.258   7.170  11.914  1.00 15.57      0.177 C
ATOM    742  C   GLN A  50      -8.071   6.533  12.611  1.00 15.75      0.241 C
ATOM    743  O   GLN A  50      -8.075   5.326  12.887  1.00 18.01     -0.271 OA
ATOM    744  CB  GLN A  50      -9.344   6.626  10.475  1.00 19.47      0.044 C
ATOM    747  CG  GLN A  50     -10.638   7.053   9.771  1.00 36.62      0.105 C
ATOM    750  CD  GLN A  50     -10.930   6.158   8.574  1.00 50.44      0.243 C
ATOM    751  NE2 GLN A  50     -10.617   6.622   7.365  1.00 45.14     -0.370 N
ATOM    752  1HE2 GLN A  50     -10.210   7.549   7.238  1.00  0.00      0.159 HD
ATOM    753  2HE2 GLN A  50     -10.813   6.023   6.563  1.00  0.00      0.159 HD
ATOM    754  OE1 GLN A  50     -11.425   5.031   8.728  1.00 55.72     -0.274 OA
ATOM    755  N   ASN A  51      -7.008   7.270  12.928  1.00 14.15     -0.346 N
ATOM    756  HN  ASN A  51      -6.976   8.255  12.665  1.00  0.00      0.163 HD
ATOM    757  CA  ASN A  51      -5.890   6.674  13.649  1.00 10.61      0.185 C
ATOM    759  C   ASN A  51      -5.296   7.764  14.537  1.00 13.23      0.243 C
ATOM    760  O   ASN A  51      -4.293   8.368  14.240  1.00  9.74     -0.271 OA
ATOM    761  CB  ASN A  51      -4.796   6.043  12.772  1.00 12.01      0.137 C
ATOM    764  CG  ASN A  51      -3.704   5.426  13.613  1.00 17.20      0.217 C
ATOM    765  ND2 ASN A  51      -2.574   5.049  13.050  1.00 15.79     -0.370 N
ATOM    766  1HD2 ASN A  51      -2.434   5.150  12.045  1.00  0.00      0.159 HD
ATOM    767  2HD2 ASN A  51      -1.836   4.632  13.618  1.00  0.00      0.159 HD
ATOM    768  OD1 ASN A  51      -3.877   5.301  14.851  1.00 15.67     -0.274 OA
ATOM    769  N   PRO A  52      -5.871   7.962  15.722  1.00 13.15     -0.337 N
ATOM    770  CA  PRO A  52      -5.381   8.948  16.664  1.00 12.98      0.179 C
ATOM    772  C   PRO A  52      -4.016   8.607  17.212  1.00 14.11      0.241 C
ATOM    773  O   PRO A  52      -3.434   9.468  17.875  1.00 14.64     -0.271 OA
ATOM    774  CB  PRO A  52      -6.421   8.908  17.815  1.00 14.31      0.037 C
ATOM    777  CG  PRO A  52      -7.652   8.436  17.103  1.00 16.56      0.022 C
ATOM    780  CD  PRO A  52      -7.156   7.350  16.162  1.00 12.57      0.127 C
ATOM    783  N   SER A  53      -3.473   7.398  17.004  1.00 12.46     -0.344 N
ATOM    784  HN  SER A  53      -4.028   6.683  16.533  1.00  0.00      0.163 HD
ATOM    785  CA  SER A  53      -2.127   7.073  17.425  1.00 11.06      0.200 C
ATOM    787  C   SER A  53      -1.079   7.199  16.332  1.00 14.31      0.243 C
ATOM    788  O   SER A  53       0.093   6.857  16.540  1.00 13.33     -0.271 OA
ATOM    789  CB  SER A  53      -2.105   5.609  17.954  1.00 17.41      0.199 C
ATOM    792  OG  SER A  53      -3.004   5.590  19.066  1.00 20.64     -0.398 OA
ATOM    793  HG  SER A  53      -2.991   4.697  19.389  1.00  0.00      0.209 HD
ATOM    794  N   TRP A  54      -1.397   7.760  15.171  1.00 10.45     -0.346 N
ATOM    795  HN  TRP A  54      -2.352   8.077  15.006  1.00  0.00      0.163 HD
ATOM    796  CA  TRP A  54      -0.369   7.929  14.112  1.00  6.83      0.181 C
ATOM    798  C   TRP A  54       0.862   8.604  14.656  1.00 10.90      0.241 C
ATOM    799  O   TRP A  54       0.777   9.692  15.220  1.00 11.46     -0.271 OA
ATOM    800  CB  TRP A  54      -0.980   8.727  12.949  1.00  5.71      0.075 C
ATOM    803  CG  TRP A  54      -0.034   9.102  11.872  1.00 11.06     -0.028 A
ATOM    804  CD1 TRP A  54       1.148   8.554  11.437  1.00 14.10      0.096 A
ATOM    806  CD2 TRP A  54      -0.243  10.277  11.030  1.00  8.79     -0.002 A
ATOM    807  CE2 TRP A  54       0.820  10.347  10.135  1.00 10.10      0.042 A
ATOM    808  CE3 TRP A  54      -1.295  11.218  10.986  1.00 11.75      0.014 A
ATOM    810  NE1 TRP A  54       1.676   9.296  10.374  1.00  9.29     -0.365 N
ATOM    811  HE1 TRP A  54       2.539   9.094   9.868  1.00  0.00      0.165 HD
ATOM    812  CZ2 TRP A  54       0.875  11.352   9.153  1.00 14.87      0.030 A
ATOM    814  CZ3 TRP A  54      -1.233  12.247  10.039  1.00 10.57      0.001 A
ATOM    816  CH2 TRP A  54      -0.128  12.270   9.151  1.00 17.19      0.002 A
ATOM    818  N   ALA A  55       2.043   7.997  14.534  1.00  7.48     -0.346 N
ATOM    819  HN  ALA A  55       2.134   7.155  13.966  1.00  0.00      0.163 HD
ATOM    820  CA  ALA A  55       3.197   8.549  15.220  1.00 10.90      0.172 C
ATOM    822  C   ALA A  55       3.549   9.956  14.768  1.00 13.97      0.240 C
ATOM    823  O   ALA A  55       4.204  10.666  15.546  1.00 13.02     -0.271 OA
ATOM    824  CB  ALA A  55       4.366   7.577  14.864  1.00 13.15      0.042 C
ATOM    828  N   ASP A  56       3.297  10.314  13.497  1.00  9.36     -0.346 N
ATOM    829  HN  ASP A  56       2.804   9.682  12.866  1.00  0.00      0.163 HD
ATOM    830  CA  ASP A  56       3.747  11.638  13.035  1.00  5.81      0.186 C
ATOM    832  C   ASP A  56       2.640  12.690  12.985  1.00 10.39      0.241 C
ATOM    833  O   ASP A  56       2.856  13.749  12.391  1.00  8.46     -0.271 OA
ATOM    834  CB  ASP A  56       4.436  11.535  11.664  1.00 11.23      0.147 C
ATOM    837  CG  ASP A  56       5.454  12.618  11.404  1.00 15.37      0.175 C
ATOM    838  OD1 ASP A  56       6.117  13.116  12.327  1.00 11.40     -0.648 OA
ATOM    839  OD2 ASP A  56       5.618  13.013  10.224  1.00 11.14     -0.648 OA
ATOM    840  N   ARG A  57       1.505  12.505  13.654  1.00 10.44     -0.346 N
ATOM    841  HN  ARG A  57       1.364  11.623  14.147  1.00  0.00      0.163 HD
ATOM    842  CA  ARG A  57       0.462  13.508  13.708  1.00 10.14      0.176 C
ATOM    844  C   ARG A  57       0.960  14.778  14.436  1.00  8.31      0.241 C
ATOM    845  O   ARG A  57       1.824  14.714  15.295  1.00  7.22     -0.271 OA
ATOM    846  CB  ARG A  57      -0.789  13.003  14.466  1.00  8.28      0.036 C
ATOM    849  CG  ARG A  57      -0.468  12.805  15.992  1.00  6.67      0.023 C
ATOM    852  CD  ARG A  57      -1.599  12.028  16.663  1.00  9.75      0.138 C
ATOM    855  NE  ARG A  57      -1.359  11.903  18.122  1.00 11.08     -0.227 N
ATOM    856  HE  ARG A  57      -1.821  12.578  18.731  1.00  0.00      0.177 HD
ATOM    857  CZ  ARG A  57      -0.607  11.002  18.691  1.00 13.67      0.665 C
ATOM    858  NH1 ARG A  57       0.038  10.080  17.974  1.00 10.85     -0.235 N
ATOM    859  1HH1 ARG A  57      -0.036  10.078  16.957  1.00  0.00      0.174 HD
ATOM    860  2HH1 ARG A  57       0.626   9.375  18.419  1.00  0.00      0.174 HD
ATOM    861  NH2 ARG A  57      -0.509  11.004  20.033  1.00 11.16     -0.235 N
ATOM    862  1HH2 ARG A  57      -1.002  11.709  20.581  1.00  0.00      0.174 HD
ATOM    863  2HH2 ARG A  57       0.078  10.299  20.478  1.00  0.00      0.174 HD
ATOM    864  N   ASP A  58       0.413  15.942  14.083  1.00  7.98     -0.346 N
ATOM    865  HN  ASP A  58      -0.176  15.984  13.251  1.00  0.00      0.163 HD
ATOM    866  CA  ASP A  58       0.637  17.151  14.856  1.00  8.66      0.186 C
ATOM    868  C   ASP A  58      -0.040  16.854  16.213  1.00 11.65      0.241 C
ATOM    869  O   ASP A  58      -1.022  16.113  16.295  1.00  9.89     -0.271 OA
ATOM    870  CB  ASP A  58      -0.061  18.372  14.253  1.00  8.80      0.147 C
ATOM    873  CG  ASP A  58       0.574  18.904  12.988  1.00 12.64      0.175 C
ATOM    874  OD1 ASP A  58       1.777  18.644  12.756  1.00  9.03     -0.648 OA
ATOM    875  OD2 ASP A  58      -0.085  19.627  12.185  1.00 11.63     -0.648 OA
ATOM    876  N   ARG A  59       0.425  17.507  17.275  1.00  7.53     -0.346 N
ATOM    877  HN  ARG A  59       1.237  18.112  17.154  1.00  0.00      0.163 HD
ATOM    878  CA  ARG A  59      -0.160  17.402  18.583  1.00  8.24      0.176 C
ATOM    880  C   ARG A  59      -0.868  18.705  18.946  1.00  9.55      0.241 C
ATOM    881  O   ARG A  59      -0.246  19.758  18.824  1.00 12.77     -0.271 OA
ATOM    882  CB  ARG A  59       0.946  17.170  19.625  1.00  9.76      0.036 C
ATOM    885  CG  ARG A  59       1.180  15.680  19.929  1.00 15.32      0.023 C
ATOM    888  CD  ARG A  59       1.755  14.867  18.775  1.00 13.56      0.138 C
ATOM    891  NE  ARG A  59       2.260  13.537  19.217  1.00 12.32     -0.227 N
ATOM    892  HE  ARG A  59       2.173  13.290  20.203  1.00  0.00      0.177 HD
ATOM    893  CZ  ARG A  59       2.817  12.656  18.394  1.00 16.00      0.665 C
ATOM    894  NH1 ARG A  59       3.005  12.851  17.108  1.00 12.68     -0.235 N
ATOM    895  1HH1 ARG A  59       2.686  13.716  16.671  1.00  0.00      0.174 HD
ATOM    896  2HH1 ARG A  59       3.433  12.174  16.476  1.00  0.00      0.174 HD
ATOM    897  NH2 ARG A  59       3.233  11.527  18.964  1.00 12.11     -0.235 N
ATOM    898  1HH2 ARG A  59       3.087  11.376  19.962  1.00  0.00      0.174 HD
ATOM    899  2HH2 ARG A  59       3.661  10.850  18.332  1.00  0.00      0.174 HD
ATOM    900  N   PHE A  60      -2.103  18.594  19.404  1.00  7.30     -0.346 N
ATOM    901  HN  PHE A  60      -2.527  17.668  19.456  1.00  0.00      0.163 HD
ATOM    902  CA  PHE A  60      -2.884  19.752  19.839  1.00 11.01      0.180 C
ATOM    904  C   PHE A  60      -3.177  19.651  21.338  1.00 11.23      0.241 C
ATOM    905  O   PHE A  60      -3.581  18.592  21.826  1.00 11.21     -0.271 OA
ATOM    906  CB  PHE A  60      -4.224  19.813  19.076  1.00  9.89      0.073 C
ATOM    909  CG  PHE A  60      -5.141  20.915  19.552  1.00 15.31     -0.056 A
ATOM    910  CD1 PHE A  60      -4.996  22.210  19.087  1.00 13.85      0.007 A
ATOM    912  CD2 PHE A  60      -6.156  20.615  20.474  1.00 13.11      0.007 A
ATOM    914  CE1 PHE A  60      -5.847  23.190  19.568  1.00 14.71      0.001 A
ATOM    916  CE2 PHE A  60      -7.006  21.604  20.925  1.00 18.67      0.001 A
ATOM    918  CZ  PHE A  60      -6.857  22.892  20.478  1.00 12.01      0.000 A
ATOM    920  N   VAL A  61      -2.997  20.772  22.057  1.00  5.88     -0.346 N
ATOM    921  HN  VAL A  61      -2.723  21.635  21.587  1.00  0.00      0.163 HD
ATOM    922  CA  VAL A  61      -3.188  20.768  23.494  1.00  7.92      0.180 C
ATOM    924  C   VAL A  61      -4.104  21.935  23.908  1.00 11.44      0.241 C
ATOM    925  O   VAL A  61      -3.772  23.096  23.655  1.00  8.01     -0.271 OA
ATOM    926  CB  VAL A  61      -1.852  20.914  24.244  1.00 10.83      0.009 C
ATOM    928  CG1 VAL A  61      -2.083  21.096  25.768  1.00  9.86      0.012 C
ATOM    932  CG2 VAL A  61      -1.019  19.639  24.037  1.00 10.90      0.012 C
ATOM    936  N   LEU A  62      -5.205  21.647  24.572  1.00  9.41     -0.346 N
ATOM    937  HN  LEU A  62      -5.452  20.671  24.736  1.00  0.00      0.163 HD
ATOM    938  CA  LEU A  62      -6.081  22.707  25.079  1.00  8.52      0.177 C
ATOM    940  C   LEU A  62      -5.706  22.983  26.544  1.00 13.63      0.241 C
ATOM    941  O   LEU A  62      -6.165  22.285  27.467  1.00 11.77     -0.271 OA
ATOM    942  CB  LEU A  62      -7.530  22.196  25.087  1.00  9.25      0.038 C
ATOM    945  CG  LEU A  62      -8.612  23.165  25.549  1.00 13.40     -0.020 C
ATOM    947  CD1 LEU A  62      -8.732  24.288  24.543  1.00 12.83      0.009 C
ATOM    951  CD2 LEU A  62      -9.937  22.381  25.627  1.00 20.61      0.009 C
ATOM    955  N   SER A  63      -4.826  23.959  26.747  1.00  9.40     -0.344 N
ATOM    956  HN  SER A  63      -4.481  24.501  25.955  1.00  0.00      0.163 HD
ATOM    957  CA  SER A  63      -4.346  24.264  28.100  1.00 11.61      0.200 C
ATOM    959  C   SER A  63      -5.422  24.876  28.983  1.00 12.36      0.243 C
ATOM    960  O   SER A  63      -5.465  24.674  30.226  1.00 13.19     -0.271 OA
ATOM    961  CB  SER A  63      -3.079  25.127  28.001  1.00  9.35      0.199 C
ATOM    964  OG  SER A  63      -2.344  25.057  29.229  1.00  9.59     -0.398 OA
ATOM    965  HG  SER A  63      -1.560  25.591  29.168  1.00  0.00      0.209 HD
ATOM    966  N   ASN A  64      -6.330  25.661  28.375  1.00 10.32     -0.345 N
ATOM    967  HN  ASN A  64      -6.241  25.864  27.379  1.00  0.00      0.163 HD
ATOM    968  CA  ASN A  64      -7.451  26.228  29.141  1.00 13.23      0.185 C
ATOM    970  C   ASN A  64      -8.504  25.121  29.118  1.00 13.23      0.241 C
ATOM    971  O   ASN A  64      -9.473  25.168  28.390  1.00 15.54     -0.271 OA
ATOM    972  CB  ASN A  64      -7.955  27.521  28.526  1.00 15.60      0.137 C
ATOM    975  CG  ASN A  64      -7.901  27.686  27.024  1.00 15.97      0.217 C
ATOM    976  ND2 ASN A  64      -8.454  28.792  26.525  1.00 20.91     -0.370 N
ATOM    977  1HD2 ASN A  64      -8.869  29.500  27.131  1.00  0.00      0.159 HD
ATOM    978  2HD2 ASN A  64      -8.418  28.903  25.512  1.00  0.00      0.159 HD
ATOM    979  OD1 ASN A  64      -7.395  26.823  26.285  1.00 13.74     -0.274 OA
ATOM    980  N   GLY A  65      -8.302  24.003  29.809  1.00 18.00     -0.351 N
ATOM    981  HN  GLY A  65      -7.512  24.006  30.455  1.00  0.00      0.163 HD
ATOM    982  CA  GLY A  65      -9.072  22.790  29.748  1.00 16.33      0.225 C
ATOM    985  C   GLY A  65     -10.516  22.887  30.142  1.00 17.42      0.236 C
ATOM    986  O   GLY A  65     -11.339  22.045  29.770  1.00 14.60     -0.272 OA
ATOM    987  N   HIS A  66     -10.898  23.906  30.921  1.00 12.71     -0.346 N
ATOM    988  HN  HIS A  66     -10.206  24.561  31.285  1.00  0.00      0.163 HD
ATOM    989  CA  HIS A  66     -12.316  24.075  31.248  1.00 13.08      0.182 C
ATOM    991  C   HIS A  66     -13.129  24.293  29.977  1.00 16.12      0.241 C
ATOM    992  O   HIS A  66     -14.322  24.007  29.961  1.00 14.35     -0.271 OA
ATOM    993  CB  HIS A  66     -12.461  25.318  32.150  1.00 15.30      0.093 C
ATOM    996  CG  HIS A  66     -11.779  26.575  31.668  1.00 14.32      0.028 A
ATOM    997  CD2 HIS A  66     -12.342  27.633  31.011  1.00 18.80      0.114 A
ATOM    999  ND1 HIS A  66     -10.470  26.909  31.854  1.00 15.27     -0.354 N
ATOM   1000  HD1 HIS A  66      -9.776  26.325  32.321  1.00  0.00      0.166 HD
ATOM   1001  CE1 HIS A  66     -10.235  28.102  31.338  1.00 23.64      0.180 A
ATOM   1003  NE2 HIS A  66     -11.354  28.570  30.796  1.00 16.17     -0.360 N
ATOM   1004  HE2 HIS A  66     -11.462  29.460  30.310  1.00  0.00      0.166 HD
ATOM   1005  N   GLY A  67     -12.552  24.788  28.870  1.00 17.17     -0.351 N
ATOM   1007  HN  GLY A  67     -11.580  25.096  28.883  1.00  0.00      0.163 HD
ATOM   1007  CA  GLY A  67     -13.358  24.878  27.628  1.00 18.65      0.225 C
ATOM   1010  C   GLY A  67     -13.409  23.553  26.887  1.00 14.53      0.236 C
ATOM   1011  O   GLY A  67     -13.311  23.488  25.665  1.00 13.99     -0.272 OA
ATOM   1012  N   SER A  68     -13.667  22.431  27.555  1.00 13.07     -0.344 N
ATOM   1013  HN  SER A  68     -13.895  22.521  28.545  1.00  0.00      0.163 HD
ATOM   1014  CA  SER A  68     -13.652  21.109  27.005  1.00 11.60      0.200 C
ATOM   1016  C   SER A  68     -14.640  20.867  25.883  1.00  9.61      0.243 C
ATOM   1017  O   SER A  68     -14.250  20.106  24.969  1.00 12.89     -0.271 OA
ATOM   1018  CB  SER A  68     -13.916  20.089  28.155  1.00 12.89      0.199 C
ATOM   1021  OG  SER A  68     -15.071  20.490  28.905  1.00 15.56     -0.398 OA
ATOM   1022  HG  SER A  68     -15.232  19.869  29.605  1.00  0.00      0.209 HD
ATOM   1023  N   MET A  69     -15.804  21.507  25.882  1.00  9.77     -0.346 N
ATOM   1024  HN  MET A  69     -16.058  22.141  26.639  1.00  0.00      0.163 HD
ATOM   1025  CA  MET A  69     -16.724  21.267  24.739  1.00 12.28      0.177 C
ATOM   1027  C   MET A  69     -16.062  21.691  23.444  1.00 12.41      0.241 C
ATOM   1028  O   MET A  69     -16.481  21.277  22.361  1.00 10.36     -0.271 OA
ATOM   1029  CB  MET A  69     -18.057  22.017  24.948  1.00 11.12      0.045 C
ATOM   1032  CG  MET A  69     -19.095  21.189  25.732  1.00 11.76      0.076 C
ATOM   1035  SD  MET A  69     -19.277  19.487  25.074  1.00 17.68     -0.173 SA
ATOM   1036  CE  MET A  69     -19.764  19.845  23.371  1.00 15.36      0.089 C
ATOM   1040  N   LEU A  70     -15.093  22.621  23.465  1.00 12.91     -0.346 N
ATOM   1041  HN  LEU A  70     -14.835  23.046  24.356  1.00  0.00      0.163 HD
ATOM   1042  CA  LEU A  70     -14.397  23.043  22.252  1.00 15.10      0.177 C
ATOM   1044  C   LEU A  70     -13.680  21.848  21.628  1.00 15.35      0.241 C
ATOM   1045  O   LEU A  70     -13.859  21.572  20.443  1.00  9.86     -0.271 OA
ATOM   1046  CB  LEU A  70     -13.410  24.176  22.548  1.00 12.17      0.038 C
ATOM   1049  CG  LEU A  70     -12.499  24.549  21.354  1.00 22.12     -0.020 C
ATOM   1051  CD1 LEU A  70     -13.298  25.284  20.305  1.00 25.39      0.009 C
ATOM   1055  CD2 LEU A  70     -11.357  25.439  21.846  1.00 22.71      0.009 C
ATOM   1059  N   ILE A  71     -12.907  21.080  22.428  1.00 10.75     -0.346 N
ATOM   1060  HN  ILE A  71     -12.787  21.305  23.416  1.00  0.00      0.163 HD
ATOM   1061  CA  ILE A  71     -12.248  19.916  21.833  1.00 10.97      0.180 C
ATOM   1063  C   ILE A  71     -13.239  18.794  21.519  1.00 10.28      0.241 C
ATOM   1064  O   ILE A  71     -13.070  18.124  20.475  1.00 12.75     -0.271 OA
ATOM   1065  CB  ILE A  71     -11.062  19.473  22.705  1.00 14.32      0.013 C
ATOM   1067  CG1 ILE A  71     -10.170  18.522  21.878  1.00 17.49      0.002 C
ATOM   1070  CG2 ILE A  71     -11.537  18.836  24.008  1.00 18.20      0.012 C
ATOM   1074  CD1 ILE A  71      -8.910  18.090  22.582  1.00 29.86      0.005 C
ATOM   1078  N   TYR A  72     -14.298  18.586  22.327  1.00  9.53     -0.346 N
ATOM   1079  HN  TYR A  72     -14.441  19.151  23.164  1.00  0.00      0.163 HD
ATOM   1080  CA  TYR A  72     -15.249  17.509  21.960  1.00 13.01      0.180 C
ATOM   1082  C   TYR A  72     -16.007  17.834  20.672  1.00 13.68      0.241 C
ATOM   1083  O   TYR A  72     -16.204  16.926  19.860  1.00 11.81     -0.271 OA
ATOM   1084  CB  TYR A  72     -16.251  17.217  23.079  1.00  8.87      0.073 C
ATOM   1087  CG  TYR A  72     -15.610  16.834  24.398  1.00 11.86     -0.056 A
ATOM   1088  CD1 TYR A  72     -14.522  15.990  24.413  1.00 11.75      0.010 A
ATOM   1090  CD2 TYR A  72     -16.124  17.278  25.613  1.00 15.01      0.010 A
ATOM   1092  CE1 TYR A  72     -13.944  15.601  25.604  1.00 15.51      0.037 A
ATOM   1094  CE2 TYR A  72     -15.553  16.880  26.822  1.00 14.47      0.037 A
ATOM   1096  CZ  TYR A  72     -14.451  16.066  26.796  1.00 15.94      0.065 A
ATOM   1097  OH  TYR A  72     -13.813  15.673  27.939  1.00 11.54     -0.361 OA
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ATOM   1098  HH  TYR A  72      -13.049  15.109  27.921  1.00  0.00     0.217 HD
ATOM   1099  N   SER A  73      -16.332  19.123  20.468  1.00 12.58    -0.344 N
ATOM   1100  HN  SER A  73      -16.133  19.824  21.181  1.00  0.00     0.163 HD
ATOM   1101  CA  SER A  73      -16.973  19.507  19.213  1.00 11.78     0.200 C
ATOM   1103  C   SER A  73      -16.050  19.224  18.026  1.00 14.09     0.243 C
ATOM   1104  O   SER A  73      -16.454  18.694  16.972  1.00 13.78    -0.271 OA
ATOM   1105  CB  SER A  73      -17.251  21.029  19.235  1.00 11.13     0.199 C
ATOM   1108  OG  SER A  73      -18.324  21.268  20.152  1.00 15.93    -0.398 OA
ATOM   1109  HG  SER A  73      -18.495  22.202  20.166  1.00  0.00     0.209 HD
ATOM   1110  N   LEU A  74      -14.786  19.645  18.135  1.00 10.53    -0.346 N
ATOM   1111  HN  LEU A  74      -14.487  20.115  18.989  1.00  0.00     0.163 HD
ATOM   1112  CA  LEU A  74      -13.813  19.442  17.040  1.00  9.96     0.177 C
ATOM   1114  C   LEU A  74      -13.612  17.970  16.711  1.00 12.88     0.241 C
ATOM   1115  O   LEU A  74      -13.575  17.586  15.534  1.00 11.03    -0.271 OA
ATOM   1116  CB  LEU A  74      -12.454  20.075  17.428  1.00  8.84     0.038 C
ATOM   1119  CG  LEU A  74      -12.399  21.615  17.414  1.00 15.53    -0.020 C
ATOM   1121  CD1 LEU A  74      -11.161  22.108  18.162  1.00 12.60     0.009 C
ATOM   1125  CD2 LEU A  74      -12.373  22.113  15.950  1.00 10.97     0.009 C
ATOM   1129  N   LEU A  75      -13.465  17.103  17.710  1.00 11.11    -0.346 N
ATOM   1130  HN  LEU A  75      -13.491  17.435  18.674  1.00  0.00     0.163 HD
ATOM   1131  CA  LEU A  75      -13.265  15.670  17.440  1.00 11.87     0.177 C
ATOM   1133  C   LEU A  75      -14.492  15.068  16.761  1.00 11.09     0.241 C
ATOM   1134  O   LEU A  75      -14.395  14.268  15.810  1.00 12.52    -0.271 OA
ATOM   1135  CB  LEU A  75      -12.979  14.919  18.773  1.00  9.46     0.038 C
ATOM   1138  CG  LEU A  75      -11.661  15.358  19.449  1.00 13.36    -0.020 C
ATOM   1140  CD1 LEU A  75      -11.628  14.762  20.874  1.00 15.40     0.009 C
ATOM   1144  CD2 LEU A  75      -10.415  14.874  18.718  1.00 10.31     0.009 C
ATOM   1148  N   HIS A  76      -15.686  15.420  17.271  1.00 11.07    -0.346 N
ATOM   1149  HN  HIS A  76      -15.728  16.044  18.077  1.00  0.00     0.163 HD
ATOM   1150  CA  HIS A  76      -16.939  14.909  16.673  1.00 13.74     0.182 C
ATOM   1152  C   HIS A  76      -17.055  15.385  15.217  1.00 16.07     0.241 C
ATOM   1153  O   HIS A  76      -17.254  14.562  14.315  1.00 14.46    -0.271 OA
ATOM   1154  CB  HIS A  76      -18.147  15.437  17.448  1.00 14.67     0.093 C
ATOM   1157  CG  HIS A  76      -19.434  15.053  16.774  1.00 14.85     0.028 A
ATOM   1158  CD2 HIS A  76      -20.307  15.810  16.074  1.00 17.81     0.114 A
ATOM   1160  ND1 HIS A  76      -19.885  13.734  16.717  1.00 17.36    -0.354 N
ATOM   1161  HD1 HIS A  76      -19.433  12.923  17.139  1.00  0.00     0.166 HD
ATOM   1162  CE1 HIS A  76      -21.007  13.728  16.016  1.00 25.72     0.180 A
ATOM   1164  NE2 HIS A  76      -21.272  14.961  15.616  1.00 18.47    -0.360 N
ATOM   1165  HE2 HIS A  76      -22.076  15.235  15.051  1.00  0.00     0.166 HD
ATOM   1166  N   LEU A  77      -16.991  16.700  14.998  1.00 12.05    -0.346 N
ATOM   1167  HN  LEU A  77      -16.853  17.337  15.782  1.00  0.00     0.163 HD
ATOM   1168  CA  LEU A  77      -17.116  17.231  13.651  1.00 14.63     0.177 C
ATOM   1170  C   LEU A  77      -16.089  16.725  12.649  1.00 16.69     0.241 C
ATOM   1171  O   LEU A  77      -16.492  16.575  11.468  1.00 15.11    -0.271 OA
ATOM   1172  CB  LEU A  77      -17.025  18.779  13.726  1.00 11.18     0.038 C
ATOM   1175  CG  LEU A  77      -18.243  19.471  14.380  1.00 12.32    -0.020 C
ATOM   1177  CD1 LEU A  77      -17.864  20.921  14.717  1.00 15.28     0.009 C
ATOM   1181  CD2 LEU A  77      -19.491  19.397  13.517  1.00 18.96     0.009 C
ATOM   1185  N   THR A  78      -14.807  16.513  12.984  1.00 11.45    -0.344 N
ATOM   1186  HN  THR A  78      -14.517  16.650  13.952  1.00  0.00     0.163 HD
ATOM   1187  CA  THR A  78      -13.820  16.093  12.000  1.00 14.82     0.205 C
ATOM   1189  C   THR A  78      -13.823  14.571  11.736  1.00 13.86     0.243 C
ATOM   1190  O   THR A  78      -13.133  14.129  10.814  1.00 13.58    -0.271 OA
ATOM   1191  CB  THR A  78      -12.371  16.546  12.344  1.00 15.83     0.146 C
ATOM   1193  CG2 THR A  78      -12.275  18.063  12.392  1.00 10.99     0.042 C
ATOM   1197  OG1 THR A  78      -12.075  16.015  13.649  1.00 13.70    -0.393 OA
ATOM   1198  HG1 THR A  78      -11.191  16.291  13.859  1.00  0.00     0.210 HD
ATOM   1199  N   GLY A  79      -14.586  13.788  12.471  1.00 16.49    -0.350 N
ATOM   1200  HN  GLY A  79      -15.104  14.172  13.261  1.00  0.00     0.163 HD
ATOM   1201  CA  GLY A  79      -14.686  12.359  12.146  1.00 16.98     0.225 C
ATOM   1204  C   GLY A  79      -14.101  11.406  13.144  1.00 18.51     0.236 C
ATOM   1205  O   GLY A  79      -14.027  10.217  12.809  1.00 14.22    -0.272 OA
ATOM   1206  N   TYR A  80      -13.669  11.855  14.331  1.00 12.81    -0.346 N
ATOM   1207  HN  TYR A  80      -13.714  12.850  14.551  1.00  0.00     0.163 HD
ATOM   1208  CA  TYR A  80      -13.134  10.911  15.307  1.00 11.52     0.180 C
ATOM   1210  C   TYR A  80      -14.284  10.019  15.810  1.00 12.85     0.241 C
ATOM   1211  O   TYR A  80      -15.444  10.445  15.700  1.00 16.08    -0.271 OA
ATOM   1212  CB  TYR A  80      -12.521  11.614  16.545  1.00 11.00     0.073 C
ATOM   1215  CG  TYR A  80      -11.176  12.215  16.188  1.00 11.48    -0.056 A
ATOM   1216  CD1 TYR A  80      -11.100  13.355  15.432  1.00 10.61     0.010 A
ATOM   1218  CD2 TYR A  80       -9.995  11.592  16.617  1.00 14.73     0.010 A
ATOM   1220  CE1 TYR A  80       -9.862  13.896  15.092  1.00  7.46     0.037 A
ATOM   1222  CE2 TYR A  80       -8.752  12.130  16.298  1.00 13.80     0.037 A
ATOM   1224  CZ  TYR A  80       -8.710  13.271  15.528  1.00 14.51     0.065 A
ATOM   1225  OH  TYR A  80       -7.492  13.841  15.184  1.00 15.80    -0.361 OA
ATOM   1226  HH  TYR A  80       -7.463  14.628  14.653  1.00  0.00     0.217 HD
ATOM   1227  N   ASP A  81      -13.900   8.945  16.528  1.00 14.61    -0.345 N
ATOM   1228  HN  ASP A  81      -12.911   8.737  16.662  1.00  0.00     0.163 HD
ATOM   1229  CA  ASP A  81      -14.931   8.081  17.113  1.00 20.34     0.186 C
ATOM   1231  C   ASP A  81      -15.520   8.656  18.396  1.00 21.38     0.241 C
ATOM   1232  O   ASP A  81      -15.190   8.223  19.501  1.00 19.20    -0.271 OA
ATOM   1233  CB  ASP A  81      -14.329   6.701  17.378  1.00 25.78     0.147 C
ATOM   1236  CG  ASP A  81      -15.326   5.677  17.903  1.00 38.52     0.175 C
ATOM   1237  OD1 ASP A  81      -16.554   5.831  17.722  1.00 40.52    -0.648 OA
ATOM   1238  OD2 ASP A  81      -14.880   4.691  18.535  1.00 41.69    -0.648 OA
ATOM   1239  N   LEU A  82      -16.367   9.676  18.271  1.00 15.69    -0.346 N
ATOM   1240  HN  LEU A  82      -16.589  10.001  17.330  1.00  0.00     0.163 HD
ATOM   1241  CA  LEU A  82      -16.998  10.359  19.397  1.00 15.70     0.177 C
ATOM   1243  C   LEU A  82      -18.390  10.789  18.933  1.00 15.90     0.243 C
ATOM   1244  O   LEU A  82      -18.603  11.865  18.361  1.00 16.43    -0.271 OA
ATOM   1245  CB  LEU A  82      -16.130  11.577  19.784  1.00 15.72     0.038 C
ATOM   1248  CG  LEU A  82      -16.683  12.290  21.039  1.00 19.08    -0.020 C
ATOM   1250  CD1 LEU A  82      -16.488  11.367  22.240  1.00 18.52     0.009 C
ATOM   1254  CD2 LEU A  82      -15.911  13.582  21.274  1.00 18.54     0.009 C
ATOM   1258  N   PRO A  83      -19.370   9.894  19.068  1.00 16.38    -0.337 N
ATOM   1259  CA  PRO A  83      -20.685  10.106  18.512  1.00 19.39     0.179 C
ATOM   1261  C   PRO A  83      -21.472  11.187  19.208  1.00 18.72     0.241 C
ATOM   1262  O   PRO A  83      -21.151  11.540  20.361  1.00 16.28    -0.271 OA
ATOM   1263  CB  PRO A  83      -21.378   8.735  18.616  1.00 20.73     0.037 C
ATOM   1266  CG  PRO A  83      -20.556   7.910  19.522  1.00 21.06     0.022 C
ATOM   1269  CD  PRO A  83      -19.172   8.515  19.603  1.00 21.01     0.127 C
ATOM   1272  N   MET A  84      -22.527  11.678  18.547  1.00 16.13    -0.346 N
ATOM   1273  HN  MET A  84      -22.746  11.315  17.619  1.00  0.00     0.163 HD
ATOM   1274  CA  MET A  84      -23.369  12.716  19.120  1.00 14.01     0.177 C
ATOM   1276  C   MET A  84      -23.967  12.323  20.452  1.00 18.76     0.241 C
ATOM   1277  O   MET A  84      -24.087  13.143  21.374  1.00 18.32    -0.271 OA
ATOM   1278  CB  MET A  84      -24.541  13.097  18.171  1.00 17.76     0.045 C
ATOM   1281  CG  MET A  84      -25.288  14.341  18.730  1.00 18.50     0.076 C
ATOM   1284  SD  MET A  84      -24.301  15.839  18.621  1.00 23.49    -0.173 SA
ATOM   1285  CE  MET A  84      -24.149  16.140  16.879  1.00 24.23     0.089 C
ATOM   1289  N   GLU A  85      -24.313  11.026  20.630  1.00 18.52    -0.346 N
ATOM   1290  HN  GLU A  85      -24.215  10.347  19.875  1.00  0.00     0.163 HD
ATOM   1291  CA  GLU A  85      -24.830  10.630  21.936  1.00 18.89     0.177 C
ATOM   1293  C   GLU A  85      -23.829  10.960  23.066  1.00 18.31     0.241 C
ATOM   1294  O   GLU A  85      -24.342  11.201  24.160  1.00 22.08    -0.271 OA
ATOM   1295  CB  GLU A  85      -25.103   9.131  21.996  1.00 22.34     0.045 C
ATOM   1298  CG  GLU A  85      -26.209   8.746  22.969  1.00 58.93     0.116 C
ATOM   1301  CD  GLU A  85      -25.941   7.409  23.643  1.00 77.21     0.172 C
ATOM   1302  OE1 GLU A  85      -25.397   6.489  22.984  1.00 87.16    -0.648 OA
ATOM   1303  OE2 GLU A  85      -26.277   7.275  24.845  1.00 85.83    -0.648 OA
ATOM   1304  N   GLU A  86      -22.514  10.881  22.867  1.00 16.33    -0.346 N
ATOM   1305  HN  GLU A  86      -22.146  10.588  21.962  1.00  0.00     0.163 HD
ATOM   1306  CA  GLU A  86      -21.594  11.224  23.975  1.00 13.94     0.177 C
ATOM   1308  C   GLU A  86      -21.612  12.713  24.249  1.00 14.53     0.241 C
ATOM   1309  O   GLU A  86      -21.508  13.114  25.420  1.00 17.00    -0.271 OA
ATOM   1310  CB  GLU A  86      -20.166  10.770  23.625  1.00 17.71     0.045 C
ATOM   1313  CG  GLU A  86      -20.100   9.249  23.479  1.00 17.86     0.116 C
ATOM   1316  CD  GLU A  86      -20.213   8.559  24.833  1.00 28.10     0.172 C
ATOM   1317  OE1 GLU A  86      -20.198   9.132  25.943  1.00 17.64    -0.648 OA
ATOM   1318  OE2 GLU A  86      -20.337   7.324  24.810  1.00 21.80    -0.648 OA
ATOM   1319  N   LEU A  87      -21.806  13.570  23.223  1.00 14.44    -0.346 N
ATOM   1320  HN  LEU A  87      -21.898  13.199  22.277  1.00  0.00     0.163 HD
ATOM   1321  CA  LEU A  87      -21.887  15.000  23.429  1.00 17.16     0.177 C
ATOM   1323  C   LEU A  87      -23.140  15.325  24.236  1.00 19.92     0.241 C
ATOM   1324  O   LEU A  87      -23.185  16.269  25.000  1.00 17.35    -0.271 OA
ATOM   1325  CB  LEU A  87      -21.888  15.860  22.156  1.00 17.66     0.038 C
ATOM   1328  CG  LEU A  87      -20.758  15.714  21.141  1.00 28.93    -0.020 C
ATOM   1330  CD1 LEU A  87      -20.614  16.971  20.265  1.00 23.12     0.009 C
ATOM   1334  CD2 LEU A  87      -19.412  15.404  21.720  1.00 24.50     0.009 C
ATOM   1338  N   LYS A  88      -24.217  14.546  24.046  1.00 17.13    -0.346 N
ATOM   1339  HN  LYS A  88      -24.180  13.815  23.336  1.00  0.00     0.163 HD
ATOM   1340  CA  LYS A  88      -25.425  14.712  24.816  1.00 17.89     0.176 C
ATOM   1342  C   LYS A  88      -25.226  14.252  26.273  1.00 20.63     0.241 C
ATOM   1343  O   LYS A  88      -26.105  14.612  27.060  1.00 22.03    -0.271 OA
ATOM   1344  CB  LYS A  88      -26.621  13.910  24.217  1.00 17.56     0.035 C
ATOM   1347  CG  LYS A  88      -26.937  14.575  22.844  1.00 22.80     0.004 C
ATOM   1350  CD  LYS A  88      -28.402  14.398  22.515  1.00 39.31     0.027 C
ATOM   1353  CE  LYS A  88      -28.653  13.015  21.957  1.00 42.91     0.229 C
ATOM   1356  NZ  LYS A  88      -29.469  13.125  20.705  1.00 58.88    -0.079 N
ATOM   1357  HZ1 LYS A  88      -29.638  12.192  20.329  1.00  0.00     0.274 HD
ATOM   1358  HZ2 LYS A  88      -29.041  13.747  20.019  1.00  0.00     0.274 HD
ATOM   1359  HZ3 LYS A  88      -30.334  13.645  20.852  1.00  0.00     0.274 HD
ATOM   1360  N   ASN A  89      -24.208  13.461  26.560  1.00 15.21    -0.346 N
ATOM   1361  HN  ASN A  89      -23.603  13.153  25.799  1.00  0.00     0.163 HD
ATOM   1362  CA  ASN A  89      -23.908  13.009  27.908  1.00 18.27     0.185 C
ATOM   1364  C   ASN A  89      -22.689  13.690  28.536  1.00 14.67     0.241 C
ATOM   1365  O   ASN A  89      -22.012  13.094  29.384  1.00 16.70    -0.271 OA
ATOM   1366  CB  ASN A  89      -23.649  11.487  27.867  1.00 15.67     0.137 C
ATOM   1369  CG  ASN A  89      -25.021  10.809  27.762  1.00 29.22     0.217 C
ATOM   1370  ND2 ASN A  89      -25.106   9.758  26.969  1.00 38.73    -0.370 N
ATOM   1371 1HD2 ASN A  89      -24.294   9.407  26.461  1.00  0.00     0.159 HD
ATOM   1372 2HD2 ASN A  89      -26.018   9.307  26.899  1.00  0.00     0.159 HD
ATOM   1373  OD1 ASN A  89      -26.003  11.234  28.376  1.00 35.38    -0.274 OA
ATOM   1374  N   PHE A  90      -22.449  14.909  28.128  1.00 14.46    -0.346 N
ATOM   1375  HN  PHE A  90      -23.049  15.313  27.409  1.00  0.00     0.163 HD
ATOM   1376  CA  PHE A  90      -21.344  15.721  28.669  1.00 13.87     0.180 C
ATOM   1378  C   PHE A  90      -21.517  15.782  30.178  1.00 13.18     0.241 C
ATOM   1379  O   PHE A  90      -22.607  16.103  30.672  1.00 14.64    -0.271 OA
ATOM   1380  CB  PHE A  90      -21.397  17.140  28.126  1.00 10.55     0.073 C
ATOM   1383  CG  PHE A  90      -20.413  18.172  28.586  1.00 16.07    -0.056 A
ATOM   1384  CD1 PHE A  90      -19.051  17.974  28.523  1.00 13.09     0.007 A
ATOM   1386  CD2 PHE A  90      -20.874  19.385  29.093  1.00 14.29     0.007 A
ATOM   1388  CE1 PHE A  90      -18.144  18.946  28.936  1.00 10.69     0.001 A
ATOM   1390  CE2 PHE A  90      -19.993  20.352  29.514  1.00 15.27     0.001 A
ATOM   1392  CZ  PHE A  90      -18.611  20.167  29.408  1.00  9.79     0.000 A
ATOM   1394  N   ARG A  91      -20.413  15.484  30.860  1.00 13.42    -0.346 N
ATOM   1395  HN  ARG A  91      -19.585  15.185  30.344  1.00  0.00     0.163 HD
ATOM   1396  CA  ARG A  91      -20.338  15.567  32.316  1.00 14.37     0.176 C
ATOM   1398  C   ARG A  91      -21.164  14.487  33.010  1.00 17.18     0.241 C
ATOM   1399  O   ARG A  91      -21.354  14.635  34.198  1.00 13.96    -0.271 OA
ATOM   1400  CB  ARG A  91      -20.674  16.996  32.828  1.00 14.32     0.036 C
ATOM   1403  CG  ARG A  91      -19.540  17.999  32.566  1.00 12.06     0.023 C
ATOM   1406  CD  ARG A  91      -19.856  19.472  32.912  1.00 10.11     0.138 C
ATOM   1409  NE  ARG A  91      -18.562  20.157  32.830  1.00 12.66    -0.227 N
ATOM   1410  HE  ARG A  91      -18.157  20.299  31.905  1.00  0.00     0.177 HD
ATOM   1411  CZ  ARG A  91      -17.880  20.606  33.884  1.00 18.28     0.665 C
ATOM   1412  NH1 ARG A  91      -18.364  20.589  35.114  1.00 14.55    -0.235 N
ATOM   1413 1HH1 ARG A  91      -17.842  20.932  35.920  1.00  0.00     0.174 HD
ATOM   1414 2HH1 ARG A  91      -19.307  20.217  35.229  1.00  0.00     0.174 HD
ATOM   1415  NH2 ARG A  91      -16.658  21.088  33.735  1.00 14.14    -0.235 N
ATOM   1416 1HH2 ARG A  91      -16.136  21.431  34.541  1.00  0.00     0.174 HD
ATOM   1417 2HH2 ARG A  91      -16.285  21.101  32.786  1.00  0.00     0.174 HD
ATOM   1418  N   GLN A  92      -21.597  13.419  32.313  1.00 13.85    -0.346 N
ATOM   1419  HN  GLN A  92      -21.365  13.346  31.322  1.00  0.00     0.163 HD
ATOM   1420  CA  GLN A  92      -22.378  12.378  32.927  1.00 18.64     0.177 C
ATOM   1422  C   GLN A  92      -21.501  11.160  33.172  1.00 17.84     0.241 C
ATOM   1423  O   GLN A  92      -20.469  10.891  32.547  1.00 15.77    -0.271 OA
ATOM   1424  CB  GLN A  92      -23.610  12.032  32.050  1.00 15.45     0.044 C
ATOM   1427  CG  GLN A  92      -24.477  13.252  31.759  1.00 15.21     0.105 C
ATOM   1430  CD  GLN A  92      -24.880  14.033  32.990  1.00 24.89     0.215 C
ATOM   1431  NE2 GLN A  92      -24.578  15.328  33.038  1.00 20.85    -0.370 N
ATOM   1432 1HE2 GLN A  92      -24.850  15.855  33.868  1.00  0.00     0.159 HD
ATOM   1433 2HE2 GLN A  92      -24.104  15.813  32.277  1.00  0.00     0.159 HD
ATOM   1434  OE1 GLN A  92      -25.457  13.443  33.916  1.00 24.81    -0.274 OA
ATOM   1435  N   LEU A  93      -21.975  10.383  34.148  1.00 17.90    -0.346 N
ATOM   1436  HN  LEU A  93      -22.878  10.604  34.567  1.00  0.00     0.163 HD
ATOM   1437  CA  LEU A  93      -21.234   9.229  34.628  1.00 17.04     0.177 C
ATOM   1439  C   LEU A  93      -20.873   8.257  33.513  1.00 19.90     0.241 C
ATOM   1440  O   LEU A  93      -21.752   7.783  32.797  1.00 20.56    -0.271 OA
ATOM   1441  CB  LEU A  93      -22.082   8.455  35.658  1.00 20.20     0.038 C
ATOM   1444  CG  LEU A  93      -21.336   7.299  36.354  1.00 27.68    -0.020 C
ATOM   1446  CD1 LEU A  93      -20.213   7.788  37.260  1.00 26.98     0.009 C
ATOM   1450  CD2 LEU A  93      -22.354   6.520  37.169  1.00 31.78     0.009 C
ATOM   1454  N   HIS A  94      -19.585   7.996  33.411  1.00 15.74    -0.346 N
ATOM   1455  HN  HIS A  94      -18.956   8.467  34.062  1.00  0.00     0.163 HD
ATOM   1456  CA  HIS A  94      -18.992   7.089  32.442  1.00 22.79     0.182 C
ATOM   1458  C   HIS A  94      -19.117   7.534  30.981  1.00 23.93     0.241 C
ATOM   1459  O   HIS A  94      -18.852   6.678  30.103  1.00 22.02    -0.271 OA
ATOM   1460  CB  HIS A  94      -19.593   5.669  32.594  1.00 29.45     0.093 C
ATOM   1463  CG  HIS A  94      -19.329   5.073  33.952  1.00 37.17     0.028 A
ATOM   1464  CD2 HIS A  94      -18.266   5.255  34.782  1.00 34.78     0.114 A
ATOM   1466  ND1 HIS A  94      -20.207   4.219  34.589  1.00 39.10    -0.354 N
ATOM   1467  HD1 HIS A  94      -21.101   3.894  34.221  1.00  0.00     0.166 HD
ATOM   1468  CE1 HIS A  94      -19.688   3.898  35.754  1.00 40.95     0.180 A
ATOM   1470  NE2 HIS A  94      -18.513   4.501  35.892  1.00 45.40    -0.360 N
ATOM   1471  HE2 HIS A  94      -17.894   4.414  36.698  1.00  0.00     0.166 HD
ATOM   1472  N   SER A  95      -19.447   8.775  30.695  1.00 17.25    -0.344 N
ATOM   1473  HN  SER A  95      -19.658   9.432  31.446  1.00  0.00     0.163 HD
ATOM   1474  CA  SER A  95      -19.512   9.218  29.286  1.00 17.63     0.200 C
ATOM   1476  C   SER A  95      -18.086   9.391  28.786  1.00 20.69     0.243 C
ATOM   1477  O   SER A  95      -17.150   9.426  29.588  1.00 18.87    -0.271 OA
ATOM   1478  CB  SER A  95      -20.252  10.541  29.083  1.00 22.19     0.199 C
ATOM   1481  OG  SER A  95      -19.495  11.675  29.553  1.00 21.38    -0.398 OA
ATOM   1482  HG  SER A  95      -19.955  12.497  29.427  1.00  0.00     0.209 HD
ATOM   1483  N   LYS A  96      -17.899   9.551  27.463  1.00 16.46    -0.346 N
ATOM   1484  HN  LYS A  96      -18.705   9.495  26.840  1.00  0.00     0.163 HD
ATOM   1485  CA  LYS A  96      -16.591   9.800  26.895  1.00 15.03     0.176 C
ATOM   1487  C   LYS A  96      -16.359  11.308  26.810  1.00 12.93     0.241 C
ATOM   1488  O   LYS A  96      -15.377  11.751  26.201  1.00 16.04    -0.271 OA
ATOM   1489  CB  LYS A  96      -16.448   9.209  25.485  1.00 20.66     0.035 C
ATOM   1492  CG  LYS A  96      -16.269   7.680  25.529  1.00 26.34     0.004 C
ATOM   1495  CD  LYS A  96      -16.411   7.162  24.106  1.00 41.14     0.027 C
ATOM   1498  CE  LYS A  96      -16.249   5.663  23.960  1.00 58.32     0.229 C
ATOM   1501  NZ  LYS A  96      -16.155   5.270  22.515  1.00 66.48    -0.079 N
ATOM   1502  HZ1 LYS A  96      -16.046   4.261  22.417  1.00  0.00     0.274 HD
ATOM   1503  HZ2 LYS A  96      -15.412   5.777  22.035  1.00  0.00     0.274 HD
ATOM   1504  HZ3 LYS A  96      -16.950   5.616  21.979  1.00  0.00     0.274 HD
ATOM   1505  N   THR A  97      -17.165  12.121  27.493  1.00 11.31    -0.344 N
ATOM   1506  HN  THR A  97      -17.946  11.716  28.009  1.00  0.00     0.163 HD
ATOM   1507  CA  THR A  97      -16.973  13.579  27.532  1.00 10.67     0.205 C
ATOM   1509  C   THR A  97      -16.965  14.119  28.959  1.00 13.11     0.246 C
ATOM   1510  O   THR A  97      -17.876  14.851  29.332  1.00 12.24    -0.271 OA
ATOM   1511  CB  THR A  97      -18.095  14.255  26.705  1.00 13.34     0.146 C
ATOM   1513  CG2 THR A  97      -17.956  13.972  25.197  1.00 11.61     0.042 C
ATOM   1517  OG1 THR A  97      -19.322  13.638  27.151  1.00 14.71    -0.393 OA
ATOM   1518  HG1 THR A  97      -19.408  13.813  28.081  1.00  0.00     0.210 HD
ATOM   1519  N   PRO A  98      -15.982  13.761  29.786  1.00 13.41    -0.337 N
ATOM   1520  CA  PRO A  98      -15.854  14.293  31.132  1.00 16.06     0.179 C
ATOM   1522  C   PRO A  98      -15.731  15.813  31.122  1.00 14.47     0.241 C
ATOM   1523  O   PRO A  98      -15.349  16.425  30.109  1.00 12.83    -0.271 OA
ATOM   1524  CB  PRO A  98      -14.562  13.648  31.651  1.00 15.41     0.037 C
ATOM   1527  CG  PRO A  98      -13.796  13.159  30.469  1.00 12.80     0.022 C
ATOM   1530  CD  PRO A  98      -14.817  12.945  29.361  1.00 12.16     0.127 C
ATOM   1533  N   GLY A  99      -15.973  16.438  32.277  1.00 13.44    -0.351 N
ATOM   1534  HN  GLY A  99      -16.233  15.874  33.086  1.00  0.00     0.163 HD
ATOM   1535  CA  GLY A  99      -15.885  17.890  32.445  1.00 14.61     0.225 C
ATOM   1538  C   GLY A  99      -14.572  18.494  31.984  1.00 12.48     0.236 C
ATOM   1539  O   GLY A  99      -14.565  19.581  31.394  1.00 13.49    -0.272 OA
ATOM   1540  N   HIS A 100      -13.424  17.903  32.198  1.00 11.47    -0.346 N
ATOM   1541  HN  HIS A 100      -13.429  17.074  32.792  1.00  0.00     0.163 HD
ATOM   1542  CA  HIS A 100      -12.126  18.336  31.653  1.00 14.08     0.182 C
ATOM   1544  C   HIS A 100      -11.644  17.176  30.781  1.00 10.34     0.243 C
ATOM   1545  O   HIS A 100      -11.951  16.014  31.122  1.00 12.69    -0.271 OA
ATOM   1546  CB  HIS A 100      -11.165  18.679  32.822  1.00 13.11     0.093 C
ATOM   1549  CG  HIS A 100      -11.691  19.915  33.523  1.00 13.19     0.028 A
ATOM   1550  CD2 HIS A 100      -11.421  21.219  33.269  1.00 16.87     0.114 A
ATOM   1552  ND1 HIS A 100      -12.588  19.883  34.570  1.00 16.47    -0.354 N
ATOM   1553  HD1 HIS A 100      -12.980  19.043  34.995  1.00  0.00     0.166 HD
ATOM   1554  CE1 HIS A 100      -12.855  21.139  34.932  1.00 17.82     0.180 A
ATOM   1556  NE2 HIS A 100      -12.156  21.976  34.176  1.00 16.45    -0.360 N
ATOM   1557  HE2 HIS A 100      -12.157  22.994  34.247  1.00  0.00     0.166 HD
ATOM   1558  N   PRO A 101      -10.946  17.436  29.708  1.00 11.83    -0.337 N
ATOM   1559  CA  PRO A 101      -10.527  16.350  28.779  1.00 14.07     0.179 C
ATOM   1561  C   PRO A 101       -9.566  15.396  29.442  1.00 14.39     0.241 C
ATOM   1562  O   PRO A 101       -8.655  15.836  30.187  1.00 12.76    -0.271 OA
ATOM   1563  CB  PRO A 101       -9.849  17.091  27.620  1.00 14.79     0.037 C
ATOM   1566  CG  PRO A 101      -10.339  18.512  27.700  1.00 13.66     0.022 C
ATOM   1569  CD  PRO A 101      -10.423  18.739  29.227  1.00 11.97     0.127 C
ATOM   1572  N   GLU A 102       -9.693  14.103  29.183  1.00 13.12    -0.346 N
ATOM   1573  HN  GLU A 102      -10.403  13.790  28.521  1.00  0.00     0.163 HD
ATOM   1574  CA  GLU A 102       -8.825  13.114  29.837  1.00 14.69     0.177 C
ATOM   1576  C   GLU A 102       -8.136  12.224  28.811  1.00 15.49     0.241 C
ATOM   1577  O   GLU A 102       -8.829  11.561  28.032  1.00 15.05    -0.271 OA
ATOM   1578  CB  GLU A 102       -9.653  12.237  30.791  1.00 12.30     0.045 C
ATOM   1581  CG  GLU A 102      -10.123  12.964  32.066  1.00 13.89     0.116 C
ATOM   1584  CD  GLU A 102      -11.025  12.078  32.922  1.00 21.60     0.172 C
ATOM   1585  OE1 GLU A 102      -10.842  10.834  32.945  1.00 21.59    -0.648 OA
ATOM   1586  OE2 GLU A 102      -11.969  12.559  33.570  1.00 14.39    -0.648 OA
ATOM   1587  N   VAL A 103       -6.798  12.171  28.853  1.00 12.86    -0.346 N
ATOM   1588  HN  VAL A 103       -6.278  12.703  29.551  1.00  0.00     0.163 HD
ATOM   1589  CA  VAL A 103       -6.094  11.332  27.875  1.00 13.93     0.180 C
ATOM   1591  C   VAL A 103       -6.405   9.874  28.168  1.00 19.82     0.241 C
ATOM   1592  O   VAL A 103       -6.623   9.460  29.310  1.00 16.95    -0.271 OA
ATOM   1593  CB  VAL A 103       -4.589  11.600  27.828  1.00 10.98     0.009 C
ATOM   1595  CG1 VAL A 103       -3.943  11.307  29.214  1.00  9.81     0.012 C
ATOM   1599  CG2 VAL A 103       -3.829  10.794  26.769  1.00 11.07     0.012 C
ATOM   1603  N   GLY A 104       -6.521   9.055  27.105  1.00 19.18    -0.351 N
ATOM   1604  HN  GLY A 104       -6.459   9.412  26.152  1.00  0.00     0.163 HD
ATOM   1605  CA  GLY A 104       -6.742   7.615  27.374  1.00 26.64     0.225 C
ATOM   1608  C   GLY A 104       -8.215   7.265  27.437  1.00 30.52     0.236 C
ATOM   1609  O   GLY A 104       -8.560   6.093  27.256  1.00 35.87    -0.272 OA
ATOM   1610  N   LYS A 105       -9.109   8.211  27.698  1.00 27.53    -0.346 N
ATOM   1611  HN  LYS A 105       -8.786   9.170  27.829  1.00  0.00     0.163 HD
ATOM   1612  CA  LYS A 105      -10.525   7.932  27.803  1.00 28.83     0.176 C
ATOM   1614  C   LYS A 105      -11.274   8.298  26.523  1.00 28.78     0.241 C
ATOM   1615  O   LYS A 105      -12.312   7.702  26.233  1.00 32.72    -0.271 OA
ATOM   1616  CB  LYS A 105      -11.123   8.692  28.996  1.00 34.12     0.035 C
ATOM   1619  CG  LYS A 105      -12.627   8.575  29.106  1.00 42.67     0.004 C
ATOM   1622  CD  LYS A 105      -13.279   9.209  30.302  1.00 46.51     0.027 C
ATOM   1625  CE  LYS A 105      -14.067   8.247  31.168  1.00 62.44     0.229 C
ATOM   1628  NZ  LYS A 105      -15.032   7.365  30.452  1.00 44.66    -0.079 N
ATOM   1629  HZ1 LYS A 105      -15.562   6.717  31.035  1.00  0.00     0.274 HD
ATOM   1630  HZ2 LYS A 105      -14.550   6.852  29.714  1.00  0.00     0.274 HD
ATOM   1631  HZ3 LYS A 105      -15.671   7.932  29.894  1.00  0.00     0.274 HD
ATOM   1632  N   THR A 106      -10.869   9.373  25.861  1.00 19.56    -0.344 N
ATOM   1633  HN  THR A 106      -10.043   9.870  26.194  1.00  0.00     0.163 HD
ATOM   1634  CA  THR A 106      -11.557   9.874  24.675  1.00 17.16     0.205 C
ATOM   1636  C   THR A 106      -10.574   9.857  23.506  1.00 20.18     0.243 C
ATOM   1637  O   THR A 106       -9.462  10.361  23.704  1.00 14.89    -0.271 OA
ATOM   1638  CB  THR A 106      -11.987  11.329  24.943  1.00 19.70     0.146 C
ATOM   1640  CG2 THR A 106      -12.700  11.910  23.733  1.00 16.10     0.042 C
ATOM   1644  OG1 THR A 106      -12.786  11.361  26.143  1.00 18.94    -0.393 OA
ATOM   1645  HG1 THR A 106      -13.051  12.258  26.308  1.00  0.00     0.210 HD
ATOM   1646  N   ALA A 107      -10.968   9.277  22.373  1.00 17.59    -0.346 N
ATOM   1647  HN  ALA A 107      -11.900   8.873  22.281  1.00  0.00     0.163 HD
ATOM   1648  CA  ALA A 107      -10.002   9.242  21.256  1.00 18.18     0.172 C
ATOM   1650  C   ALA A 107       -9.603  10.629  20.800  1.00 15.21     0.240 C
ATOM   1651  O   ALA A 107      -10.495  11.454  20.598  1.00 16.20    -0.271 OA
ATOM   1652  CB  ALA A 107      -10.632   8.488  20.084  1.00 20.31     0.042 C
ATOM   1656  N   GLY A 108       -8.330  10.892  20.491  1.00 14.32    -0.351 N
ATOM   1657  HN  GLY A 108       -7.626  10.164  20.611  1.00  0.00     0.163 HD
ATOM   1658  CA  GLY A 108       -7.926  12.205  19.984  1.00 14.66     0.225 C
ATOM   1661  C   GLY A 108       -7.448  13.185  21.057  1.00 13.06     0.236 C
ATOM   1662  O   GLY A 108       -6.813  14.181  20.739  1.00 17.47    -0.272 OA
ATOM   1663  N   VAL A 109       -7.699  12.890  22.341  1.00  8.78    -0.346 N
ATOM   1664  HN  VAL A 109       -8.164  12.017  22.591  1.00  0.00     0.163 HD
ATOM   1665  CA  VAL A 109       -7.284  13.865  23.404  1.00  8.88     0.180 C
ATOM   1667  C   VAL A 109       -5.854  13.551  23.724  1.00  9.71     0.241 C
ATOM   1668  O   VAL A 109       -5.547  12.366  23.999  1.00 12.33    -0.271 OA
ATOM   1669  CB  VAL A 109       -8.121  13.713  24.687  1.00 16.86     0.009 C
ATOM   1671  CG1 VAL A 109       -7.582  14.605  25.834  1.00  8.95     0.012 C
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ATOM   1675  CG2 VAL A 109      -9.564  14.151  24.403  1.00 18.88      0.012 C
ATOM   1679  N   GLU A 110      -4.966  14.510  23.704  1.00  8.37     -0.346 N
ATOM   1680  HN  GLU A 110      -5.272  15.474  23.571  1.00  0.00      0.163 HD
ATOM   1681  CA  GLU A 110      -3.551  14.225  23.868  1.00  8.29      0.177 C
ATOM   1683  C   GLU A 110      -3.034  14.299  25.311  1.00 10.37      0.241 C
ATOM   1684  O   GLU A 110      -1.928  13.774  25.531  1.00  8.93     -0.271 OA
ATOM   1685  CB  GLU A 110      -2.698  15.211  23.051  1.00 10.73      0.045 C
ATOM   1688  CG  GLU A 110      -3.043  15.176  21.571  1.00 12.30      0.116 C
ATOM   1691  CD  GLU A 110      -2.464  13.956  20.849  1.00 15.38      0.172 C
ATOM   1692  OE1 GLU A 110      -1.694  13.147  21.416  1.00 17.17     -0.648 OA
ATOM   1693  OE2 GLU A 110      -2.720  13.803  19.636  1.00 13.92     -0.648 OA
ATOM   1694  N   THR A 111      -3.707  15.013  26.179  1.00 11.58     -0.344 N
ATOM   1695  HN  THR A 111      -4.544  15.518  25.889  1.00  0.00      0.163 HD
ATOM   1696  CA  THR A 111      -3.244  15.081  27.581  1.00  7.50      0.205 C
ATOM   1698  C   THR A 111      -4.454  15.424  28.434  1.00 12.85      0.243 C
ATOM   1699  O   THR A 111      -5.477  15.864  27.864  1.00 12.90     -0.271 OA
ATOM   1700  CB  THR A 111      -2.154  16.202  27.702  1.00  9.38      0.146 C
ATOM   1702  CG2 THR A 111      -2.687  17.562  27.296  1.00 12.60      0.042 C
ATOM   1706  OG1 THR A 111      -1.724  16.247  29.071  1.00  9.38     -0.393 OA
ATOM   1707  HG1 THR A 111      -1.391  15.396  29.331  1.00  0.00      0.210 HD
ATOM   1708  N   THR A 112      -4.359  15.293  29.743  1.00 11.01     -0.344 N
ATOM   1709  HN  THR A 112      -3.488  14.937  30.127  1.00  0.00      0.163 HD
ATOM   1710  CA  THR A 112      -5.453  15.638  30.655  1.00  6.81      0.205 C
ATOM   1712  C   THR A 112      -5.205  17.049  31.181  1.00 10.02      0.243 C
ATOM   1713  O   THR A 112      -4.117  17.290  31.729  1.00 10.79     -0.271 OA
ATOM   1714  CB  THR A 112      -5.480  14.621  31.814  1.00 11.08      0.146 C
ATOM   1716  CG2 THR A 112      -6.590  14.930  32.853  1.00  9.01      0.042 C
ATOM   1720  OG1 THR A 112      -5.714  13.335  31.219  1.00 11.37     -0.393 OA
ATOM   1721  HG1 THR A 112      -5.731  12.709  31.933  1.00  0.00      0.210 HD
ATOM   1722  N   THR A 113      -6.085  18.001  30.923  1.00  9.23     -0.344 N
ATOM   1723  HN  THR A 113      -6.917  17.791  30.371  1.00  0.00      0.163 HD
ATOM   1724  CA  THR A 113      -5.864  19.363  31.432  1.00 10.49      0.205 C
ATOM   1726  C   THR A 113      -7.007  19.744  32.363  1.00 14.37      0.243 C
ATOM   1727  O   THR A 113      -7.807  18.899  32.768  1.00 13.98     -0.271 OA
ATOM   1728  CB  THR A 113      -5.717  20.424  30.314  1.00 16.53      0.146 C
ATOM   1730  CG2 THR A 113      -4.436  20.167  29.530  1.00 18.60      0.042 C
ATOM   1734  OG1 THR A 113      -6.817  20.265  29.438  1.00 11.67     -0.393 OA
ATOM   1735  HG1 THR A 113      -7.616  20.425  29.927  1.00  0.00      0.210 HD
ATOM   1736  N   GLY A 114      -6.945  20.984  32.892  1.00 11.31     -0.350 N
ATOM   1737  HN  GLY A 114      -6.294  21.690  32.548  1.00  0.00      0.163 HD
ATOM   1738  CA  GLY A 114      -7.892  21.253  34.014  1.00 11.24      0.225 C
ATOM   1741  C   GLY A 114      -7.105  22.094  35.021  1.00 11.30      0.238 C
ATOM   1742  O   GLY A 114      -7.468  23.242  35.281  1.00 15.12     -0.272 OA
ATOM   1743  N   PRO A 115      -6.001  21.583  35.508  1.00 11.22     -0.337 N
ATOM   1744  CA  PRO A 115      -5.127  22.357  36.400  1.00  9.73      0.179 C
ATOM   1746  C   PRO A 115      -4.438  23.348  35.459  1.00  9.86      0.241 C
ATOM   1747  O   PRO A 115      -3.598  23.011  34.614  1.00  9.23     -0.271 OA
ATOM   1748  CB  PRO A 115      -4.167  21.344  36.996  1.00 13.48      0.037 C
ATOM   1751  CG  PRO A 115      -4.834  20.016  36.755  1.00 16.18      0.022 C
ATOM   1754  CD  PRO A 115      -5.481  20.192  35.377  1.00 13.81      0.127 C
ATOM   1757  N   LEU A 116      -4.710  24.638  35.694  1.00 11.56     -0.346 N
ATOM   1758  HN  LEU A 116      -5.299  24.920  36.478  1.00  0.00      0.163 HD
ATOM   1759  CA  LEU A 116      -4.125  25.640  34.774  1.00  9.43      0.177 C
ATOM   1761  C   LEU A 116      -2.619  25.701  34.754  1.00 12.04      0.240 C
ATOM   1762  O   LEU A 116      -1.921  25.502  35.718  1.00  9.81     -0.271 OA
ATOM   1763  CB  LEU A 116      -4.666  27.044  35.107  1.00 12.13      0.038 C
ATOM   1766  CG  LEU A 116      -6.177  27.172  34.897  1.00 11.40     -0.020 C
ATOM   1768  CD1 LEU A 116      -6.706  28.453  35.558  1.00 14.19      0.009 C
ATOM   1772  CD2 LEU A 116      -6.517  27.214  33.397  1.00 14.26      0.009 C
ATOM   1776  N   GLY A 117      -2.061  25.971  33.560  1.00  7.72     -0.351 N
ATOM   1777  HN  GLY A 117      -2.690  26.099  32.767  1.00  0.00      0.163 HD
ATOM   1778  CA  GLY A 117      -0.655  26.094  33.311  1.00  7.73      0.225 C
ATOM   1781  C   GLY A 117       0.018  24.786  32.884  1.00  9.08      0.236 C
ATOM   1782  O   GLY A 117       1.071  24.815  32.244  1.00  7.63     -0.272 OA
ATOM   1783  N   GLN A 118      -0.537  23.616  33.255  1.00  8.47     -0.346 N
ATOM   1784  HN  GLN A 118      -1.424  23.603  33.758  1.00  0.00      0.163 HD
ATOM   1785  CA  GLN A 118       0.144  22.366  32.930  1.00  8.38      0.177 C
ATOM   1787  C   GLN A 118      -0.012  21.975  31.466  1.00  9.23      0.240 C
ATOM   1788  O   GLN A 118       0.894  21.305  30.983  1.00  7.19     -0.271 OA
ATOM   1789  CB  GLN A 118      -0.356  21.233  33.884  1.00  7.84      0.044 C
ATOM   1792  CG  GLN A 118       0.278  21.528  35.261  1.00 12.83      0.105 C
ATOM   1795  CD  GLN A 118       0.101  20.359  36.227  1.00 10.13      0.215 C
ATOM   1796  NE2 GLN A 118      -0.640  20.557  37.298  1.00 10.48     -0.370 N
ATOM   1797 1HE2 GLN A 118      -0.758  19.776  37.943  1.00  0.00      0.159 HD
ATOM   1798 2HE2 GLN A 118      -1.075  21.455  37.508  1.00  0.00      0.159 HD
ATOM   1799  OE1 GLN A 118       0.619  19.290  35.977  1.00  8.02     -0.274 OA
ATOM   1800  N   GLY A 119      -1.099  22.368  30.804  1.00  8.20     -0.351 N
ATOM   1801  HN  GLY A 119      -1.828  22.893  31.288  1.00  0.00      0.163 HD
ATOM   1802  CA  GLY A 119      -1.253  22.044  29.362  1.00  8.80      0.225 C
ATOM   1805  C   GLY A 119      -0.070  22.595  28.546  1.00  8.46      0.236 C
ATOM   1806  O   GLY A 119       0.557  21.882  27.756  1.00 10.07     -0.272 OA
ATOM   1807  N   ILE A 120       0.202  23.899  28.681  1.00  5.96     -0.346 N
ATOM   1808  HN  ILE A 120      -0.377  24.476  29.291  1.00  0.00      0.163 HD
ATOM   1809  CA  ILE A 120       1.337  24.510  27.951  1.00  5.07      0.180 C
ATOM   1811  C   ILE A 120       2.638  23.857  28.379  1.00  8.58      0.241 C
ATOM   1812  O   ILE A 120       3.504  23.597  27.499  1.00  7.18     -0.271 OA
ATOM   1813  CB  ILE A 120       1.389  26.040  28.103  1.00 10.35      0.013 C
ATOM   1815  CG1 ILE A 120       2.539  26.686  27.295  1.00 11.52      0.002 C
ATOM   1818  CG2 ILE A 120       1.583  26.443  29.579  1.00 12.28      0.012 C
ATOM   1822  CD1 ILE A 120       2.300  26.486  25.777  1.00 13.71      0.005 C
ATOM   1826  N   ALA A 121       2.815  23.443  29.650  1.00  5.65     -0.346 N
ATOM   1827  HN  ALA A 121       2.104  23.645  30.353  1.00  0.00      0.163 HD
ATOM   1828  CA  ALA A 121       4.013  22.710  30.024  1.00  6.82      0.172 C
ATOM   1830  C   ALA A 121       4.122  21.388  29.255  1.00  5.93      0.240 C
ATOM   1831  O   ALA A 121       5.222  20.986  28.795  1.00  6.65     -0.271 OA
ATOM   1832  CB  ALA A 121       4.031  22.432  31.533  1.00  5.61      0.042 C
ATOM   1836  N   ASN A 122       3.037  20.621  29.154  1.00  5.84     -0.346 N
ATOM   1837  HN  ASN A 122       2.167  20.927  29.589  1.00  0.00      0.163 HD
ATOM   1838  CA  ASN A 122       3.069  19.356  28.436  1.00  4.90      0.185 C
ATOM   1840  C   ASN A 122       3.373  19.611  26.939  1.00  5.17      0.241 C
ATOM   1841  O   ASN A 122       4.079  18.853  26.302  1.00 10.07     -0.271 OA
ATOM   1842  CB  ASN A 122       1.679  18.719  28.515  1.00  4.40      0.137 C
ATOM   1845  CG  ASN A 122       1.184  18.300  29.877  1.00  8.47      0.217 C
ATOM   1846  ND2 ASN A 122       2.030  18.159  30.874  1.00  8.06     -0.370 N
ATOM   1847 1HD2 ASN A 122       3.030  18.313  30.743  1.00  0.00      0.159 HD
ATOM   1848 2HD2 ASN A 122       1.695  17.876  31.795  1.00  0.00      0.159 HD
ATOM   1849  OD1 ASN A 122      -0.053  18.109  30.039  1.00 10.98     -0.274 OA
ATOM   1850  N   ALA A 123       2.809  20.710  26.412  1.00  6.66     -0.346 N
ATOM   1851  HN  ALA A 123       2.223  21.325  26.977  1.00  0.00      0.163 HD
ATOM   1852  CA  ALA A 123       3.070  21.001  24.970  1.00  8.26      0.172 C
ATOM   1854  C   ALA A 123       4.532  21.257  24.737  1.00  7.20      0.240 C
ATOM   1855  O   ALA A 123       5.163  20.875  23.743  1.00  5.32     -0.271 OA
ATOM   1856  CB  ALA A 123       2.219  22.200  24.543  1.00  6.72      0.042 C
ATOM   1860  N   VAL A 124       5.187  21.994  25.674  1.00  8.91     -0.346 N
ATOM   1861  HN  VAL A 124       4.665  22.383  26.459  1.00  0.00      0.163 HD
ATOM   1862  CA  VAL A 124       6.628  22.239  25.576  1.00  7.25      0.180 C
ATOM   1864  C   VAL A 124       7.323  20.876  25.612  1.00  5.09      0.241 C
ATOM   1865  O   VAL A 124       8.239  20.690  24.810  1.00  8.51     -0.271 OA
ATOM   1866  CB  VAL A 124       7.165  23.198  26.660  1.00  6.81      0.009 C
ATOM   1868  CG1 VAL A 124       8.665  23.161  26.861  1.00  5.33      0.012 C
ATOM   1872  CG2 VAL A 124       6.717  24.667  26.447  1.00  5.73      0.012 C
ATOM   1876  N   GLY A 125       6.904  19.927  26.455  1.00  7.41     -0.351 N
ATOM   1877  HN  GLY A 125       6.135  20.113  27.099  1.00  0.00      0.163 HD
ATOM   1878  CA  GLY A 125       7.570  18.596  26.446  1.00  4.89      0.225 C
ATOM   1881  C   GLY A 125       7.298  17.886  25.128  1.00  7.10      0.236 C
ATOM   1882  O   GLY A 125       8.247  17.224  24.636  1.00  8.18     -0.272 OA
ATOM   1883  N   MET A 126       6.109  18.022  24.557  1.00  6.29     -0.346 N
ATOM   1884  HN  MET A 126       5.381  18.576  25.009  1.00  0.00      0.163 HD
ATOM   1885  CA  MET A 126       5.852  17.353  23.253  1.00  6.11      0.177 C
ATOM   1887  C   MET A 126       6.756  17.930  22.163  1.00 11.07      0.241 C
ATOM   1888  O   MET A 126       7.196  17.175  21.320  1.00  7.53     -0.271 OA
ATOM   1889  CB  MET A 126       4.374  17.570  22.799  1.00  5.45      0.045 C
ATOM   1892  CG  MET A 126       3.527  16.659  23.748  1.00  5.84      0.076 C
ATOM   1895  SD  MET A 126       1.781  17.111  23.526  1.00 12.50     -0.173 SA
ATOM   1896  CE  MET A 126       1.017  16.109  24.792  1.00 15.85      0.089 C
ATOM   1900  N   ALA A 127       6.939  19.229  22.148  1.00  7.63     -0.346 N
ATOM   1901  HN  ALA A 127       6.458  19.822  22.841  1.00  0.00      0.163 HD
ATOM   1902  CA  ALA A 127       7.808  19.901  21.169  1.00  9.40      0.172 C
ATOM   1904  C   ALA A 127       9.274  19.512  21.363  1.00  9.08      0.240 C
ATOM   1905  O   ALA A 127      10.017  19.268  20.407  1.00  7.10     -0.271 OA
ATOM   1906  CB  ALA A 127       7.646  21.427  21.277  1.00  7.16      0.042 C
ATOM   1910  N   ILE A 128       9.732  19.349  22.602  1.00  5.82     -0.346 N
ATOM   1911  HN  ILE A 128       9.117  19.582  23.382  1.00  0.00      0.163 HD
ATOM   1912  CA  ILE A 128      11.086  18.847  22.901  1.00  8.30      0.180 C
ATOM   1914  C   ILE A 128      11.242  17.433  22.340  1.00  6.64      0.241 C
ATOM   1915  O   ILE A 128      12.279  17.113  21.748  1.00  8.37     -0.271 OA
ATOM   1916  CB  ILE A 128      11.440  18.857  24.400  1.00  8.89      0.013 C
ATOM   1918  CG1 ILE A 128      11.679  20.350  24.817  1.00 11.19      0.002 C
ATOM   1921  CG2 ILE A 128      12.701  18.053  24.679  1.00  8.89      0.012 C
ATOM   1925  CD1 ILE A 128      11.737  20.528  26.362  1.00  8.38      0.005 C
ATOM   1929  N   ALA A 129      10.247  16.589  22.611  1.00  6.53     -0.346 N
ATOM   1930  HN  ALA A 129       9.445  16.904  23.157  1.00  0.00      0.163 HD
ATOM   1931  CA  ALA A 129      10.306  15.209  22.215  1.00  7.53      0.172 C
ATOM   1933  C   ALA A 129      10.370  15.156  20.593  1.00 10.81      0.240 C
ATOM   1934  O   ALA A 129      11.209  14.415  20.072  1.00  8.40     -0.271 OA
ATOM   1935  CB  ALA A 129       9.085  14.425  22.633  1.00  8.82      0.042 C
ATOM   1939  N   GLU A 130       9.532  15.946  19.912  1.00  7.72     -0.346 N
ATOM   1940  HN  GLU A 130       8.889  16.578  20.390  1.00  0.00      0.163 HD
ATOM   1941  CA  GLU A 130       9.579  15.862  18.411  1.00  4.91      0.177 C
ATOM   1943  C   GLU A 130      10.957  16.287  17.933  1.00  8.89      0.241 C
ATOM   1944  O   GLU A 130      11.580  15.685  17.026  1.00  9.52     -0.271 OA
ATOM   1945  CB  GLU A 130       8.534  16.780  17.802  1.00 12.41      0.045 C
ATOM   1948  CG  GLU A 130       8.345  16.714  16.274  1.00  8.28      0.116 C
ATOM   1951  CD  GLU A 130       9.254  17.621  15.458  1.00  9.16      0.172 C
ATOM   1952  OE1 GLU A 130       9.987  18.499  15.963  1.00  8.22     -0.648 OA
ATOM   1953  OE2 GLU A 130       9.185  17.520  14.189  1.00  9.68     -0.648 OA
ATOM   1954  N   LYS A 131      11.466  17.393  18.515  1.00  7.87     -0.346 N
ATOM   1955  HN  LYS A 131      10.965  17.864  19.269  1.00  0.00      0.163 HD
ATOM   1956  CA  LYS A 131      12.762  17.905  18.036  1.00  9.19      0.176 C
ATOM   1958  C   LYS A 131      13.891  16.922  18.234  1.00 12.41      0.241 C
ATOM   1959  O   LYS A 131      14.817  16.803  17.420  1.00  9.79     -0.271 OA
ATOM   1960  CB  LYS A 131      13.102  19.219  18.790  1.00  8.27      0.035 C
ATOM   1963  CG  LYS A 131      14.413  19.865  18.280  1.00  9.70      0.004 C
ATOM   1966  CD  LYS A 131      14.714  21.136  19.105  1.00 13.10      0.027 C
ATOM   1969  CE  LYS A 131      16.018  21.754  18.604  1.00 21.99      0.229 C
ATOM   1972  NZ  LYS A 131      16.597  22.728  19.578  1.00 20.40     -0.079 N
ATOM   1973  HZ1 LYS A 131      17.468  23.141  19.243  1.00  0.00      0.274 HD
ATOM   1974  HZ2 LYS A 131      16.721  22.301  20.496  1.00  0.00      0.274 HD
ATOM   1975  HZ3 LYS A 131      15.919  23.449  19.824  1.00  0.00      0.274 HD
ATOM   1976  N   THR A 132      13.942  16.293  19.410  1.00  7.58     -0.344 N
ATOM   1977  HN  THR A 132      13.205  16.481  20.090  1.00  0.00      0.163 HD
ATOM   1978  CA  THR A 132      14.992  15.353  19.775  1.00  6.13      0.205 C
ATOM   1980  C   THR A 132      14.833  14.076  18.946  1.00 10.36      0.243 C
ATOM   1981  O   THR A 132      15.831  13.521  18.479  1.00 10.08     -0.271 OA
ATOM   1982  CB  THR A 132      14.888  15.011  21.287  1.00  9.92      0.146 C
ATOM   1984  CG2 THR A 132      16.005  14.080  21.742  1.00 13.48      0.042 C
ATOM   1988  OG1 THR A 132      14.955  16.251  22.042  1.00  9.06     -0.393 OA
ATOM   1989  HG1 THR A 132      14.891  16.042  22.967  1.00  0.00      0.210 HD
ATOM   1990  N   LEU A 133      13.633  13.584  18.780  1.00  7.76     -0.346 N
ATOM   1991  HN  LEU A 133      12.837  14.064  19.201  1.00  0.00      0.163 HD
ATOM   1992  CA  LEU A 133      13.397  12.346  17.996  1.00 11.23      0.177 C
ATOM   1994  C   LEU A 133      13.751  12.588  16.527  1.00 11.69      0.241 C
ATOM   1995  O   LEU A 133      14.407  11.752  15.910  1.00 11.37     -0.271 OA
ATOM   1996  CB  LEU A 133      11.914  11.943  18.195  1.00 10.57      0.038 C
ATOM   1999  CG  LEU A 133      11.610  10.441  17.948  1.00 20.58     -0.020 C
ATOM   2001  CD1 LEU A 133      12.251   9.580  19.029  1.00  7.57      0.009 C
ATOM   2005  CD2 LEU A 133      10.099  10.278  17.821  1.00 23.22      0.009 C
ATOM   2009  N   ALA A 134      13.391  13.762  15.988  1.00  7.25     -0.346 N
ATOM   2010  HN  ALA A 134      12.840  14.429  16.529  1.00  0.00      0.163 HD
ATOM   2011  CA  ALA A 134      13.800  14.082  14.601  1.00 10.60      0.172 C
ATOM   2013  C   ALA A 134      15.324  14.101  14.474  1.00 10.72      0.240 C
ATOM   2014  O   ALA A 134      15.878  13.510  13.532  1.00 11.59     -0.271 OA
ATOM   2015  CB  ALA A 134      13.236  15.446  14.174  1.00  6.97      0.042 C
ATOM   2019  N   ALA A 135      16.058  14.711  15.427  1.00  8.65     -0.346 N
ATOM   2020  HN  ALA A 135      15.566  15.152  16.204  1.00  0.00      0.163 HD
ATOM   2021  CA  ALA A 135      17.486  14.775  15.412  1.00 11.98      0.172 C
ATOM   2023  C   ALA A 135      18.078  13.383  15.532  1.00 11.95      0.240 C
ATOM   2024  O   ALA A 135      19.148  13.130  14.949  1.00 11.41     -0.271 OA
ATOM   2025  CB  ALA A 135      18.075  15.727  16.482  1.00  7.09      0.042 C
ATOM   2029  N   GLN A 136      17.523  12.477  16.315  1.00  7.19     -0.346 N
ATOM   2030  HN  GLN A 136      16.691  12.738  16.844  1.00  0.00      0.163 HD
ATOM   2031  CA  GLN A 136      18.035  11.135  16.461  1.00 10.52      0.177 C
ATOM   2033  C   GLN A 136      17.744  10.250  15.245  1.00 12.42      0.241 C
ATOM   2034  O   GLN A 136      18.594   9.391  14.978  1.00 14.14     -0.271 OA
ATOM   2035  CB  GLN A 136      17.464  10.414  17.701  1.00  9.03      0.044 C
ATOM   2038  CG  GLN A 136      18.074  11.084  18.974  1.00 12.63      0.105 C
ATOM   2041  CD  GLN A 136      17.504  10.498  20.268  1.00 14.13      0.215 C
ATOM   2042  NE2 GLN A 136      17.833  11.064  21.431  1.00 11.27     -0.370 N
ATOM   2043 1HE2 GLN A 136      17.453  10.673  22.293  1.00  0.00      0.159 HD
ATOM   2044 2HE2 GLN A 136      18.476  11.856  21.449  1.00  0.00      0.159 HD
ATOM   2045  OE1 GLN A 136      16.739   9.555  20.247  1.00 13.25     -0.274 OA
ATOM   2046  N   PHE A 137      16.602  10.460  14.583  1.00  9.23     -0.346 N
ATOM   2047  HN  PHE A 137      16.016  11.274  14.769  1.00  0.00      0.163 HD
ATOM   2048  CA  PHE A 137      16.234   9.457  13.574  1.00 11.01      0.180 C
ATOM   2050  C   PHE A 137      16.193   9.955  12.135  1.00 12.41      0.241 C
ATOM   2051  O   PHE A 137      16.315   9.086  11.286  1.00 14.20     -0.271 OA
ATOM   2052  CB  PHE A 137      14.829   8.898  13.907  1.00 10.89      0.073 C
ATOM   2055  CG  PHE A 137      14.926   7.903  15.045  1.00 14.57     -0.056 A
ATOM   2056  CD1 PHE A 137      15.343   6.610  14.791  1.00 13.54      0.007 A
ATOM   2058  CD2 PHE A 137      14.672   8.288  16.348  1.00 13.94      0.007 A
ATOM   2060  CE1 PHE A 137      15.457   5.673  15.798  1.00 18.07      0.001 A
ATOM   2062  CE2 PHE A 137      14.782   7.366  17.389  1.00 16.46      0.001 A
ATOM   2064  CZ  PHE A 137      15.161   6.060  17.090  1.00 11.57      0.000 A
ATOM   2066  N   ASN A 138      15.999  11.246  11.918  1.00  9.82     -0.346 N
ATOM   2067  HN  ASN A 138      15.959  11.918  12.685  1.00  0.00      0.163 HD
ATOM   2068  CA  ASN A 138      15.844  11.666  10.510  1.00 10.34      0.185 C
ATOM   2070  C   ASN A 138      17.217  11.504   9.828  1.00 13.12      0.241 C
ATOM   2071  O   ASN A 138      18.239  11.689  10.464  1.00 11.44     -0.271 OA
ATOM   2072  CB  ASN A 138      15.360  13.117  10.368  1.00 10.70      0.137 C
ATOM   2075  CG  ASN A 138      13.884  13.314  10.674  1.00 14.44      0.217 C
ATOM   2076  ND2 ASN A 138      13.432  14.570  10.788  1.00 10.87     -0.370 N
ATOM   2077 1HD2 ASN A 138      14.058  15.369  10.692  1.00  0.00      0.159 HD
ATOM   2078 2HD2 ASN A 138      12.442  14.702  10.993  1.00  0.00      0.159 HD
ATOM   2079  OD1 ASN A 138      13.122  12.341  10.791  1.00 12.05     -0.274 OA
ATOM   2080  N   ARG A 139      17.193  11.187   8.541  1.00 12.75     -0.346 N
ATOM   2081  HN  ARG A 139      16.282  11.045   8.106  1.00  0.00      0.163 HD
ATOM   2082  CA  ARG A 139      18.384  11.026   7.697  1.00 15.02      0.176 C
ATOM   2084  C   ARG A 139      18.064  11.735   6.364  1.00 15.61      0.243 C
ATOM   2085  O   ARG A 139      16.915  12.005   6.027  1.00 15.58     -0.271 OA
ATOM   2086  CB  ARG A 139      18.608   9.545   7.477  1.00 12.23      0.036 C
ATOM   2089  CG  ARG A 139      18.975   8.687   8.691  1.00 15.05      0.023 C
ATOM   2092  CD  ARG A 139      20.291   9.179   9.320  1.00 17.32      0.138 C
ATOM   2095  NE  ARG A 139      20.684   8.210  10.368  1.00 21.27     -0.227 N
ATOM   2096  HE  ARG A 139      21.187   7.362  10.106  1.00  0.00      0.177 HD
ATOM   2097  CZ  ARG A 139      20.390   8.430  11.652  1.00 27.40      0.665 C
ATOM   2098  NH1 ARG A 139      19.745   9.530  12.033  1.00 17.65     -0.235 N
ATOM   2099 1HH1 ARG A 139      19.520   9.698  13.014  1.00  0.00      0.174 HD
ATOM   2100 2HH1 ARG A 139      19.478  10.161  11.278  1.00  0.00      0.174 HD
ATOM   2101  NH2 ARG A 139      20.738   7.607  12.637  1.00 20.57     -0.235 N
ATOM   2102 1HH2 ARG A 139      20.513   7.775  13.618  1.00  0.00      0.174 HD
ATOM   2103 2HH2 ARG A 139      21.232   6.764  12.345  1.00  0.00      0.174 HD
ATOM   2104  N   PRO A 140      19.074  12.156   5.605  1.00 17.14     -0.337 N
ATOM   2105  CA  PRO A 140      18.880  12.879   4.351  1.00 18.86      0.179 C
ATOM   2107  C   PRO A 140      17.977  12.127   3.394  1.00 14.48      0.241 C
ATOM   2108  O   PRO A 140      18.155  10.938   3.143  1.00 16.57     -0.271 OA
ATOM   2109  CB  PRO A 140      20.301  13.036   3.790  1.00 20.41      0.037 C
ATOM   2112  CG  PRO A 140      21.186  12.915   4.996  1.00 21.59      0.022 C
ATOM   2115  CD  PRO A 140      20.510  11.915   5.917  1.00 19.48      0.127 C
ATOM   2118  N   GLY A 141      16.899  12.741   2.952  1.00 12.81     -0.351 N
ATOM   2119  HN  GLY A 141      16.787  13.716   3.230  1.00  0.00      0.163 HD
ATOM   2120  CA  GLY A 141      15.857  12.187   2.117  1.00 16.04      0.225 C
ATOM   2123  C   GLY A 141      14.827  11.337   2.841  1.00 16.56      0.236 C
ATOM   2124  O   GLY A 141      13.935  10.729   2.250  1.00 14.29     -0.272 OA
ATOM   2125  N   HIS A 142      14.958  11.215   4.191  1.00 14.27     -0.346 N
ATOM   2126  HN  HIS A 142      15.710  11.708   4.673  1.00  0.00      0.163 HD
ATOM   2127  CA  HIS A 142      14.032  10.384   4.955  1.00 12.81      0.182 C
ATOM   2129  C   HIS A 142      13.675  11.140   6.261  1.00 18.25      0.241 C
ATOM   2130  O   HIS A 142      14.187  10.797   7.328  1.00 19.14     -0.271 OA
ATOM   2131  CB  HIS A 142      14.756   9.093   5.389  1.00 12.91      0.093 C
ATOM   2134  CG  HIS A 142      15.195   8.239   4.228  1.00 20.96      0.028 A
ATOM   2135  CD2 HIS A 142      16.376   8.207   3.572  1.00 21.82      0.114 A
ATOM   2137  ND1 HIS A 142      14.351   7.385   3.558  1.00 24.58     -0.354 N
ATOM   2138  HD1 HIS A 142      13.375   7.214   3.800  1.00  0.00      0.166 HD
ATOM   2139  CE1 HIS A 142      15.004   6.814   2.543  1.00 24.65      0.180 A
ATOM   2141  NE2 HIS A 142      16.243   7.295   2.539  1.00 22.09     -0.360 N
ATOM   2142  HE2 HIS A 142      16.977   7.034   1.881  1.00  0.00      0.166 HD
ATOM   2143  N   ASP A 143      12.831  12.136   6.191  1.00 13.66     -0.345 N
ATOM   2144  HN  ASP A 143      12.448  12.402   5.284  1.00  0.00      0.163 HD
ATOM   2145  CA  ASP A 143      12.422  12.880   7.388  1.00 17.87      0.186 C
ATOM   2147  C   ASP A 143      11.145  12.233   7.936  1.00 15.52      0.241 C
ATOM   2148  O   ASP A 143      10.062  12.692   7.672  1.00 17.34     -0.271 OA
ATOM   2149  CB  ASP A 143      12.269  14.345   7.062  1.00 20.42      0.147 C
ATOM   2152  CG  ASP A 143      13.659  14.978   6.901  1.00 41.55      0.175 C
ATOM   2153  OD1 ASP A 143      14.748  14.378   7.042  1.00 47.85     -0.648 OA
ATOM   2154  OD2 ASP A 143      13.653  16.196   6.610  1.00 61.69     -0.648 OA
ATOM   2155  N   ILE A 144      11.321  11.128   8.669  1.00  9.83     -0.346 N
ATOM   2156  HN  ILE A 144      12.259  10.774   8.856  1.00  6.00      0.163 HD
ATOM   2157  CA  ILE A 144      10.154  10.440   9.195  1.00  9.43      0.180 C
ATOM   2159  C   ILE A 144       9.544  11.141  10.410  1.00 12.17      0.241 C
ATOM   2160  O   ILE A 144       8.478  10.713  10.856  1.00 14.23     -0.271 OA
ATOM   2161  CB  ILE A 144      10.466   8.971   9.521  1.00 17.65      0.013 C
ATOM   2163  CG1 ILE A 144      11.683   8.899  10.419  1.00 15.86      0.002 C
ATOM   2166  CG2 ILE A 144      10.653   8.224   8.193  1.00 21.64      0.012 C
ATOM   2170  CD1 ILE A 144      11.736   7.705  11.359  1.00 23.86      0.005 C
ATOM   2174  N   VAL A 145      10.252  12.091  11.031  1.00 10.93     -0.346 N
ATOM   2175  HN  VAL A 145      11.196  12.321  10.720  1.00  0.00      0.163 HD
ATOM   2176  CA  VAL A 145       9.643  12.802  12.175  1.00  8.86      0.180 C
ATOM   2178  C   VAL A 145       9.543  14.291  11.778  1.00  7.87      0.241 C
ATOM   2179  O   VAL A 145      10.564  14.914  11.541  1.00 10.67     -0.271 OA
ATOM   2180  CB  VAL A 145      10.477  12.717  13.456  1.00 10.83      0.009 C
ATOM   2182  CG1 VAL A 145       9.770  13.452  14.637  1.00  8.74      0.012 C
ATOM   2186  CG2 VAL A 145      10.730  11.274  13.875  1.00 13.54      0.012 C
ATOM   2190  N   ASP A 146       8.336  14.803  11.658  1.00  8.25     -0.345 N
ATOM   2191  HN  ASP A 146       7.517  14.213  11.806  1.00  0.00      0.163 HD
ATOM   2192  CA  ASP A 146       8.164  16.230  11.310  1.00 10.58      0.186 C
ATOM   2194  C   ASP A 146       6.739  16.612  11.629  1.00 10.55      0.241 C
ATOM   2195  O   ASP A 146       5.792  16.424  10.823  1.00 11.71     -0.271 OA
ATOM   2196  CB  ASP A 146       8.434  16.339   9.772  1.00 13.90      0.147 C
ATOM   2199  CG  ASP A 146       8.248  17.777   9.324  1.00 25.12      0.175 C
ATOM   2200  OD1 ASP A 146       8.226  18.753  10.092  1.00 14.44     -0.648 OA
ATOM   2201  OD2 ASP A 146       8.075  17.942   8.103  1.00 21.89     -0.648 OA
ATOM   2202  N   HIS A 147       6.530  17.191  12.836  1.00  8.63     -0.346 N
ATOM   2203  HN  HIS A 147       7.293  17.328  13.498  1.00  0.00      0.163 HD
ATOM   2204  CA  HIS A 147       5.157  17.614  13.152  1.00  4.98      0.182 C
ATOM   2206  C   HIS A 147       5.174  18.799  14.113  1.00  8.64      0.241 C
ATOM   2207  O   HIS A 147       6.209  18.986  14.803  1.00 10.28     -0.271 OA
ATOM   2208  CB  HIS A 147       4.326  16.474  13.758  1.00  6.70      0.093 C
ATOM   2211  CG  HIS A 147       4.937  15.684  14.865  1.00  7.81      0.028 A
ATOM   2212  CD2 HIS A 147       4.926  15.898  16.219  1.00  8.07      0.114 A
ATOM   2214  ND1 HIS A 147       5.560  14.454  14.639  1.00  7.77     -0.354 N
ATOM   2215  HD1 HIS A 147       5.684  14.003  13.733  1.00  0.00      0.166 HD
ATOM   2216  CE1 HIS A 147       5.970  13.967  15.831  1.00 11.75      0.180 A
ATOM   2218  NE2 HIS A 147       5.607  14.828  16.763  1.00  8.31     -0.360 N
ATOM   2219  HE2 HIS A 147       5.804  14.717  17.758  1.00  0.00      0.166 HD
ATOM   2220  N   TYR A 148       4.088  19.547  14.107  1.00  8.52     -0.346 N
ATOM   2221  HN  TYR A 148       3.295  19.303  13.513  1.00  0.00      0.163 HD
ATOM   2222  CA  TYR A 148       4.035  20.740  14.970  1.00  8.24      0.180 C
ATOM   2224  C   TYR A 148       3.372  20.412  16.296  1.00 10.92      0.241 C
ATOM   2225  O   TYR A 148       2.664  19.409  16.393  1.00 11.04     -0.271 OA
ATOM   2226  CB  TYR A 148       3.056  21.764  14.288  1.00  6.72      0.073 C
ATOM   2229  CG  TYR A 148       3.939  22.481  13.258  1.00 10.47     -0.056 A
ATOM   2230  CD1 TYR A 148       4.194  21.897  12.021  1.00 17.59      0.010 A
ATOM   2232  CD2 TYR A 148       4.527  23.682  13.577  1.00 14.85      0.010 A
ATOM   2234  CE1 TYR A 148       5.047  22.561  11.135  1.00 24.85      0.037 A
ATOM   2236  CE2 TYR A 148       5.358  24.353  12.701  1.00 15.96      0.037 A
ATOM   2238  CZ  TYR A 148       5.594  23.769  11.468  1.00 23.24      0.065 A
ATOM   2239  OH  TYR A 148       6.427  24.439  10.597  1.00 32.27     -0.361 OA
ATOM   2240  HH  TYR A 148       6.807  25.278  10.828  1.00  0.00      0.217 HD
ATOM   2241  N   THR A 149       3.495  21.351  17.242  1.00  8.39     -0.344 N
ATOM   2242  HN  THR A 149       4.083  22.169  17.081  1.00  0.00      0.163 HD
ATOM   2243  CA  THR A 149       2.777  21.195  18.514  1.00  6.93      0.205 C
ATOM   2245  C   THR A 149       1.982  22.495  18.680  1.00 11.02      0.243 C
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ATOM   2246  O   THR A 149       2.632  23.548  18.714  1.00 10.36     -0.271 OA
ATOM   2247  CB  THR A 149       3.747  21.048  19.691  1.00 10.43      0.146 C
ATOM   2249  CG2 THR A 149       2.889  20.836  20.964  1.00  7.31      0.042 C
ATOM   2253  OG1 THR A 149       4.581  19.903  19.470  1.00 10.23     -0.393 OA
ATOM   2254  HG1 THR A 149       5.182  19.812  20.200  1.00  0.00      0.210 HD
ATOM   2255  N   TYR A 150       0.678  22.441  18.704  1.00  8.05     -0.346 N
ATOM   2256  HN  TYR A 150       0.212  21.538  18.619  1.00  0.00      0.163 HD
ATOM   2257  CA  TYR A 150      -0.138  23.672  18.853  1.00  6.54      0.180 C
ATOM   2259  C   TYR A 150      -0.819  23.663  20.233  1.00  9.96      0.241 C
ATOM   2260  O   TYR A 150      -1.335  22.643  20.649  1.00 12.27     -0.271 OA
ATOM   2261  CB  TYR A 150      -1.267  23.636  17.814  1.00  6.58      0.073 C
ATOM   2264  CG  TYR A 150      -0.793  23.660  16.365  1.00  6.77     -0.056 A
ATOM   2265  CD1 TYR A 150      -0.331  24.845  15.824  1.00  9.15      0.010 A
ATOM   2267  CD2 TYR A 150      -0.846  22.513  15.568  1.00  9.94      0.010 A
ATOM   2269  CE1 TYR A 150       0.095  24.906  14.498  1.00 10.46      0.037 A
ATOM   2271  CE2 TYR A 150      -0.433  22.595  14.234  1.00  8.14      0.037 A
ATOM   2273  CZ  TYR A 150       0.039  23.773  13.732  1.00 10.24      0.065 A
ATOM   2274  OH  TYR A 150       0.450  23.868  12.389  1.00 13.21     -0.361 OA
ATOM   2275  HH  TYR A 150       0.779  24.688  12.040  1.00  0.00      0.217 HD
ATOM   2276  N   ALA A 151      -0.889  24.811  20.896  1.00 10.21     -0.346 N
ATOM   2277  HN  ALA A 151      -0.514  25.658  20.469  1.00  0.00      0.163 HD
ATOM   2278  CA  ALA A 151      -1.492  24.886  22.225  1.00  7.70      0.172 C
ATOM   2280  C   ALA A 151      -2.455  26.077  22.313  1.00  9.14      0.240 C
ATOM   2281  O   ALA A 151      -2.087  27.135  21.798  1.00 11.01     -0.271 OA
ATOM   2282  CB  ALA A 151      -0.374  25.174  23.232  1.00  8.82      0.042 C
ATOM   2286  N   PHE A 152      -3.582  25.962  22.981  1.00  5.21     -0.346 N
ATOM   2287  HN  PHE A 152      -3.859  25.054  23.353  1.00  0.00      0.163 HD
ATOM   2288  CA  PHE A 152      -4.434  27.117  23.193  1.00  4.33      0.180 C
ATOM   2290  C   PHE A 152      -4.291  27.466  24.687  1.00  8.43      0.241 C
ATOM   2291  O   PHE A 152      -4.242  26.493  25.468  1.00  9.85     -0.271 OA
ATOM   2292  CB  PHE A 152      -5.898  26.698  22.967  1.00  9.57      0.073 C
ATOM   2295  CG  PHE A 152      -6.353  26.750  21.521  1.00 13.77     -0.056 A
ATOM   2296  CD1 PHE A 152      -5.474  26.972  20.461  1.00  7.04      0.007 A
ATOM   2298  CD2 PHE A 152      -7.698  26.587  21.280  1.00 12.59      0.007 A
ATOM   2300  CE1 PHE A 152      -5.980  27.015  19.168  1.00 15.90      0.001 A
ATOM   2302  CE2 PHE A 152      -8.212  26.648  19.980  1.00 13.27      0.001 A
ATOM   2304  CZ  PHE A 152      -7.347  26.850  18.940  1.00 10.46      0.000 A
ATOM   2306  N   MET A 153      -4.202  28.769  25.023  1.00  7.33     -0.346 N
ATOM   2307  HN  MET A 153      -4.230  29.523  24.337  1.00  0.00      0.163 HD
ATOM   2308  CA  MET A 153      -4.058  29.009  26.491  1.00  7.31      0.177 C
ATOM   2310  C   MET A 153      -4.844  30.275  26.843  1.00 12.05      0.240 C
ATOM   2311  O   MET A 153      -5.098  31.046  25.924  1.00 10.77     -0.271 OA
ATOM   2312  CB  MET A 153      -2.608  29.329  26.844  1.00 13.68      0.045 C
ATOM   2315  CG  MET A 153      -1.397  28.605  26.370  1.00 33.05      0.076 C
ATOM   2318  SD  MET A 153       0.052  29.696  26.244  1.00 21.02     -0.173 SA
ATOM   2319  CE  MET A 153       0.259  30.077  27.978  1.00 18.94      0.089 C
ATOM   2323  N   GLY A 154      -5.124  30.487  28.133  1.00 11.30     -0.351 N
ATOM   2324  HN  GLY A 154      -4.801  29.841  28.856  1.00  0.00      0.163 HD
ATOM   2325  CA  GLY A 154      -5.922  31.695  28.488  1.00  8.87      0.225 C
ATOM   2328  C   GLY A 154      -5.203  32.525  29.559  1.00  9.58      0.236 C
ATOM   2329  O   GLY A 154      -4.037  32.279  29.885  1.00  8.44     -0.272 OA
ATOM   1440  N   ASP A 155      -5.924  33.534  30.101  1.00  8.56     -0.345 N
ATOM   1441  HN  ASP A 155      -6.903  33.681  29.855  1.00  0.00      0.163 HD
ATOM   1442  CA  ASP A 155      -5.231  34.413  31.063  1.00  7.42      0.186 C
ATOM   1443  C   ASP A 155      -4.779  33.635  32.301  1.00 11.05      0.241 C
ATOM   1444  O   ASP A 155      -3.775  33.994  32.901  1.00 11.07     -0.271 OA
ATOM   1445  CB  ASP A 155      -6.169  35.508  31.565  1.00 10.56      0.147 C
ATOM   1446  CG  ASP A 155      -6.633  36.418  30.403  1.00 11.13      0.175 C
ATOM   1447  OD1 ASP A 155      -5.800  37.037  29.774  1.00 14.23     -0.648 OA
ATOM   1448  OD2 ASP A 155      -7.849  36.452  30.185  1.00 12.16     -0.648 OA
ATOM   2342  N   GLY A 156      -5.601  32.662  32.726  1.00  6.97     -0.351 N
ATOM   2343  HN  GLY A 156      -6.465  32.465  32.221  1.00  0.00      0.163 HD
ATOM   2344  CA  GLY A 156      -5.248  31.876  33.930  1.00 11.15      0.225 C
ATOM   2347  C   GLY A 156      -3.887  31.223  33.730  1.00 12.78      0.236 C
ATOM   2348  O   GLY A 156      -3.064  31.272  34.639  1.00 10.57     -0.272 OA
ATOM   2349  N   CYS A 157      -3.622  30.583  32.595  1.00  9.21     -0.346 N
ATOM   2350  HN  CYS A 157      -4.365  30.527  31.899  1.00  0.00      0.163 HD
ATOM   2351  CA  CYS A 157      -2.352  29.959  32.276  1.00  7.21      0.186 C
ATOM   2353  C   CYS A 157      -1.203  30.981  32.300  1.00 10.21      0.241 C
ATOM   2354  O   CYS A 157      -0.122  30.710  32.840  1.00  8.70     -0.271 OA
ATOM   2355  CB  CYS A 157      -2.416  29.368  30.826  1.00  5.81      0.121 C
ATOM   2358  SG  CYS A 157      -3.583  27.906  30.832  1.00 15.40     -0.095 SA
ATOM   2359  N   MET A 158      -1.437  32.202  31.821  1.00  5.38     -0.346 N
ATOM   2360  HN  MET A 158      -2.378  32.421  31.494  1.00  0.00      0.163 HD
ATOM   2361  CA  MET A 158      -0.425  33.235  31.741  1.00  4.66      0.177 C
ATOM   2363  C   MET A 158      -0.080  33.732  33.158  1.00  8.13      0.241 C
ATOM   2364  O   MET A 158       1.066  34.083  33.386  1.00  8.89     -0.271 OA
ATOM   2365  CB  MET A 158      -0.863  34.450  30.933  1.00  5.32      0.045 C
ATOM   2368  CG  MET A 158      -1.048  34.154  29.441  1.00  8.66      0.076 C
ATOM   2371  SD  MET A 158       0.626  33.885  28.786  1.00 15.28     -0.173 SA
ATOM   2372  CE  MET A 158       0.197  33.871  26.998  1.00  9.85      0.089 C
ATOM   2376  N   MET A 159      -1.069  33.831  34.045  1.00  7.64     -0.346 N
ATOM   2377  HN  MET A 159      -2.030  33.605  33.789  1.00  0.00      0.163 HD
ATOM   2378  CA  MET A 159      -0.730  34.278  35.407  1.00  5.33      0.177 C
ATOM   2380  C   MET A 159       0.039  33.244  36.184  1.00  9.29      0.241 C
ATOM   2381  O   MET A 159       0.834  33.608  37.085  1.00  7.47     -0.271 OA
ATOM   2382  CB  MET A 159      -2.059  34.603  36.147  1.00  5.35      0.045 C
ATOM   2385  CG  MET A 159      -2.596  35.981  35.721  1.00  5.65      0.076 C
ATOM   2388  SD  MET A 159      -4.092  36.381  36.663  1.00 11.04     -0.173 SA
ATOM   2389  CE  MET A 159      -5.317  36.116  35.356  1.00 14.48      0.089 C
ATOM   2393  N   GLU A 160      -0.194  31.949  35.956  1.00  6.99     -0.346 N
ATOM   2394  HN  GLU A 160      -0.846  31.679  35.220  1.00  0.00      0.163 HD
ATOM   2395  CA  GLU A 160       0.469  30.912  36.743  1.00  7.06      0.177 C
ATOM   2397  C   GLU A 160       1.985  30.915  36.539  1.00  8.94      0.240 C
ATOM   2398  O   GLU A 160       2.473  31.061  35.430  1.00  8.02     -0.271 OA
ATOM   2399  CB  GLU A 160      -0.062  29.502  36.392  1.00  7.60      0.045 C
ATOM   2402  CG  GLU A 160      -1.453  29.215  36.881  1.00  5.36      0.116 C
ATOM   2405  CD  GLU A 160      -1.505  28.896  38.382  1.00  8.33      0.172 C
ATOM   2406  OE1 GLU A 160      -0.457  28.872  39.032  1.00  6.36     -0.648 OA
ATOM   2407  OE2 GLU A 160      -2.597  28.627  38.945  1.00 10.57     -0.648 OA
ATOM   2408  N   GLY A 161       2.709  30.715  37.628  1.00  4.71     -0.351 N
ATOM   2409  HN  GLY A 161       2.229  30.606  38.522  1.00  0.00      0.163 HD
ATOM   2410  CA  GLY A 161       4.175  30.644  37.602  1.00  6.84      0.225 C
ATOM   2413  C   GLY A 161       4.708  29.578  36.644  1.00  7.08      0.236 C
ATOM   2414  O   GLY A 161       5.760  29.812  36.015  1.00  7.85     -0.272 OA
ATOM   2415  N   ILE A 162       3.999  28.459  36.490  1.00  4.85     -0.346 N
ATOM   2416  HN  ILE A 162       3.102  28.317  36.954  1.00  0.00      0.163 HD
ATOM   2417  CA  ILE A 162       4.598  27.437  35.603  1.00  3.56      0.180 C
ATOM   2419  C   ILE A 162       4.716  27.975  34.188  1.00  7.48      0.241 C
ATOM   2420  O   ILE A 162       5.580  27.453  33.472  1.00  7.29     -0.271 OA
ATOM   2421  CB  ILE A 162       3.818  26.102  35.737  1.00  8.12      0.013 C
ATOM   2423  CG1 ILE A 162       4.536  24.930  35.107  1.00 21.21      0.002 C
ATOM   2426  CG2 ILE A 162       2.385  26.316  35.249  1.00  6.82      0.012 C
ATOM   2430  CD1 ILE A 162       3.793  23.579  35.230  1.00  8.53      0.005 C
ATOM   2434  N   SER A 163       3.888  28.914  33.728  1.00  7.89     -0.344 N
ATOM   2435  HN  SER A 163       3.148  29.287  34.323  1.00  0.00      0.163 HD
ATOM   2436  CA  SER A 163       4.057  29.413  32.330  1.00 18.75      0.200 C
ATOM   2438  C   SER A 163       5.392  30.132  32.209  1.00  8.71      0.243 C
ATOM   2439  O   SER A 163       6.041  30.022  31.148  1.00  7.39     -0.271 OA
ATOM   2440  CB  SER A 163       2.876  30.308  31.975  1.00  5.45      0.199 C
ATOM   2443  OG  SER A 163       2.897  31.573  32.653  1.00  5.77     -0.398 OA
ATOM   2444  HG  SER A 163       2.161  32.131  32.432  1.00  0.00      0.209 HD
ATOM   2445  N   HIS A 164       5.848  30.868  33.246  1.00  4.70     -0.346 N
ATOM   2446  HN  HIS A 164       5.274  31.013  34.076  1.00  0.00      0.163 HD
ATOM   2447  CA  HIS A 164       7.194  31.456  33.148  1.00  4.74      0.182 C
ATOM   2449  C   HIS A 164       8.268  30.367  33.080  1.00  9.12      0.241 C
ATOM   2450  O   HIS A 164       9.200  30.444  32.305  1.00  8.83     -0.271 OA
ATOM   2451  CB  HIS A 164       7.427  32.284  34.427  1.00  5.45      0.093 C
ATOM   2454  CG  HIS A 164       8.841  32.715  34.597  1.00  5.44      0.028 A
ATOM   2455  CD2 HIS A 164       9.766  32.428  35.564  1.00  9.51      0.114 A
ATOM   2457  ND1 HIS A 164       9.461  33.574  33.709  1.00  9.60     -0.354 N
ATOM   2458  HD1 HIS A 164       9.023  33.992  32.888  1.00  0.00      0.166 HD
ATOM   2459  CE1 HIS A 164      10.708  33.768  34.091  1.00 11.49      0.180 A
ATOM   2461  NE2 HIS A 164      10.906  33.110  35.235  1.00  9.79     -0.360 N
ATOM   2462  HE2 HIS A 164      11.770  33.115  35.778  1.00  0.00      0.166 HD
ATOM   2463  N   GLU A 165       8.198  29.331  33.953  1.00  5.25     -0.346 N
ATOM   2464  HN  GLU A 165       7.455  29.283  34.650  1.00  0.00      0.163 HD
ATOM   2465  CA  GLU A 165       9.217  28.285  33.867  1.00  5.16      0.177 C
ATOM   2467  C   GLU A 165       9.302  27.665  32.459  1.00  7.52      0.241 C
ATOM   2468  O   GLU A 165      10.405  27.524  31.940  1.00  8.47     -0.271 OA
ATOM   2469  CB  GLU A 165       8.970  27.142  34.877  1.00  4.98      0.045 C
ATOM   2472  CG  GLU A 165       9.076  27.706  36.320  1.00  5.62      0.116 C
ATOM   2475  CD  GLU A 165       8.923  26.642  37.379  1.00  9.97      0.172 C
ATOM   2476  OE1 GLU A 165       8.960  25.432  37.054  1.00 10.38     -0.648 OA
ATOM   2477  OE2 GLU A 165       8.786  27.007  38.580  1.00 21.01     -0.648 OA
ATOM   2478  N   VAL A 166       8.175  27.191  31.887  1.00  4.32     -0.346 N
ATOM   2479  HN  VAL A 166       7.254  27.383  32.282  1.00  0.00      0.163 HD
ATOM   2480  CA  VAL A 166       8.338  26.374  30.652  1.00  6.13      0.180 C
ATOM   2482  C   VAL A 166       8.477  27.272  29.429  1.00  3.90      0.241 C
ATOM   2483  O   VAL A 166       9.144  26.822  28.503  1.00  5.35     -0.271 OA
ATOM   2484  CB  VAL A 166       7.199  25.350  30.491  1.00  8.39      0.009 C
ATOM   2486  CG1 VAL A 166       7.095  24.486  31.741  1.00  6.01      0.012 C
ATOM   2490  CG2 VAL A 166       5.839  26.056  30.287  1.00  7.76      0.012 C
ATOM   2494  N   CYS A 167       7.887  28.474  29.440  1.00  6.70     -0.345 N
ATOM   2495  HN  CYS A 167       7.344  28.795  30.241  1.00  0.00      0.163 HD
ATOM   2496  CA  CYS A 167       8.062  29.319  28.227  1.00  9.86      0.186 C
ATOM   2498  C   CYS A 167       9.437  29.939  28.145  1.00  8.99      0.242 C
ATOM   2499  O   CYS A 167      10.033  30.160  27.055  1.00  8.11     -0.271 OA
ATOM   2500  CB  CYS A 167       6.932  30.385  28.171  1.00  7.25      0.121 C
ATOM   2503  SG  CYS A 167       5.313  29.602  27.881  1.00 10.43     -0.095 SA
ATOM   2504  N   SER A 168      10.057  30.197  29.335  1.00  6.69     -0.344 N
ATOM   2505  HN  SER A 168       9.562  30.049  30.213  1.00  0.00      0.163 HD
ATOM   2506  CA  SER A 168      11.431  30.685  29.338  1.00  7.41      0.200 C
ATOM   2508  C   SER A 168      12.348  29.624  28.732  1.00  7.46      0.243 C
ATOM   2509  O   SER A 168      13.215  29.869  27.878  1.00  8.43     -0.271 OA
ATOM   2510  CB  SER A 168      11.862  30.946  30.810  1.00  1.53      0.199 C
ATOM   2513  OG  SER A 168      13.242  31.208  30.935  1.00 10.32     -0.398 OA
ATOM   2514  HG  SER A 168      13.505  31.367  31.834  1.00  0.00      0.209 HD
ATOM   2515  N   LEU A 169      12.221  28.347  29.154  1.00  6.79     -0.346 N
ATOM   2516  HN  LEU A 169      11.510  28.134  29.854  1.00  0.00      0.163 HD
ATOM   2517  CA  LEU A 169      13.056  27.256  28.654  1.00  7.34      0.177 C
ATOM   2519  C   LEU A 169      12.791  26.902  27.187  1.00  8.22      0.241 C
ATOM   2520  O   LEU A 169      13.733  26.645  26.395  1.00  8.93     -0.271 OA
ATOM   2521  CB  LEU A 169      12.786  25.982  29.525  1.00  8.24      0.038 C
ATOM   2524  CG  LEU A 169      13.599  24.732  29.181  1.00 13.38     -0.020 C
ATOM   2526  CD1 LEU A 169      15.087  25.022  29.378  1.00 16.20      0.009 C
ATOM   2530  CD2 LEU A 169      13.263  23.571  30.132  1.00 18.34      0.009 C
ATOM   2534  N   ALA A 170      11.516  27.068  26.770  1.00  7.93     -0.346 N
ATOM   2535  HN  ALA A 170      10.792  27.336  27.436  1.00  0.00      0.163 HD
ATOM   2536  CA  ALA A 170      11.179  26.864  25.374  1.00  8.13      0.172 C
ATOM   2538  C   ALA A 170      11.936  27.873  24.480  1.00 10.77      0.240 C
ATOM   2539  O   ALA A 170      12.346  27.492  23.364  1.00  9.22     -0.271 OA
ATOM   2540  CB  ALA A 170       9.682  27.010  25.100  1.00  7.33      0.042 C
ATOM   2544  N   GLY A 171      12.078  29.099  24.938  1.00 11.31     -0.351 N
ATOM   2545  HN  GLY A 171      11.636  29.355  25.821  1.00  0.00      0.163 HD
ATOM   2546  CA  GLY A 171      12.863  30.114  24.202  1.00 13.15      0.225 C
ATOM   2549  C   GLY A 171      14.341  29.733  24.065  1.00 12.62      0.236 C
ATOM   2550  O   GLY A 171      14.950  29.789  22.972  1.00 11.89     -0.272 OA
ATOM   2551  N   THR A 172      14.959  29.261  25.142  1.00  9.34     -0.344 N
ATOM   2552  HN  THR A 172      14.434  29.196  26.014  1.00  0.00      0.163 HD
ATOM   2553  CA  THR A 172      16.374  28.825  25.136  1.00  8.82      0.205 C
ATOM   2555  C   THR A 172      16.610  27.683  24.183  1.00 12.25      0.243 C
ATOM   2556  O   THR A 172      17.634  27.570  23.461  1.00  9.17     -0.271 OA
ATOM   2557  CB  THR A 172      16.790  28.309  26.542  1.00 10.19      0.146 C
ATOM   2559  CG2 THR A 172      18.273  27.952  26.612  1.00 12.85      0.042 C
ATOM   2563  OG1 THR A 172      16.566  29.392  27.448  1.00 13.86     -0.393 OA
ATOM   2564  HG1 THR A 172      16.820  29.077  28.307  1.00  0.00      0.210 HD
ATOM   2565  N   LEU A 173      15.629  26.766  24.109  1.00  9.15     -0.346 N
ATOM   2566  HN  LEU A 173      14.777  26.907  24.652  1.00  0.00      0.163 HD
ATOM   2567  CA  LEU A 173      15.748  25.578  23.276  1.00 13.03      0.177 C
ATOM   2569  C   LEU A 173      15.308  25.842  21.840  1.00 10.77      0.241 C
ATOM   2570  O   LEU A 173      15.305  24.855  21.081  1.00 13.48     -0.271 OA
ATOM   2571  CB  LEU A 173      15.049  24.559  23.900  1.00  7.95      0.038 C
ATOM   2574  CG  LEU A 173      15.655  23.926  25.278  1.00 10.31     -0.020 C
ATOM   2576  CD1 LEU A 173      14.779  22.802  25.857  1.00 15.28      0.009 C
ATOM   2580  CD2 LEU A 173      17.077  23.412  25.161  1.00 16.17      0.009 C
ATOM   2584  N   LYS A 174      14.874  27.066  21.517  1.00  7.03     -0.346 N
ATOM   2585  HN  LYS A 174      14.793  27.772  22.249  1.00  0.00      0.163 HD
ATOM   2586  CA  LYS A 174      14.512  27.421  20.144  1.00  8.60      0.176 C
ATOM   2588  C   LYS A 174      13.531  26.450  19.509  1.00 14.97      0.241 C
ATOM   2589  O   LYS A 174      13.785  25.893  18.423  1.00 15.11     -0.271 OA
ATOM   2590  CB  LYS A 174      15.823  27.386  19.336  1.00 10.93      0.035 C
ATOM   2593  CG  LYS A 174      16.816  28.452  19.873  1.00 16.43      0.004 C
ATOM   2596  CD  LYS A 174      18.120  28.137  19.108  1.00 27.42      0.027 C
ATOM   2599  CE  LYS A 174      19.253  29.005  19.619  1.00 40.26      0.229 C
ATOM   2602  NZ  LYS A 174      19.106  30.394  19.091  1.00 54.98     -0.079 N
ATOM   2603  HZ1 LYS A 174      19.868  30.978  19.435  1.00  0.00      0.274 HD
ATOM   2604  HZ2 LYS A 174      18.192  30.791  19.307  1.00  0.00      0.274 HD
ATOM   2605  HZ3 LYS A 174      19.039  30.412  18.073  1.00  0.00      0.274 HD
ATOM   2606  N   LEU A 175      12.399  26.231  20.178  1.00  8.58     -0.346 N
ATOM   2607  HN  LEU A 175      12.214  26.733  21.047  1.00  0.00      0.163 HD
ATOM   2608  CA  LEU A 175      11.415  25.264  19.662  1.00  9.31      0.177 C
ATOM   2610  C   LEU A 175      10.536  25.944  18.630  1.00 11.44      0.240 C
ATOM   2611  O   LEU A 175       9.394  26.288  18.915  1.00  8.94     -0.271 OA
ATOM   2612  CB  LEU A 175      10.577  24.822  20.869  1.00  7.90      0.038 C
ATOM   2615  CG  LEU A 175      11.442  24.132  21.942  1.00 11.13     -0.020 C
ATOM   2617  CD1 LEU A 175      10.484  23.744  23.062  1.00 10.91      0.009 C
ATOM   2621  CD2 LEU A 175      12.099  22.862  21.359  1.00 13.12      0.009 C
ATOM   2625  N   GLY A 176      11.029  25.989  17.384  1.00  8.04     -0.351 N
ATOM   2626  HN  GLY A 176      11.929  25.555  17.179  1.00  0.00      0.163 HD
ATOM   2627  CA  GLY A 176      10.285  26.657  16.317  1.00  8.68      0.225 C
ATOM   2630  C   GLY A 176       8.951  26.016  15.973  1.00 12.62      0.236 C
ATOM   2631  O   GLY A 176       8.101  26.705  15.386  1.00 11.28     -0.272 OA
ATOM   2632  N   LYS A 177       8.771  24.735  16.306  1.00  7.40     -0.346 N
ATOM   2633  HN  LYS A 177       9.496  24.227  16.813  1.00  0.00      0.163 HD
ATOM   2634  CA  LYS A 177       7.521  24.068  15.935  1.00  7.61      0.176 C
ATOM   2636  C   LYS A 177       6.436  24.127  16.996  1.00 12.33      0.241 C
ATOM   2637  O   LYS A 177       5.360  23.564  16.823  1.00 11.55     -0.271 OA
ATOM   2638  CB  LYS A 177       7.769  22.616  15.505  1.00 12.16      0.035 C
ATOM   2641  CG  LYS A 177       8.644  22.583  14.233  1.00 17.75      0.004 C
ATOM   2644  CD  LYS A 177       8.593  21.158  13.690  1.00 21.60      0.027 C
ATOM   2647  CE  LYS A 177       9.608  20.836  12.627  1.00 22.56      0.229 C
ATOM   2650  NZ  LYS A 177       9.599  19.360  12.362  1.00 12.48     -0.079 N
ATOM   2651  HZ1 LYS A 177      10.287  19.142  11.641  1.00  0.00      0.274 HD
ATOM   2652  HZ2 LYS A 177       8.669  19.016  12.125  1.00  0.00      0.274 HD
ATOM   2653  HZ3 LYS A 177       9.743  18.814  13.212  1.00  0.00      0.274 HD
ATOM   2654  N   ILE A 178       6.670  24.880  18.071  1.00  8.25     -0.346 N
ATOM   2655  HN  ILE A 178       7.589  25.309  18.181  1.00  0.00      0.163 HD
ATOM   2656  CA  ILE A 178       5.649  25.114  19.104  1.00  8.08      0.177 C
ATOM   2658  C   ILE A 178       4.976  26.421  18.791  1.00  8.20      0.241 C
ATOM   2659  O   ILE A 178       5.646  27.465  18.711  1.00  8.46     -0.271 OA
ATOM   2660  CB  ILE A 178       6.381  25.287  20.449  1.00  5.42      0.038 C
ATOM   2663  CG  ILE A 178       5.488  25.623  21.651  1.00  9.67     -0.020 C
ATOM   2665  CD1 ILE A 178       4.408  24.573  21.891  1.00 10.18      0.009 C
ATOM   2669  CD2 ILE A 178       6.408  25.593  22.895  1.00  8.69      0.009 C
ATOM   2673  N   ILE A 179       3.680  26.413  18.568  1.00  8.90     -0.346 N
ATOM   2674  HN  ILE A 179       3.183  25.525  18.639  1.00  0.00      0.163 HD
ATOM   2675  CA  ILE A 179       2.910  27.618  18.222  1.00 10.49      0.180 C
ATOM   2677  C   ILE A 179       1.743  27.685  19.195  1.00 12.23      0.241 C
ATOM   2678  O   ILE A 179       0.928  26.767  19.222  1.00 10.76     -0.271 OA
ATOM   2679  CB  ILE A 179       2.409  27.523  16.758  1.00  8.50      0.013 C
ATOM   2681  CG1 ILE A 179       3.636  27.617  15.834  1.00 14.68      0.002 C
ATOM   2684  CG2 ILE A 179       1.404  28.629  16.434  1.00 14.46      0.012 C
ATOM   2688  CD1 ILE A 179       3.321  27.316  14.372  1.00 23.31      0.005 C
ATOM   2692  N   ALA A 180       1.702  28.716  20.046  1.00  6.61     -0.346 N
ATOM   2693  HN  ALA A 180       2.426  29.432  19.994  1.00  0.00      0.163 HD
ATOM   2694  CA  ALA A 180       0.655  28.841  21.040  1.00  6.22      0.172 C
ATOM   2696  C   ALA A 180      -0.262  30.005  20.671  1.00 11.15      0.240 C
ATOM   2697  O   ALA A 180       0.228  30.998  20.120  1.00 12.56     -0.271 OA
ATOM   2698  CB  ALA A 180       1.281  29.124  22.431  1.00  7.30      0.042 C
ATOM   2702  N   PHE A 181      -1.535  29.869  20.989  1.00  8.47     -0.346 N
ATOM   2703  HN  PHE A 181      -1.828  29.003  21.442  1.00  0.00      0.163 HD
ATOM   2704  CA  PHE A 181      -2.529  30.869  20.734  1.00  6.85      0.180 C
ATOM   2706  C   PHE A 181      -3.040  31.306  22.104  1.00  9.69      0.241 C
ATOM   2707  O   PHE A 181      -3.514  30.488  22.900  1.00 12.25     -0.271 OA
ATOM   2708  CB  PHE A 181      -3.770  30.325  20.002  1.00 11.47      0.073 C
ATOM   2711  CG  PHE A 181      -3.471  29.765  18.628  1.00  9.83     -0.056 A
ATOM   2712  CD1 PHE A 181      -2.841  28.550  18.475  1.00  9.25      0.007 A
ATOM   2714  CD2 PHE A 181      -3.827  30.505  17.526  1.00  9.21      0.007 A
ATOM   2716  CE1 PHE A 181      -2.576  28.027  17.204  1.00 15.12      0.001 A
ATOM   2718  CE2 PHE A 181      -3.576  29.988  16.238  1.00 11.06      0.001 A
ATOM   2720  CZ  PHE A 181      -2.953  28.770  16.105  1.00 16.72      0.000 A
ATOM   2722  N   TYR A 182      -2.990  32.615  22.312  1.00  8.82     -0.346 N
ATOM   2723  HN  TYR A 182      -2.624  33.249  21.602  1.00  0.00      0.163 HD
ATOM   2724  CA  TYR A 182      -3.487  33.125  23.620  1.00  4.45      0.180 C
ATOM   2726  C   TYR A 182      -4.848  33.765  23.450  1.00  9.45      0.241 C
ATOM   2727  O   TYR A 182      -5.020  34.685  22.627  1.00 10.76     -0.271 OA
ATOM   2728  CB  TYR A 182      -2.442  34.120  24.092  1.00  6.62      0.073 C
ATOM   2731  CG  TYR A 182      -2.853  35.005  25.263  1.00 11.01     -0.056 A
ATOM   2732  CD1 TYR A 182      -3.590  34.514  26.339  1.00 10.69      0.010 A
ATOM   2734  CD2 TYR A 182      -2.423  36.332  25.228  1.00 12.07      0.010 A
ATOM   2736  CE1 TYR A 182      -3.913  35.363  27.411  1.00 11.24      0.037 A
ATOM   2738  CE2 TYR A 182      -2.754  37.162  26.307  1.00 14.51      0.037 A
ATOM   2740  CZ  TYR A 182      -3.500  36.670  27.354  1.00 11.61      0.065 A
ATOM   2741  OH  TYR A 182      -3.796  37.563  28.374  1.00 18.17     -0.361 OA
ATOM   2742  HH  TYR A 182      -3.510  38.468  28.335  1.00  0.00      0.217 HD
ATOM   2743  N   ASP A 183      -5.800  33.273  24.231  1.00  7.76     -0.345 N
ATOM   2744  HN  ASP A 183      -5.561  32.519  24.875  1.00  0.00      0.163 HD
ATOM   2745  CA  ASP A 183      -7.181  33.764  24.211  1.00 10.75      0.186 C
ATOM   2747  C   ASP A 183      -7.244  35.035  25.049  1.00 13.05      0.241 C
ATOM   2748  O   ASP A 183      -7.480  35.040  26.261  1.00 10.98     -0.271 OA
ATOM   2749  CB  ASP A 183      -8.091  32.647  24.755  1.00 11.65      0.147 C
ATOM   2752  CG  ASP A 183      -9.580  32.925  24.633  1.00 19.13      0.175 C
ATOM   2753  OD1 ASP A 183      -9.966  33.713  23.755  1.00 23.76     -0.648 OA
ATOM   2754  OD2 ASP A 183      -10.416  32.286  25.377  1.00 16.07     -0.648 OA
ATOM   2755  N   ASP A 184      -6.919  36.195  24.443  1.00 10.80     -0.345 N
ATOM   2756  HN  ASP A 184      -6.702  36.181  23.446  1.00  0.00      0.163 HD
ATOM   2757  CA  ASP A 184      -6.864  37.480  25.156  1.00 11.01      0.186 C
ATOM   2759  C   ASP A 184      -8.238  38.104  25.231  1.00 14.70      0.241 C
ATOM   2760  O   ASP A 184      -8.661  38.911  24.386  1.00 13.34     -0.271 OA
ATOM   2761  CB  ASP A 184      -5.843  38.311  24.330  1.00 11.20      0.147 C
ATOM   2764  CG  ASP A 184      -5.545  39.653  24.985  1.00 21.83      0.175 C
ATOM   2765  OD1 ASP A 184      -6.088  39.932  26.065  1.00 15.78     -0.648 OA
ATOM   2766  OD2 ASP A 184      -4.792  40.427  24.368  1.00 21.64     -0.648 OA
ATOM   2767  N   ASN A 185      -9.047  37.678  26.236  1.00 11.31     -0.346 N
ATOM   2768  HN  ASN A 185      -8.699  37.035  26.947  1.00  0.00      0.163 HD
ATOM   2769  CA  ASN A 185      -10.434  38.163  26.278  1.00  9.94      0.185 C
ATOM   2771  C   ASN A 185      -10.689  39.105  27.458  1.00 14.72      0.241 C
ATOM   2772  O   ASN A 185      -11.835  39.507  27.687  1.00 14.02     -0.271 OA
ATOM   2773  CB  ASN A 185      -11.404  36.993  26.257  1.00  8.93      0.137 C
ATOM   2776  CG  ASN A 185      -11.270  36.032  27.446  1.00 15.95      0.217 C
ATOM   2777  ND2 ASN A 185      -11.841  34.848  27.323  1.00 14.19     -0.370 N
ATOM   2778 1HD2 ASN A 185      -12.361  34.561  26.494  1.00  0.00      0.159 HD
ATOM   2779 2HD2 ASN A 185      -11.752  34.209  28.113  1.00  0.00      0.159 HD
ATOM   2780  OD1 ASN A 185      -10.648  36.375  28.438  1.00 12.37     -0.274 OA
ATOM   2781  N   GLY A 186      -9.677  39.483  28.224  1.00 13.84     -0.351 N
ATOM   2782  HN  GLY A 186      -8.757  39.078  28.052  1.00  0.00      0.163 HD
ATOM   2783  CA  GLY A 186      -9.820  40.454  29.304  1.00 16.60      0.225 C
ATOM   2786  C   GLY A 186      -10.604  40.098  30.553  1.00 16.86      0.236 C
ATOM   2787  O   GLY A 186      -10.833  40.983  31.425  1.00 13.10     -0.272 OA
ATOM   2788  N   ILE A 187      -11.034  38.861  30.703  1.00 13.17     -0.346 N
ATOM   2789  HN  ILE A 187      -10.719  38.172  30.020  1.00  0.00      0.163 HD
ATOM   2790  CA  ILE A 187      -11.916  38.394  31.754  1.00 15.86      0.180 C
ATOM   2792  C   ILE A 187      -11.394  37.170  32.478  1.00 14.88      0.241 C
ATOM   2793  O   ILE A 187      -10.844  36.247  31.842  1.00 15.32     -0.271 OA
ATOM   2794  CB  ILE A 187      -13.260  37.976  31.064  1.00 22.73      0.013 C
ATOM   2796  CG1 ILE A 187      -14.085  39.184  30.570  1.00 21.69      0.002 C
ATOM   2799  CG2 ILE A 187      -14.155  37.122  31.938  1.00 18.54      0.012 C
ATOM   2803  CD1 ILE A 187      -14.557  40.046  31.736  1.00 23.52      0.005 C
ATOM   2807  N   SER A 188      -11.549  37.112  33.805  1.00 12.82     -0.344 N
ATOM   2808  HN  SER A 188      -11.879  37.924  34.326  1.00  0.00      0.163 HD
ATOM   2809  CA  SER A 188      -11.227  35.828  34.512  1.00 11.30      0.200 C
ATOM   2811  C   SER A 188      -12.393  35.649  35.462  1.00 14.13      0.243 C
ATOM   2812  O   SER A 188      -13.357  36.401  35.390  1.00 14.44     -0.271 OA
ATOM   2813  CB  SER A 188      -9.865  35.810  35.203  1.00 15.53      0.199 C
ATOM   2816  OG  SER A 188      -9.812  36.813  36.233  1.00 11.77     -0.398 OA
ATOM   2817  HG  SER A 188      -8.965  36.802  36.663  1.00  0.00      0.209 HD
ATOM   2818  N   ILE A 189      -12.341  34.707  36.423  1.00 14.74     -0.346 N
ATOM   2819  HN  ILE A 189      -11.489  34.171  36.584  1.00  0.00      0.163 HD
ATOM   2820  CA  ILE A 189      -13.537  34.473  37.229  1.00 14.48      0.180 C
ATOM   2822  C   ILE A 189      -13.879  35.660  38.103  1.00 13.04      0.241 C
ATOM   2823  O   ILE A 189      -15.097  35.979  38.207  1.00 13.55     -0.271 OA
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ATOM   2824  CB  ILE A 189     -13.316  33.202  38.083  1.00 13.95     0.013 C
ATOM   2826  CG1 ILE A 189     -13.412  31.976  37.117  1.00 16.96     0.002 C
ATOM   2829  CG2 ILE A 189     -14.302  33.085  39.214  1.00 15.79     0.012 C
ATOM   2833  CD1 ILE A 189     -13.158  30.686  37.913  1.00 22.82     0.005 C
ATOM   2837  N   ASP A 190     -12.878  36.352  38.648  1.00 10.34    -0.345 N
ATOM   2838  HN  ASP A 190     -11.901  36.124  38.466  1.00  0.00     0.163 HD
ATOM   2839  CA  ASP A 190     -13.274  37.476  39.537  1.00 13.42     0.186 C
ATOM   2841  C   ASP A 190     -13.886  38.649  38.745  1.00 16.61     0.241 C
ATOM   2842  O   ASP A 190     -14.387  39.601  39.406  1.00 15.09    -0.271 OA
ATOM   2843  CB  ASP A 190     -12.086  37.991  40.362  1.00 14.80     0.147 C
ATOM   2846  CG  ASP A 190     -11.758  37.171  41.607  1.00 19.62     0.175 C
ATOM   2847  OD1 ASP A 190     -12.486  36.171  41.875  1.00 13.77    -0.648 OA
ATOM   2848  OD2 ASP A 190     -10.793  37.531  42.335  1.00 14.26    -0.648 OA
ATOM   2849  N   GLY A 191     -13.680  38.764  37.430  1.00 14.84    -0.351 N
ATOM   2850  HN  GLY A 191     -13.168  38.036  36.932  1.00  0.00     0.163 HD
ATOM   2851  CA  GLY A 191     -14.186  39.932  36.695  1.00 18.53     0.225 C
ATOM   2854  C   GLY A 191     -13.157  40.394  35.647  1.00 19.82     0.236 C
ATOM   2855  O   GLY A 191     -12.427  39.572  35.095  1.00 14.77    -0.272 OA
ATOM   2856  N   HIS A 192     -13.120  41.690  35.372  1.00 15.68    -0.346 N
ATOM   2857  HN  HIS A 192     -13.762  42.320  35.853  1.00  0.00     0.163 HD
ATOM   2858  CA  HIS A 192     -12.180  42.236  34.395  1.00 17.32     0.182 C
ATOM   2860  C   HIS A 192     -10.775  42.130  34.962  1.00 19.80     0.241 C
ATOM   2861  O   HIS A 192     -10.532  42.658  36.057  1.00 13.79    -0.271 OA
ATOM   2862  CB  HIS A 192     -12.547  43.699  34.103  1.00 22.19     0.093 C
ATOM   2865  CG  HIS A 192     -13.821  43.732  33.297  1.00 27.67     0.028 A
ATOM   2866  CD2 HIS A 192     -15.121  43.661  33.659  1.00 37.55     0.114 A
ATOM   2868  ND1 HIS A 192     -13.793  43.835  31.923  1.00 36.45    -0.354 N
ATOM   2869  HD1 HIS A 192     -12.951  43.900  31.351  1.00  0.00     0.166 HD
ATOM   2870  CE1 HIS A 192     -15.026  43.836  31.468  1.00 41.32     0.180 A
ATOM   2872  NE2 HIS A 192     -15.841  43.737  32.497  1.00 38.93    -0.360 N
ATOM   2873  HE2 HIS A 192     -16.859  43.719  32.437  1.00  0.00     0.166 HD
ATOM   2874  N   VAL A 193      -9.857  41.539  34.197  1.00 15.81    -0.346 N
ATOM   2875  HN  VAL A 193     -10.091  41.285  33.237  1.00  0.00     0.163 HD
ATOM   2876  CA  VAL A 193      -8.532  41.252  34.707  1.00 16.00     0.180 C
ATOM   2878  C   VAL A 193      -7.616  42.411  35.006  1.00 17.56     0.241 C
ATOM   2879  O   VAL A 193      -6.663  42.173  35.754  1.00 15.80    -0.271 OA
ATOM   2880  CB  VAL A 193      -7.724  40.326  33.740  1.00 20.74     0.009 C
ATOM   2882  CG1 VAL A 193      -8.501  39.042  33.530  1.00 15.39     0.012 C
ATOM   2886  CG2 VAL A 193      -7.384  41.016  32.434  1.00 15.49     0.012 C
ATOM   2890  N   GLU A 194      -7.863  43.636  34.569  1.00 12.45    -0.346 N
ATOM   2891  HN  GLU A 194      -8.701  43.819  34.018  1.00  0.00     0.163 HD
ATOM   2892  CA  GLU A 194      -6.937  44.730  34.874  1.00 14.96     0.177 C
ATOM   2894  C   GLU A 194      -6.785  44.986  36.379  1.00 16.99     0.240 C
ATOM   2895  O   GLU A 194      -5.758  45.575  36.754  1.00 18.19    -0.271 OA
ATOM   2896  CB  GLU A 194      -7.356  46.067  34.269  1.00 23.10     0.045 C
ATOM   2899  CG  GLU A 194      -7.734  45.901  32.794  1.00 42.42     0.116 C
ATOM   2902  CD  GLU A 194      -9.248  45.649  32.827  1.00 52.11     0.172 C
ATOM   2903  OE1 GLU A 194      -9.943  46.496  33.437  1.00 64.18    -0.648 OA
ATOM   2904  OE2 GLU A 194      -9.635  44.596  32.305  1.00 38.58    -0.648 OA
ATOM   2905  N   GLY A 195      -7.696  44.561  37.227  1.00 17.11    -0.351 N
ATOM   2906  HN  GLY A 195      -8.548  44.113  36.889  1.00  0.00     0.163 HD
ATOM   2907  CA  GLY A 195      -7.469  44.741  38.679  1.00 13.54     0.225 C
ATOM   2910  C   GLY A 195      -6.333  43.894  39.231  1.00 14.76     0.236 C
ATOM   2911  O   GLY A 195      -5.864  44.135  40.365  1.00 17.01    -0.272 OA
ATOM   2912  N   TRP A 196      -5.941  42.821  38.540  1.00 11.59    -0.346 N
ATOM   2913  HN  TRP A 196      -6.337  42.646  37.617  1.00  0.00     0.163 HD
ATOM   2914  CA  TRP A 196      -4.952  41.893  39.087  1.00  8.91     0.181 C
ATOM   2916  C   TRP A 196      -4.016  41.337  38.025  1.00 11.91     0.241 C
ATOM   2917  O   TRP A 196      -3.140  40.532  38.398  1.00 12.37    -0.271 OA
ATOM   2918  CB  TRP A 196      -5.691  40.711  39.797  1.00  9.20     0.075 C
ATOM   2921  CG  TRP A 196      -6.788  40.103  38.984  1.00 11.39    -0.028 A
ATOM   2922  CD1 TRP A 196      -6.711  39.074  38.085  1.00 12.60     0.096 A
ATOM   2924  CD2 TRP A 196      -8.177  40.468  39.039  1.00 11.05    -0.002 A
ATOM   2925  CE2 TRP A 196      -8.866  39.675  38.124  1.00 14.41     0.042 A
ATOM   2926  CE3 TRP A 196      -8.862  41.476  39.751  1.00 12.02     0.014 A
ATOM   2928  NE1 TRP A 196      -7.956  38.794  37.567  1.00 13.50    -0.365 N
ATOM   2929  HE1 TRP A 196      -8.170  38.063  36.889  1.00  0.00     0.165 HD
ATOM   2930  CZ2 TRP A 196     -10.241  39.796  37.929  1.00 13.27     0.030 A
ATOM   2932  CZ3 TRP A 196     -10.226  41.601  39.549  1.00 15.36     0.001 A
ATOM   2934  CH2 TRP A 196     -10.893  40.760  38.647  1.00 15.52     0.002 A
ATOM   2936  N   PHE A 197      -4.128  41.769  36.759  1.00  9.41    -0.346 N
ATOM   2937  HN  PHE A 197      -4.811  42.486  36.515  1.00  0.00     0.163 HD
ATOM   2938  CA  PHE A 197      -3.248  41.191  35.728  1.00  9.50     0.180 C
ATOM   2940  C   PHE A 197      -2.940  42.302  34.718  1.00 11.77     0.241 C
ATOM   2941  O   PHE A 197      -3.809  42.544  33.872  1.00 10.25    -0.271 OA
ATOM   2942  CB  PHE A 197      -3.899  39.967  35.085  1.00  9.69     0.073 C
ATOM   2945  CG  PHE A 197      -3.056  39.310  34.008  1.00  7.95    -0.056 A
ATOM   2946  CD1 PHE A 197      -1.701  39.102  34.160  1.00 11.24     0.007 A
ATOM   2948  CD2 PHE A 197      -3.719  38.880  32.862  1.00 16.73     0.007 A
ATOM   2950  CE1 PHE A 197      -0.990  38.481  33.144  1.00 15.51     0.001 A
ATOM   2952  CE2 PHE A 197      -3.010  38.237  31.860  1.00 17.10     0.001 A
ATOM   2954  CZ  PHE A 197      -1.654  38.068  32.001  1.00 13.18     0.000 A
ATOM   2956  N   THR A 198      -1.773  42.949  34.837  1.00 11.46    -0.344 N
ATOM   2957  HN  THR A 198      -1.085  42.661  35.533  1.00  0.00     0.163 HD
ATOM   2958  CA  THR A 198      -1.503  44.100  33.928  1.00 12.30     0.205 C
ATOM   2960  C   THR A 198      -0.225  43.929  33.128  1.00 15.26     0.243 C
ATOM   2961  O   THR A 198       0.272  44.922  32.543  1.00 12.48    -0.271 OA
ATOM   2962  CB  THR A 198      -1.380  45.414  34.771  1.00 10.42     0.146 C
ATOM   2964  CG2 THR A 198      -2.727  45.772  35.424  1.00 13.25     0.042 C
ATOM   2968  OG1 THR A 198      -0.508  45.177  35.850  1.00 13.26    -0.393 OA
ATOM   2969  HG1 THR A 198       0.323  44.956  35.447  1.00  0.00     0.210 HD
ATOM   2970  N   ASP A 199       0.312  42.715  33.017  1.00  8.03    -0.345 N
ATOM   2971  HN  ASP A 199      -0.159  41.923  33.455  1.00  0.00     0.163 HD
ATOM   2972  CA  ASP A 199       1.543  42.486  32.294  1.00  5.89     0.186 C
ATOM   2974  C   ASP A 199       1.445  42.971  30.836  1.00  9.74     0.241 C
ATOM   2975  O   ASP A 199       0.390  42.725  30.237  1.00  8.52    -0.271 OA
ATOM   2976  CB  ASP A 199       1.857  40.969  32.074  1.00  8.71     0.147 C
ATOM   2979  CG  ASP A 199       2.198  40.279  33.400  1.00 14.80     0.175 C
ATOM   2980  OD1 ASP A 199       2.149  40.922  34.443  1.00 11.19    -0.648 OA
ATOM   2981  OD2 ASP A 199       2.474  39.077  33.401  1.00 10.65    -0.648 OA
ATOM   2982  N   ASP A 200       2.550  43.395  30.297  1.00  9.43    -0.345 N
ATOM   2983  HN  ASP A 200       3.371  43.584  30.872  1.00  0.00     0.163 HD
ATOM   2984  CA  ASP A 200       2.591  43.601  28.807  1.00  7.81     0.186 C
ATOM   2986  C   ASP A 200       3.045  42.209  28.348  1.00  7.92     0.241 C
ATOM   2987  O   ASP A 200       4.212  41.857  28.304  1.00  8.52    -0.271 OA
ATOM   2988  CB  ASP A 200       3.615  44.698  28.480  1.00  9.00     0.147 C
ATOM   2991  CG  ASP A 200       3.765  44.880  26.982  1.00 19.15     0.175 C
ATOM   2992  OD1 ASP A 200       3.392  43.977  26.223  1.00  9.76    -0.648 OA
ATOM   2993  OD2 ASP A 200       4.317  45.861  26.492  1.00 13.69    -0.648 OA
ATOM   2994  N   THR A 201       2.053  41.312  28.078  1.00  8.15    -0.344 N
ATOM   2995  HN  THR A 201       1.078  41.610  28.080  1.00  0.00     0.163 HD
ATOM   2996  CA  THR A 201       2.400  39.905  27.782  1.00 10.33     0.205 C
ATOM   2998  C   THR A 201       3.253  39.778  26.551  1.00  9.36     0.243 C
ATOM   2999  O   THR A 201       4.155  38.941  26.487  1.00  8.18    -0.271 OA
ATOM   3000  CB  THR A 201       1.071  39.121  27.726  1.00  9.60     0.146 C
ATOM   3002  CG2 THR A 201       1.240  37.670  27.275  1.00 13.49     0.042 C
ATOM   3006  OG1 THR A 201       0.598  39.117  29.079  1.00 10.70    -0.393 OA
ATOM   3007  HG1 THR A 201       0.493  40.019  29.359  1.00  0.00     0.210 HD
ATOM   3008  N   ALA A 202       3.019  40.605  25.502  1.00  8.62    -0.346 N
ATOM   3009  HN  ALA A 202       2.254  41.279  25.518  1.00  0.00     0.163 HD
ATOM   3010  CA  ALA A 202       3.910  40.491  24.345  1.00  5.63     0.172 C
ATOM   3012  C   ALA A 202       5.338  40.760  24.693  1.00  9.70     0.240 C
ATOM   3013  O   ALA A 202       6.277  40.064  24.254  1.00  9.01    -0.271 OA
ATOM   3014  CB  ALA A 202       3.424  41.486  23.241  1.00  9.95     0.042 C
ATOM   3018  N   MET A 203       5.609  41.837  25.498  1.00  8.60    -0.346 N
ATOM   3019  HN  MET A 203       4.851  42.400  25.883  1.00  0.00     0.163 HD
ATOM   3020  CA  MET A 203       7.002  42.165  25.795  1.00  8.33     0.177 C
ATOM   3022  C   MET A 203       7.623  41.083  26.684  1.00  9.21     0.241 C
ATOM   3023  O   MET A 203       8.795  40.751  26.547  1.00  8.22    -0.271 OA
ATOM   3024  CB  MET A 203       7.011  43.528  26.537  1.00  7.52     0.045 C
ATOM   3027  CG  MET A 203       8.375  43.991  27.014  1.00 20.46     0.076 C
ATOM   3030  SD  MET A 203       8.251  45.600  27.899  1.00 24.61    -0.173 SA
ATOM   3031  CE  MET A 203       7.376  46.597  26.688  1.00 22.75     0.089 C
ATOM   3035  N   ARG A 204       6.805  40.513  27.566  1.00  8.34    -0.346 N
ATOM   3036  HN  ARG A 204       5.843  40.831  27.683  1.00  0.00     0.163 HD
ATOM   3037  CA  ARG A 204       7.360  39.385  28.379  1.00 10.62     0.176 C
ATOM   3039  C   ARG A 204       7.819  38.240  27.510  1.00  7.08     0.241 C
ATOM   3040  O   ARG A 204       8.874  37.613  27.740  1.00  7.40    -0.271 OA
ATOM   3041  CB  ARG A 204       6.207  38.953  29.307  1.00  6.24     0.036 C
ATOM   3044  CG  ARG A 204       6.550  37.706  30.148  1.00  9.72     0.023 C
ATOM   3047  CD  ARG A 204       5.288  37.207  30.861  1.00  9.18     0.138 C
ATOM   3050  NE  ARG A 204       5.371  35.831  31.300  1.00  9.52    -0.227 N
ATOM   3051  HE  ARG A 204       6.320  35.481  31.430  1.00  0.00     0.177 HD
ATOM   3052  CZ  ARG A 204       4.416  34.951  31.561  1.00  8.85     0.665 C
ATOM   3053  NH1 ARG A 204       3.095  35.169  31.410  1.00  6.73    -0.235 N
ATOM   3054 1HH1 ARG A 204       2.778  36.081  31.081  1.00  0.00     0.174 HD
ATOM   3055 2HH1 ARG A 204       2.360  34.491  31.611  1.00  0.00     0.174 HD
ATOM   3056  NH2 ARG A 204       4.833  33.752  31.994  1.00  9.24    -0.235 N
ATOM   3057 1HH2 ARG A 204       5.833  33.587  32.108  1.00  0.00     0.174 HD
ATOM   3058 2HH2 ARG A 204       4.098  33.074  32.195  1.00  0.00     0.174 HD
ATOM   3059  N   PHE A 205       7.003  37.817  26.505  1.00  4.76    -0.346 N
ATOM   3060  HN  PHE A 205       6.123  38.305  26.339  1.00  0.00     0.163 HD
ATOM   3061  CA  PHE A 205       7.357  36.692  25.668  1.00  6.80     0.180 C
ATOM   3063  C   PHE A 205       8.491  37.036  24.715  1.00 10.18     0.241 C
ATOM   3064  O   PHE A 205       9.363  36.194  24.481  1.00  8.73    -0.271 OA
ATOM   3065  CB  PHE A 205       6.126  36.128  24.888  1.00  6.73     0.073 C
ATOM   3068  CG  PHE A 205       5.418  35.104  25.765  1.00 12.01    -0.056 A
ATOM   3069  CD1 PHE A 205       4.711  35.506  26.873  1.00  9.96     0.007 A
ATOM   3071  CD2 PHE A 205       5.532  33.757  25.450  1.00 11.53     0.007 A
ATOM   3073  CE1 PHE A 205       4.075  34.560  27.700  1.00 10.74     0.001 A
ATOM   3075  CE2 PHE A 205       4.876  32.814  26.244  1.00  9.98     0.001 A
ATOM   3077  CZ  PHE A 205       4.163  33.217  27.349  1.00  9.37     0.000 A
ATOM   3079  N   GLU A 206       8.620  38.303  24.273  1.00  7.87    -0.346 N
ATOM   3080  HN  GLU A 206       7.893  38.996  24.451  1.00  0.00     0.163 HD
ATOM   3081  CA  GLU A 206       9.844  38.662  23.523  1.00  9.17     0.177 C
ATOM   3083  C   GLU A 206      11.088  38.542  24.390  1.00 10.08     0.241 C
ATOM   3084  O   GLU A 206      12.206  38.199  23.911  1.00  8.94    -0.271 OA
ATOM   3085  CB  GLU A 206       9.644  40.169  23.131  1.00  8.45     0.045 C
ATOM   3088  CG  GLU A 206       8.805  40.059  21.849  1.00 15.31     0.116 C
ATOM   3091  CD  GLU A 206       8.496  41.406  21.243  1.00 27.18     0.172 C
ATOM   3092  OE1 GLU A 206       8.487  42.428  21.943  1.00 23.08    -0.648 OA
ATOM   3093  OE2 GLU A 206       8.215  41.332  20.039  1.00 25.02    -0.648 OA
ATOM   3094  N   ALA A 207      10.912  38.795  25.701  1.00 10.64    -0.346 N
ATOM   3095  HN  ALA A 207       9.999  39.080  26.056  1.00  0.00     0.163 HD
ATOM   3096  CA  ALA A 207      12.065  38.653  26.619  1.00  9.35     0.172 C
ATOM   3098  C   ALA A 207      12.465  37.186  26.778  1.00 10.50     0.240 C
ATOM   3099  O   ALA A 207      13.626  36.924  27.133  1.00 10.37    -0.271 OA
ATOM   3100  CB  ALA A 207      11.691  39.207  28.012  1.00  8.49     0.042 C
ATOM   3104  N   TYR A 208      11.554  36.241  26.550  1.00  5.64    -0.346 N
ATOM   3105  HN  TYR A 208      10.584  36.516  26.394  1.00  0.00     0.163 HD
ATOM   3106  CA  TYR A 208      11.900  34.827  26.516  1.00  7.33     0.180 C
ATOM   3108  C   TYR A 208      12.517  34.415  25.169  1.00 12.26     0.241 C
ATOM   3109  O   TYR A 208      12.837  33.255  24.937  1.00 11.20    -0.271 OA
ATOM   3110  CB  TYR A 208      10.632  33.958  26.709  1.00  8.90     0.073 C
ATOM   3113  CG  TYR A 208       9.904  34.083  28.026  1.00 12.81    -0.056 A
ATOM   3114  CD1 TYR A 208      10.636  34.391  29.194  1.00 12.32     0.010 A
ATOM   3116  CD2 TYR A 208       8.543  33.862  28.129  1.00  7.95     0.010 A
ATOM   3118  CE1 TYR A 208       9.950  34.488  30.401  1.00 13.41     0.037 A
ATOM   3120  CE2 TYR A 208       7.855  33.983  29.352  1.00  8.87     0.037 A
ATOM   3122  CZ  TYR A 208       8.595  34.274  30.487  1.00 10.56     0.065 A
ATOM   3123  OH  TYR A 208       7.964  34.405  31.704  1.00 10.84    -0.361 OA
ATOM   3124  HH  TYR A 208       8.471  34.604  32.482  1.00  0.00     0.217 HD
ATOM   3125  N   GLY A 209      12.606  35.296  24.186  1.00  8.47    -0.351 N
ATOM   3126  HN  GLY A 209      12.307  36.261  24.324  1.00  0.00     0.163 HD
ATOM   3127  CA  GLY A 209      13.149  34.852  22.878  1.00  9.35     0.225 C
ATOM   3130  C   GLY A 209      12.018  34.247  22.023  1.00 13.94     0.236 C
ATOM   3131  O   GLY A 209      12.331  33.582  21.042  1.00 12.99    -0.272 OA
ATOM   3132  N   TRP A 210      10.738  34.494  22.248  1.00  8.46    -0.346 N
ATOM   3133  HN  TRP A 210      10.469  35.058  23.054  1.00  0.00     0.163 HD
ATOM   3134  CA  TRP A 210       9.707  33.971  21.359  1.00  7.82     0.181 C
ATOM   3136  C   TRP A 210       9.462  34.987  20.227  1.00 12.19     0.241 C
ATOM   3137  O   TRP A 210       9.643  36.215  20.389  1.00 11.89    -0.271 OA
ATOM   3138  CB  TRP A 210       8.362  33.831  22.124  1.00  7.30     0.075 C
ATOM   3141  CG  TRP A 210       8.318  32.643  23.049  1.00  7.12    -0.028 A
ATOM   3142  CD1 TRP A 210       9.301  32.250  23.936  1.00  6.65     0.096 A
ATOM   3144  CD2 TRP A 210       7.292  31.654  23.142  1.00  6.39    -0.002 A
ATOM   3145  CE2 TRP A 210       7.642  30.742  24.126  1.00  7.65     0.042 A
ATOM   3146  CE3 TRP A 210       6.064  31.487  22.462  1.00  8.40     0.014 A
ATOM   3148  NE1 TRP A 210       8.876  31.090  24.589  1.00  8.91    -0.365 N
ATOM   3149  HE1 TRP A 210       9.405  30.584  25.299  1.00  0.00     0.165 HD
ATOM   3150  CZ2 TRP A 210       6.826  29.645  24.450  1.00  6.80     0.030 A
ATOM   3152  CZ3 TRP A 210       5.227  30.433  22.811  1.00 16.12     0.001 A
ATOM   3154  CH2 TRP A 210       5.620  29.502  23.796  1.00  9.79     0.002 A
ATOM   3156  N   HIS A 211       8.891  34.530  19.144  1.00 10.52    -0.346 N
ATOM   3157  HN  HIS A 211       8.830  33.517  19.038  1.00  0.00     0.163 HD
ATOM   3158  CA  HIS A 211       8.327  35.361  18.062  1.00  9.70     0.182 C
ATOM   3160  C   HIS A 211       6.909  35.689  18.479  1.00 10.62     0.241 C
ATOM   3161  O   HIS A 211       6.124  34.797  18.903  1.00 12.05    -0.271 OA
ATOM   3162  CB  HIS A 211       8.332  34.493  16.786  1.00  9.99     0.093 C
ATOM   3165  CG  HIS A 211       7.408  34.967  15.690  1.00 11.48     0.028 A
ATOM   3166  CD2 HIS A 211       7.390  36.126  14.998  1.00 13.39     0.114 A
ATOM   3168  ND1 HIS A 211       6.394  34.181  15.167  1.00 11.60    -0.354 N
ATOM   3169  HD1 HIS A 211       6.172  33.234  15.473  1.00  0.00     0.166 HD
ATOM   3170  CE1 HIS A 211       5.757  34.835  14.216  1.00 16.58     0.180 A
ATOM   3172  NE2 HIS A 211       6.345  36.026  14.077  1.00 13.57    -0.360 N
ATOM   3173  HE2 HIS A 211       6.075  36.746  13.407  1.00  0.00     0.166 HD
ATOM   3174  N   VAL A 212       6.463  36.945  18.519  1.00  7.72    -0.346 N
ATOM   3175  HN  VAL A 212       7.065  37.705  18.202  1.00  0.00     0.163 HD
ATOM   3176  CA  VAL A 212       5.128  37.242  19.010  1.00  5.32     0.180 C
ATOM   3178  C   VAL A 212       4.327  37.989  17.940  1.00 11.35     0.241 C
ATOM   3179  O   VAL A 212       4.939  38.865  17.299  1.00 13.17    -0.271 OA
ATOM   3180  CB  VAL A 212       5.219  38.148  20.265  1.00 12.39     0.009 C
ATOM   3182  CG1 VAL A 212       3.801  38.565  20.661  1.00 10.14     0.012 C
ATOM   3186  CG2 VAL A 212       5.948  37.427  21.400  1.00 17.00     0.012 C
ATOM   3190  N   ILE A 213       3.096  37.662  17.707  1.00 11.40    -0.346 N
ATOM   3191  HN  ILE A 213       2.714  36.858  18.205  1.00  0.00     0.163 HD
ATOM   3192  CA  ILE A 213       2.208  38.378  16.766  1.00  9.73     0.180 C
ATOM   3194  C   ILE A 213       1.105  39.004  17.621  1.00 13.59     0.241 C
ATOM   3195  O   ILE A 213       0.374  38.296  18.300  1.00  9.53    -0.271 OA
ATOM   3196  CB  ILE A 213       1.584  37.468  15.700  1.00 13.57     0.013 C
ATOM   3198  CG1 ILE A 213       2.701  36.827  14.864  1.00 17.73     0.002 C
ATOM   3201  CG2 ILE A 213       0.640  38.301  14.784  1.00  7.15     0.012 C
ATOM   3205  CD1 ILE A 213       2.198  35.946  13.722  1.00 15.59     0.005 C
ATOM   3209  N   ARG A 214       1.077  40.331  17.686  1.00 11.15    -0.346 N
ATOM   3210  HN  ARG A 214       1.716  40.865  17.097  1.00  0.00     0.163 HD
ATOM   3211  CA  ARG A 214       0.167  41.051  18.568  1.00 11.21     0.176 C
ATOM   3213  C   ARG A 214      -1.152  41.372  17.894  1.00 12.98     0.241 C
ATOM   3214  O   ARG A 214      -1.158  41.386  16.638  1.00 11.76    -0.271 OA
ATOM   3215  CB  ARG A 214       0.865  42.442  18.746  1.00 10.72     0.036 C
ATOM   3218  CG  ARG A 214       1.938  42.465  19.875  1.00 13.81     0.023 C
ATOM   3221  CD  ARG A 214       2.763  43.771  19.649  1.00 18.13     0.138 C
ATOM   3224  NE  ARG A 214       3.745  43.952  20.728  1.00 18.86    -0.227 N
ATOM   3225  HE  ARG A 214       3.464  44.521  21.526  1.00  0.00     0.177 HD
ATOM   3226  CZ  ARG A 214       4.967  43.435  20.748  1.00 25.26     0.665 C
ATOM   3227  NH1 ARG A 214       5.449  42.636  19.788  1.00 18.51    -0.235 N
ATOM   3228 1HH1 ARG A 214       4.866  42.418  18.980  1.00  0.00     0.174 HD
ATOM   3229 2HH1 ARG A 214       6.388  42.239  19.803  1.00  0.00     0.174 HD
ATOM   3230  NH2 ARG A 214       5.730  43.720  21.806  1.00 24.06    -0.235 N
ATOM   3231 1HH2 ARG A 214       5.363  44.329  22.537  1.00  0.00     0.174 HD
ATOM   3232 2HH2 ARG A 214       6.669  43.323  21.821  1.00  0.00     0.174 HD
ATOM   3233  N   ASP A 215      -2.186  41.642  18.687  1.00  8.91    -0.346 N
ATOM   3234  HN  ASP A 215      -2.094  41.424  19.679  1.00  0.00     0.163 HD
ATOM   3235  CA  ASP A 215      -3.430  42.223  18.237  1.00 12.24     0.186 C
ATOM   3237  C   ASP A 215      -4.140  41.539  17.088  1.00 15.91     0.241 C
ATOM   3238  O   ASP A 215      -4.598  42.194  16.148  1.00 14.41    -0.271 OA
ATOM   3239  CB  ASP A 215      -3.131  43.704  17.813  1.00 13.17     0.147 C
ATOM   3242  CG  ASP A 215      -2.709  44.528  19.050  1.00 12.89     0.175 C
ATOM   3243  OD1 ASP A 215      -3.399  44.446  20.088  1.00 18.85    -0.648 OA
ATOM   3244  OD2 ASP A 215      -1.669  45.180  18.992  1.00 12.15    -0.648 OA
ATOM   3245  N   ILE A 216      -4.188  40.216  17.093  1.00 12.21    -0.346 N
ATOM   3246  HN  ILE A 216      -3.720  39.716  17.849  1.00  0.00     0.163 HD
ATOM   3247  CA  ILE A 216      -4.875  39.443  16.075  1.00  9.35     0.180 C
ATOM   3249  C   ILE A 216      -6.362  39.497  16.388  1.00 10.88     0.241 C
ATOM   3250  O   ILE A 216      -6.761  39.315  17.535  1.00 12.00    -0.271 OA
ATOM   3251  CB  ILE A 216      -4.418  37.973  16.035  1.00  8.38     0.013 C
ATOM   3253  CG1 ILE A 216      -2.909  37.913  15.672  1.00 12.87     0.002 C
ATOM   3256  CG2 ILE A 216      -5.225  37.231  14.982  1.00 14.30     0.012 C
ATOM   3260  CD1 ILE A 216      -2.298  36.560  16.050  1.00 10.91     0.005 C
ATOM   3264  N   ASP A 217      -7.185  39.865  15.394  1.00 10.62    -0.345 N
ATOM   3265  HN  ASP A 217      -6.785  40.160  14.503  1.00  0.00     0.163 HD
ATOM   3266  CA  ASP A 217      -8.633  39.856  15.550  1.00 14.25     0.186 C
ATOM   3268  C   ASP A 217      -9.023  38.370  15.576  1.00 15.13     0.241 C
ATOM   3269  O   ASP A 217      -9.015  37.724  14.515  1.00 13.27    -0.271 OA
ATOM   3270  CB  ASP A 217      -9.366  40.529  14.386  1.00 12.65     0.147 C
ATOM   3273  CG  ASP A 217     -10.859  40.588  14.579  1.00 13.62     0.175 C
ATOM   3274  OD1 ASP A 217     -11.433  39.834  15.365  1.00 10.71    -0.648 OA
ATOM   3275  OD2 ASP A 217     -11.498  41.453  13.912  1.00 14.61    -0.648 OA
ATOM   3276  N   GLY A 218      -9.410  37.904  16.779  1.00 12.06    -0.351 N
ATOM   3277  HN  GLY A 218      -9.499  38.540  17.572  1.00  0.00     0.163 HD
ATOM   3278  CA  GLY A 218      -9.703  36.476  16.942  1.00 10.43     0.225 C
ATOM   3281  C   GLY A 218     -11.032  36.044  16.333  1.00 12.38     0.236 C
ATOM   3282  O   GLY A 218     -11.369  34.854  16.441  1.00 13.12    -0.272 OA
ATOM   3283  N   HIS A 219     -11.810  36.980  15.759  1.00 10.40    -0.346 N
ATOM   3284  HN  HIS A 219     -11.526  37.959  15.775  1.00  0.00     0.163 HD
ATOM   3285  CA  HIS A 219     -13.067  36.591  15.111  1.00 11.74     0.182 C
ATOM   3287  C   HIS A 219     -12.965  36.801  13.605  1.00 15.72     0.241 C
ATOM   3288  O   HIS A 219     -13.973  36.742  12.895  1.00 16.55    -0.271 OA
ATOM   3289  CB  HIS A 219     -14.263  37.332  15.732  1.00  9.19     0.093 C
ATOM   3292  CG  HIS A 219     -14.352  37.001  17.201  1.00 11.58     0.028 A
ATOM   3293  CD2 HIS A 219     -14.188  37.766  18.308  1.00 16.70     0.114 A
ATOM   3295  ND1 HIS A 219     -14.580  35.695  17.603  1.00 11.96    -0.354 N
ATOM   3296  HD1 HIS A 219     -14.718  34.886  16.997  1.00  0.00     0.166 HD
ATOM   3297  CE1 HIS A 219     -14.584  35.701  18.937  1.00 15.75     0.180 A
ATOM   3299  NE2 HIS A 219     -14.348  36.915  19.400  1.00 15.66    -0.360 N
ATOM   3300  HE2 HIS A 219     -14.293  37.182  20.383  1.00  0.00     0.166 HD
ATOM   3301  N   ASP A 220     -11.778  37.004  13.072  1.00  9.74    -0.345 N
ATOM   3302  HN  ASP A 220     -10.958  36.994  13.678  1.00  0.00     0.163 HD
ATOM   3303  CA  ASP A 220     -11.595  37.243  11.642  1.00 13.71     0.186 C
ATOM   3305  C   ASP A 220     -10.718  36.162  11.043  1.00 12.80     0.241 C
ATOM   3306  O   ASP A 220      -9.496  36.166  11.244  1.00 12.45    -0.271 OA
ATOM   3307  CB  ASP A 220     -10.936  38.649  11.446  1.00 11.80     0.147 C
ATOM   3310  CG  ASP A 220     -10.831  38.936   9.947  1.00 17.95     0.175 C
ATOM   3311  OD1 ASP A 220     -11.856  38.902   9.242  1.00 17.22    -0.648 OA
ATOM   3312  OD2 ASP A 220      -9.749  39.209   9.440  1.00 14.50    -0.648 OA
ATOM   3313  N   ALA A 221     -11.307  35.147  10.390  1.00 14.12    -0.346 N
ATOM   3314  HN  ALA A 221     -12.323  35.151  10.299  1.00  0.00     0.163 HD
ATOM   3315  CA  ALA A 221     -10.553  34.029   9.800  1.00 18.20     0.172 C
ATOM   3317  C   ALA A 221      -9.339  34.413   8.995  1.00 13.59     0.240 C
ATOM   3318  O   ALA A 221      -8.263  33.829   9.117  1.00 12.12    -0.271 OA
ATOM   3319  CB  ALA A 221     -11.536  33.176   8.944  1.00 13.59     0.042 C
ATOM   3323  N   ALA A 222      -9.432  35.432   8.075  1.00 12.60    -0.346 N
ATOM   3324  HN  ALA A 222     -10.310  35.933   7.938  1.00  0.00     0.163 HD
ATOM   3325  CA  ALA A 222      -8.255  35.775   7.307  1.00 16.22     0.172 C
ATOM   3327  C   ALA A 222      -7.098  36.282   8.155  1.00 12.15     0.240 C
ATOM   3328  O   ALA A 222      -5.942  36.031   7.820  1.00 14.81    -0.271 OA
ATOM   3329  CB  ALA A 222      -8.602  36.863   6.257  1.00 21.18     0.042 C
ATOM   3333  N   SER A 223      -7.368  37.089   9.204  1.00 12.39    -0.344 N
ATOM   3334  HN  SER A 223      -8.331  37.358   9.408  1.00  0.00     0.163 HD
ATOM   3335  CA  SER A 223      -6.285  37.572  10.039  1.00 11.57     0.200 C
ATOM   3337  C   SER A 223      -5.611  36.397  10.765  1.00 13.71     0.243 C
ATOM   3338  O   SER A 223      -4.407  36.370  10.941  1.00 12.16    -0.271 OA
ATOM   3339  CB  SER A 223      -6.816  38.500  11.184  1.00 14.22     0.199 C
ATOM   3342  OG  SER A 223      -7.392  39.621  10.535  1.00 20.49    -0.398 OA
ATOM   3343  HG  SER A 223      -7.714  40.184  11.229  1.00  0.00     0.209 HD
ATOM   3344  N   ILE A 224      -6.457  35.480  11.227  1.00 14.13    -0.346 N
ATOM   3345  HN  ILE A 224      -7.461  35.572  11.074  1.00  0.00     0.163 HD
ATOM   3346  CA  ILE A 224      -5.903  34.318  11.972  1.00 11.31     0.180 C
ATOM   3348  C   ILE A 224      -5.048  33.456  11.042  1.00 12.45     0.241 C
ATOM   3349  O   ILE A 224      -3.935  33.004  11.323  1.00 14.34    -0.271 OA
ATOM   3350  CB  ILE A 224      -7.054  33.513  12.559  1.00 14.12     0.013 C
ATOM   3352  CG1 ILE A 224      -7.856  34.234  13.659  1.00 11.92     0.002 C
ATOM   3355  CG2 ILE A 224      -6.490  32.214  13.168  1.00 17.55     0.012 C
ATOM   3359  CD1 ILE A 224      -9.274  33.756  13.785  1.00 12.83     0.005 C
ATOM   3363  N   LYS A 225      -5.594  33.191   9.813  1.00  9.85    -0.346 N
ATOM   3364  HN  LYS A 225      -6.517  33.549   9.568  1.00  0.00     0.163 HD
ATOM   3365  CA  LYS A 225      -4.827  32.382   8.854  1.00  9.43     0.176 C
ATOM   3367  C   LYS A 225      -3.467  32.950   8.547  1.00 12.61     0.241 C
ATOM   3368  O   LYS A 225      -2.415  32.290   8.481  1.00 10.54    -0.271 OA
ATOM   3369  CB  LYS A 225      -5.657  32.141   7.593  1.00 15.24     0.035 C
ATOM   3372  CG  LYS A 225      -4.929  31.208   6.621  1.00 20.52     0.004 C
ATOM   3375  CD  LYS A 225      -6.018  30.602   5.721  1.00 32.30     0.027 C
ATOM   3378  CE  LYS A 225      -5.343  29.670   4.705  1.00 38.24     0.229 C
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ATOM   3381  NZ  LYS A 225      -4.984  30.488   3.507  1.00 48.07   -0.079 N
ATOM   3382  HZ1 LYS A 225      -4.535  29.869   2.832  1.00  0.00    0.274 HD
ATOM   3383  HZ2 LYS A 225      -4.414  31.301   3.739  1.00  0.00    0.274 HD
ATOM   3384  HZ3 LYS A 225      -5.781  30.990   3.116  1.00  0.00    0.274 HD
ATOM   3385  N   ARG A 226      -3.399  34.272   8.295  1.00 12.26   -0.346 N
ATOM   3386  HN  ARG A 226      -4.251  34.832   8.326  1.00  0.00    0.163 HD
ATOM   3387  CA  ARG A 226      -2.139  34.913   7.981  1.00 12.36    0.176 C
ATOM   3389  C   ARG A 226      -1.169  34.853   9.162  1.00  9.86    0.241 C
ATOM   3390  O   ARG A 226       0.034  34.696   8.975  1.00 11.49   -0.271 OA
ATOM   3391  CB  ARG A 226      -2.475  36.362   7.612  1.00 18.74    0.036 C
ATOM   3394  CG  ARG A 226      -1.351  37.336   7.387  1.00 41.66    0.023 C
ATOM   3397  CD  ARG A 226      -1.939  38.725   7.087  1.00 63.09    0.138 C
ATOM   3400  NE  ARG A 226      -3.107  38.682   6.212  1.00 70.56   -0.227 N
ATOM   3401  HE  ARG A 226      -3.032  38.087   5.389  1.00  0.00    0.177 HD
ATOM   3402  CZ  ARG A 226      -4.259  39.331   6.368  1.00 72.30    0.665 C
ATOM   3403  NH1 ARG A 226      -4.446  40.127   7.413  1.00 74.21   -0.235 N
ATOM   3404 1HH1 ARG A 226      -5.329  40.624   7.533  1.00  0.00    0.174 HD
ATOM   3405 2HH1 ARG A 226      -3.697  40.237   8.097  1.00  0.00    0.174 HD
ATOM   3406  NH2 ARG A 226      -5.235  39.188   5.476  1.00 70.97   -0.235 N
ATOM   3407 1HH2 ARG A 226      -6.118  39.685   5.596  1.00  0.00    0.174 HD
ATOM   3408 2HH2 ARG A 226      -5.091  38.576   4.673  1.00  0.00    0.174 HD
ATOM   3409  N   ALA A 227      -1.690  34.984  10.395  1.00 11.19   -0.346 N
ATOM   3410  HN  ALA A 227      -2.690  35.126  10.534  1.00  0.00    0.163 HD
ATOM   3411  CA  ALA A 227      -0.762  34.915  11.538  1.00 13.39    0.172 C
ATOM   3413  C   ALA A 227      -0.204  33.506  11.676  1.00  9.11    0.240 C
ATOM   3414  O   ALA A 227       0.968  33.341  11.999  1.00 10.55   -0.271 OA
ATOM   3415  CB  ALA A 227      -1.548  35.275  12.807  1.00 15.44    0.042 C
ATOM   3419  N   VAL A 228      -1.041  32.477  11.387  1.00  8.98   -0.346 N
ATOM   3420  HN  VAL A 228      -2.006  32.628  11.092  1.00  0.00    0.163 HD
ATOM   3421  CA  VAL A 228      -0.462  31.118  11.528  1.00  6.37    0.180 C
ATOM   3423  C   VAL A 228       0.605  30.893  10.471  1.00  8.05    0.241 C
ATOM   3424  O   VAL A 228       1.659  30.273  10.653  1.00 10.87   -0.271 OA
ATOM   3425  CB  VAL A 228      -1.572  30.065  11.462  1.00 12.58    0.009 C
ATOM   3427  CG1 VAL A 228      -0.966  28.647  11.418  1.00 13.31    0.012 C
ATOM   3431  CG2 VAL A 228      -2.518  30.213  12.654  1.00 15.44    0.012 C
ATOM   3435  N   GLU A 229       0.324  31.335   9.211  1.00  9.12   -0.346 N
ATOM   3436  HN  GLU A 229      -0.582  31.752   8.998  1.00  0.00    0.163 HD
ATOM   3437  CA  GLU A 229       1.334  31.202   8.179  1.00  7.77    0.177 C
ATOM   3439  C   GLU A 229       2.648  31.842   8.558  1.00 11.66    0.241 C
ATOM   3440  O   GLU A 229       3.717  31.292   8.308  1.00 13.90   -0.271 OA
ATOM   3441  CB  GLU A 229       0.884  31.915   6.861  1.00 13.73    0.045 C
ATOM   3444  CG  GLU A 229      -0.287  31.059   6.369  1.00 13.76    0.116 C
ATOM   3447  CD  GLU A 229      -0.913  31.670   5.114  1.00 32.43    0.172 C
ATOM   3448  OE1 GLU A 229      -0.724  32.864   4.810  1.00 31.38   -0.648 OA
ATOM   3449  OE2 GLU A 229      -1.638  30.916   4.454  1.00 33.36   -0.648 OA
ATOM   3450  N   GLU A 230       2.539  33.067   9.122  1.00 13.79   -0.346 N
ATOM   3451  HN  GLU A 230       1.632  33.513   9.260  1.00  0.00    0.163 HD
ATOM   3452  CA  GLU A 230       3.780  33.720   9.524  1.00 14.36    0.177 C
ATOM   3454  C   GLU A 230       4.519  32.941  10.627  1.00 15.51    0.241 C
ATOM   3455  O   GLU A 230       5.763  32.866  10.641  1.00 14.82   -0.271 OA
ATOM   3456  CB  GLU A 230       3.466  35.148   9.984  1.00 17.83    0.045 C
ATOM   3459  CG  GLU A 230       4.716  35.922  10.369  1.00 33.93    0.116 C
ATOM   3462  CD  GLU A 230       4.455  37.254  11.050  1.00 45.25    0.172 C
ATOM   3463  OE1 GLU A 230       3.449  37.954  10.758  1.00 41.66   -0.648 OA
ATOM   3464  OE2 GLU A 230       5.297  37.615  11.922  1.00 34.28   -0.648 OA
ATOM   3465  N   ALA A 231       3.785  32.441  11.619  1.00 11.60   -0.346 N
ATOM   3466  HN  ALA A 231       2.773  32.569  11.626  1.00  0.00    0.163 HD
ATOM   3467  CA  ALA A 231       4.451  31.697  12.712  1.00 12.05    0.172 C
ATOM   3469  C   ALA A 231       5.109  30.416  12.221  1.00 11.24    0.240 C
ATOM   3470  O   ALA A 231       6.203  29.987  12.645  1.00 12.57   -0.271 OA
ATOM   3471  CB  ALA A 231       3.355  31.332  13.750  1.00 11.70    0.042 C
ATOM   3475  N   ARG A 232       4.464  29.770  11.226  1.00 11.61   -0.346 N
ATOM   3476  HN  ARG A 232       3.593  30.150  10.854  1.00  0.00    0.163 HD
ATOM   3477  CA  ARG A 232       5.006  28.538  10.681  1.00 12.51    0.176 C
ATOM   3479  C   ARG A 232       6.323  28.784   9.958  1.00 15.11    0.241 C
ATOM   3480  O   ARG A 232       7.204  27.918   9.915  1.00 17.10   -0.271 OA
ATOM   3481  CB  ARG A 232       3.998  27.805   9.775  1.00 12.80    0.036 C
ATOM   3484  CG  ARG A 232       2.986  27.009  10.598  1.00 13.61    0.023 C
ATOM   3487  CD  ARG A 232       1.777  26.632   9.743  1.00 22.91    0.138 C
ATOM   3490  NE  ARG A 232       2.284  25.816   8.611  1.00 29.75   -0.227 N
ATOM   3491  HE  ARG A 232       2.525  26.269   7.728  1.00  0.00    0.177 HD
ATOM   3492  CZ  ARG A 232       2.426  24.504   8.737  1.00 38.77    0.665 C
ATOM   3493  NH1 ARG A 232       2.077  23.890   9.859  1.00 30.70   -0.235 N
ATOM   3494 1HH1 ARG A 232       2.186  22.881   9.956  1.00  0.00    0.174 HD
ATOM   3495 2HH1 ARG A 232       1.713  24.439  10.638  1.00  0.00    0.174 HD
ATOM   3496  NH2 ARG A 232       2.896  23.795   7.730  1.00 40.31   -0.235 N
ATOM   3497 1HH2 ARG A 232       3.005  22.786   7.827  1.00  0.00    0.174 HD
ATOM   3498 2HH2 ARG A 232       3.165  24.267   6.867  1.00  0.00    0.174 HD
ATOM   3499  N   ALA A 233       6.536  29.967   9.421  1.00 13.82   -0.346 N
ATOM   3500  HN  ALA A 233       5.824  30.688   9.537  1.00  0.00    0.163 HD
ATOM   3501  CA  ALA A 233       7.741  30.295   8.669  1.00 18.97    0.172 C
ATOM   3503  C   ALA A 233       8.897  30.717   9.564  1.00 21.01    0.240 C
ATOM   3504  O   ALA A 233      10.004  30.830   9.060  1.00 16.18   -0.271 OA
ATOM   3505  CB  ALA A 233       7.483  31.396   7.637  1.00 19.19    0.042 C
ATOM   3509  N   VAL A 234       8.648  30.951  10.851  1.00 15.89   -0.346 N
ATOM   3510  HN  VAL A 234       7.688  30.903  11.193  1.00  0.00    0.163 HD
ATOM   3511  CA  VAL A 234       9.732  31.277  11.787  1.00 12.08    0.180 C
ATOM   3513  C   VAL A 234      10.181  29.941  12.343  1.00 15.76    0.241 C
ATOM   3514  O   VAL A 234       9.411  29.297  13.095  1.00 15.72   -0.271 OA
ATOM   3515  CB  VAL A 234       9.210  32.213  12.885  1.00 13.18    0.009 C
ATOM   3517  CG1 VAL A 234      10.314  32.497  13.921  1.00 18.42    0.012 C
ATOM   3521  CG2 VAL A 234       8.725  33.539  12.280  1.00 16.05    0.012 C
ATOM   3525  N   THR A 235      11.370  29.443  11.949  1.00 14.85   -0.344 N
ATOM   3526  HN  THR A 235      12.006  29.979  11.358  1.00  0.00    0.163 HD
ATOM   3527  CA  THR A 235      11.703  28.097  12.410  1.00 15.57    0.205 C
ATOM   3529  C   THR A 235      12.614  27.995  13.610  1.00 11.44    0.241 C
ATOM   3530  O   THR A 235      12.796  26.869  14.068  1.00 18.75   -0.271 OA
ATOM   3531  CB  THR A 235      12.427  27.350  11.233  1.00 22.89    0.146 C
ATOM   3533  CG2 THR A 235      11.437  27.248  10.097  1.00 21.38    0.042 C
ATOM   3537  OG1 THR A 235      13.559  28.157  10.908  1.00 23.12   -0.393 OA
ATOM   3538  HG1 THR A 235      14.182  28.221  11.623  1.00  0.00    0.210 HD
ATOM   3539  N   ASP A 236      13.123  29.111  14.104  1.00 15.25   -0.345 N
ATOM   3540  HN  ASP A 236      12.880  30.020  13.710  1.00  0.00    0.163 HD
ATOM   3541  CA  ASP A 236      14.045  29.001  15.221  1.00 17.12    0.186 C
ATOM   3543  C   ASP A 236      13.542  29.569  16.536  1.00 15.66    0.241 C
ATOM   3544  O   ASP A 236      14.343  29.747  17.457  1.00 16.69   -0.271 OA
ATOM   3545  CB  ASP A 236      15.358  29.683  14.830  1.00 22.44    0.147 C
ATOM   3548  CG  ASP A 236      16.180  31.130  14.449  1.00 21.93    0.175 C
ATOM   3549  OD1 ASP A 236      14.071  31.627  14.155  1.00 25.01   -0.648 OA
ATOM   3550  OD2 ASP A 236      16.216  31.838  14.437  1.00 47.16   -0.648 OA
ATOM   3551  N   LYS A 237      12.290  30.001  16.624  1.00 14.96   -0.346 N
ATOM   3552  HN  LYS A 237      11.697  29.976  15.795  1.00  0.00    0.163 HD
ATOM   3553  CA  LYS A 237      11.735  30.515  17.886  1.00 11.64    0.176 C
ATOM   3555  C   LYS A 237      10.288  30.009  17.975  1.00 10.30    0.243 C
ATOM   3556  O   LYS A 237       9.585  29.990  16.979  1.00 10.91   -0.271 OA
ATOM   3557  CB  LYS A 237      11.572  32.052  17.842  1.00 12.05    0.035 C
ATOM   3560  CG  LYS A 237      12.870  32.826  17.667  1.00 12.87    0.004 C
ATOM   3563  CD  LYS A 237      12.508  34.309  17.505  1.00 14.55    0.027 C
ATOM   3566  CE  LYS A 237      13.875  35.009  17.421  1.00 34.89    0.229 C
ATOM   3569  NZ  LYS A 237      14.127  35.853  18.617  1.00 46.20   -0.079 N
ATOM   3570  HZ1 LYS A 237      15.034  36.317  18.561  1.00  0.00    0.274 HD
ATOM   3571  HZ2 LYS A 237      14.035  35.316  19.479  1.00  0.00    0.274 HD
ATOM   3572  HZ3 LYS A 237      13.373  36.523  18.767  1.00  0.00    0.274 HD
ATOM   3573  N   PRO A 238       9.794  29.693  19.169  1.00 10.57   -0.337 N
ATOM   3574  CA  PRO A 238       8.408  29.345  19.385  1.00 12.50    0.179 A
ATOM   3576  C   PRO A 238       7.568  30.599  19.108  1.00  7.64    0.241 C
ATOM   3577  O   PRO A 238       8.102  31.731  19.264  1.00 10.23   -0.271 OA
ATOM   3578  CB  PRO A 238       8.297  28.972  20.858  1.00  8.75    0.037 A
ATOM   3581  CG  PRO A 238       9.620  29.280  21.449  1.00 10.76    0.022 A
ATOM   3584  CD  PRO A 238      10.614  29.733  20.423  1.00  9.31    0.127 A
ATOM   3587  N   SER A 239       6.317  30.509  18.711  1.00  7.32   -0.344 N
ATOM   3588  HN  SER A 239       5.886  29.592  18.597  1.00  0.00    0.163 HD
ATOM   3589  CA  SER A 239       5.545  31.711  18.434  1.00  4.90    0.200 C
ATOM   3591  C   SER A 239       4.353  31.848  19.378  1.00 10.01    0.243 C
ATOM   3592  O   SER A 239       3.699  30.839  19.658  1.00  9.29   -0.271 OA
ATOM   3593  CB  SER A 239       4.896  31.565  17.025  1.00 12.59    0.199 C
ATOM   3596  OG  SER A 239       5.943  31.580  16.091  1.00 11.89   -0.398 OA
ATOM   3597  HG  SER A 239       5.547  31.491  15.231  1.00  0.00    0.209 HD
ATOM   3598  N   LEU A 240       4.041  33.067  19.795  1.00  6.69   -0.346 N
ATOM   3599  HN  LEU A 240       4.674  33.840  19.590  1.00  0.00    0.163 HD
ATOM   3600  CA  LEU A 240       2.820  33.328  20.537  1.00  7.29    0.177 C
ATOM   3602  C   LEU A 240       1.895  34.232  19.695  1.00  9.71    0.241 C
ATOM   3603  O   LEU A 240       2.323  35.319  19.255  1.00 11.53   -0.271 OA
ATOM   3604  CB  LEU A 240       3.167  34.006  21.882  1.00  5.50    0.038 C
ATOM   3607  CG  LEU A 240       1.917  34.407  22.667  1.00 13.97   -0.020 C
ATOM   3609  CD1 LEU A 240       1.301  33.150  23.296  1.00 12.20    0.009 C
ATOM   3613  CD2 LEU A 240       2.277  35.401  23.765  1.00 12.98    0.009 C
ATOM   3617  N   LEU A 241       0.710  33.763  19.374  1.00  8.02   -0.346 N
ATOM   3618  HN  LEU A 241       0.489  32.812  19.670  1.00  0.00    0.163 HD
ATOM   3619  CA  LEU A 241      -0.320  34.489  18.628  1.00  9.80    0.177 C
ATOM   3621  C   LEU A 241      -1.332  35.042  19.644  1.00 12.87    0.241 C
ATOM   3622  O   LEU A 241      -2.087  34.336  20.312  1.00  9.52   -0.271 OA
ATOM   3623  CB  LEU A 241      -1.008  33.574  17.630  1.00  8.54    0.038 C
ATOM   3626  CG  LEU A 241      -0.160  32.745  16.629  1.00 22.31   -0.020 C
ATOM   3628  CD1 LEU A 241      -1.035  32.221  15.475  1.00 24.67    0.009 C
ATOM   3632  CD2 LEU A 241       0.998  33.496  16.078  1.00 23.02    0.009 C
ATOM   3636  N   MET A 242      -1.301  36.377  19.816  1.00  7.87   -0.346 N
ATOM   3637  HN  MET A 242      -0.670  36.956  19.262  1.00  0.00    0.163 HD
ATOM   3638  CA  MET A 242      -2.194  36.989  20.819  1.00  7.11    0.177 C
ATOM   3640  C   MET A 242      -3.483  37.340  20.087  1.00 12.05    0.241 C
ATOM   3641  O   MET A 242      -3.459  38.245  19.270  1.00 12.59   -0.271 OA
ATOM   3642  CB  MET A 242      -1.511  38.285  21.516  1.00 12.18    0.045 C
ATOM   3645  CG  MET A 242      -0.172  37.877  21.958  1.00 15.54    0.076 C
ATOM   3648  SD  MET A 242       0.620  39.317  22.700  1.00 20.42   -0.173 SA
ATOM   3649  CE  MET A 242      -0.452  39.600  24.093  1.00 15.81    0.089 C
ATOM   3653  N   CYS A 243      -4.559  36.631  20.392  1.00  9.52   -0.345 N
ATOM   3654  HN  CYS A 243      -4.492  35.963  21.130  1.00  0.00    0.163 HD
ATOM   3655  CA  CYS A 243      -5.814  36.714  19.679  1.00 10.87    0.186 C
ATOM   3657  C   CYS A 243      -6.855  37.383  20.600  1.00  9.18    0.241 C
ATOM   3658  O   CYS A 243      -7.234  36.886  21.656  1.00 10.97   -0.271 OA
ATOM   3659  CB  CYS A 243      -6.384  35.281  19.438  1.00 10.95    0.121 C
ATOM   3662  SG  CYS A 243      -5.254  34.409  18.303  1.00 15.35   -0.095 SA
ATOM   3663  N   LYS A 244      -7.203  38.583  20.147  1.00  7.95   -0.346 N
ATOM   3664  HN  LYS A 244      -6.756  38.993  19.327  1.00  0.00    0.163 HD
ATOM   3665  CA  LYS A 244      -8.270  39.298  20.888  1.00 10.91    0.176 C
ATOM   3667  C   LYS A 244      -9.591  38.635  20.574  1.00 15.56    0.241 C
ATOM   3668  O   LYS A 244     -10.079  38.566  19.419  1.00 13.94   -0.271 OA
ATOM   3669  CB  LYS A 244      -8.216  40.769  20.437  1.00 19.14    0.035 C
ATOM   3672  CG  LYS A 244      -9.352  41.554  21.103  1.00 29.60    0.004 C
ATOM   3675  CD  LYS A 244      -8.874  42.316  22.323  1.00 52.95    0.027 C
ATOM   3678  CE  LYS A 244      -9.728  43.565  22.546  1.00 53.85    0.229 C
ATOM   3681  NZ  LYS A 244      -9.019  44.785  22.063  1.00 69.23   -0.079 N
ATOM   3682  HZ1 LYS A 244      -9.589  45.618  22.212  1.00  0.00    0.274 HD
ATOM   3683  HZ2 LYS A 244      -8.732  44.693  21.089  1.00  0.00    0.274 HD
ATOM   3684  HZ3 LYS A 244      -8.096  44.878  22.488  1.00  0.00    0.274 HD
ATOM   3685  N   THR A 245     -10.305  38.125  21.598  1.00 11.24   -0.344 N
ATOM   3686  HN  THR A 245      -9.927  38.191  22.543  1.00  0.00    0.163 HD
ATOM   3687  CA  THR A 245     -11.599  37.483  21.401  1.00 12.55    0.205 C
ATOM   3689  C   THR A 245     -12.634  38.016  22.403  1.00 12.86    0.243 C
ATOM   3690  O   THR A 245     -12.287  38.702  23.380  1.00 14.95   -0.271 OA
ATOM   3691  CB  THR A 245     -11.578  35.948  21.638  1.00 16.65    0.146 C
ATOM   3693  CG2 THR A 245     -10.522  35.219  20.816  1.00 11.04    0.042 C
ATOM   3697  OG1 THR A 245     -11.204  35.765  23.015  1.00 21.70   -0.393 OA
ATOM   3698  HG1 THR A 245     -11.862  36.219  23.527  1.00  0.00    0.210 HD
ATOM   3699  N   ILE A 246     -13.900  37.762  22.144  1.00 13.70   -0.346 N
ATOM   3700  HN  ILE A 246     -14.145  37.294  21.272  1.00  0.00    0.163 HD
ATOM   3701  CA  ILE A 246     -14.965  38.136  23.079  1.00 14.50    0.180 C
ATOM   3703  C   ILE A 246     -15.464  36.854  23.759  1.00 19.05    0.241 C
ATOM   3704  O   ILE A 246     -15.986  35.959  23.074  1.00 19.50   -0.271 OA
ATOM   3705  CB  ILE A 246     -16.112  38.859  22.380  1.00 18.29    0.013 C
ATOM   3707  CG1 ILE A 246     -15.545  40.188  21.800  1.00 21.76    0.002 C
ATOM   3710  CG2 ILE A 246     -17.289  39.191  23.295  1.00 20.22    0.012 C
ATOM   3714  CD1 ILE A 246     -16.437  40.695  20.664  1.00 29.03    0.005 C
ATOM   3718  N   ILE A 247     -15.352  36.777  25.081  1.00 15.84   -0.346 N
ATOM   3719  HN  ILE A 247     -14.955  37.555  25.607  1.00  0.00    0.163 HD
ATOM   3720  CA  ILE A 247     -15.805  35.558  25.787  1.00 12.25    0.180 C
ATOM   3722  C   ILE A 247     -17.283  35.372  25.571  1.00 15.44    0.241 C
ATOM   3723  O   ILE A 247     -17.989  36.398  25.552  1.00 16.18   -0.271 OA
ATOM   3724  CB  ILE A 247     -15.395  35.547  27.277  1.00 14.93    0.013 C
ATOM   3726  CG1 ILE A 247     -15.637  34.143  27.883  1.00 18.45    0.002 C
ATOM   3729  CG2 ILE A 247     -16.147  36.618  28.051  1.00 17.91    0.012 C
ATOM   3733  CD1 ILE A 247     -15.048  34.001  29.310  1.00 18.52    0.005 C
ATOM   3737  N   GLY A 248     -17.763  34.158  25.237  1.00 16.79   -0.351 N
ATOM   3738  HN  GLY A 248     -17.141  33.358  25.122  1.00  0.00    0.163 HD
ATOM   3739  CA  GLY A 248     -19.206  34.028  25.046  1.00 18.39    0.225 C
ATOM   3742  C   GLY A 248     -19.694  34.684  23.745  1.00 21.18    0.236 C
ATOM   3743  O   GLY A 248     -20.877  35.016  23.670  1.00 20.90   -0.272 OA
ATOM   3744  N   PHE A 249     -18.832  34.913  22.784  1.00 17.30   -0.346 N
ATOM   3745  HN  PHE A 249     -17.859  34.651  22.942  1.00  0.00    0.163 HD
ATOM   3746  CA  PHE A 249     -19.179  35.520  21.501  1.00 19.53    0.180 C
ATOM   3748  C   PHE A 249     -20.482  34.947  20.945  1.00 18.06    0.241 C
ATOM   3749  O   PHE A 249     -20.592  33.735  20.740  1.00 22.83   -0.271 OA
ATOM   3750  CB  PHE A 249     -18.042  35.307  20.480  1.00 20.40    0.073 C
ATOM   3753  CG  PHE A 249     -18.297  35.920  19.119  1.00 22.99   -0.056 A
ATOM   3754  CD1 PHE A 249     -19.054  35.275  18.160  1.00 24.05    0.007 A
ATOM   3756  CD2 PHE A 249     -17.773  37.152  18.799  1.00 23.81    0.007 A
ATOM   3758  CE1 PHE A 249     -19.309  35.852  16.922  1.00 24.87    0.001 A
ATOM   3760  CE2 PHE A 249     -18.003  37.744  17.554  1.00 29.48    0.001 A
ATOM   3762  CZ  PHE A 249     -18.773  37.082  16.605  1.00 25.01    0.000 A
ATOM   3764  N   GLY A 250     -21.446  35.820  20.668  1.00 20.70   -0.351 N
ATOM   3765  HN  GLY A 250     -21.285  36.813  20.836  1.00  0.00    0.163 HD
ATOM   3766  CA  GLY A 250     -22.734  35.384  20.127  1.00 21.54    0.225 C
ATOM   3769  C   GLY A 250     -23.850  35.727  21.115  1.00 25.97    0.236 C
ATOM   3770  O   GLY A 250     -24.972  36.033  20.692  1.00 21.97   -0.272 OA
ATOM   3771  N   SER A 251     -23.557  35.637  22.419  1.00 22.13   -0.344 N
ATOM   3772  HN  SER A 251     -22.615  35.392  22.723  1.00  0.00    0.163 HD
ATOM   3773  CA  SER A 251     -24.619  35.898  23.407  1.00 24.85    0.200 C
ATOM   3775  C   SER A 251     -24.804  37.396  23.594  1.00 27.69    0.245 C
ATOM   3776  O   SER A 251     -23.898  38.131  23.958  1.00 27.03   -0.271 OA
ATOM   3777  CB  SER A 251     -24.271  35.231  24.730  1.00 25.24    0.199 C
ATOM   3780  OG  SER A 251     -24.932  35.817  25.825  1.00 32.21   -0.398 OA
ATOM   3781  HG  SER A 251     -24.715  35.401  26.651  1.00  0.00    0.209 HD
ATOM   3782  N   PRO A 252     -26.006  37.883  23.310  1.00 31.63   -0.337 N
ATOM   3783  CA  PRO A 252     -26.275  39.317  23.378  1.00 31.53    0.179 C
ATOM   3785  C   PRO A 252     -26.068  39.910  24.760  1.00 32.77    0.241 C
ATOM   3786  O   PRO A 252     -25.540  41.013  24.942  1.00 31.63   -0.271 OA
ATOM   3787  CB  PRO A 252     -27.720  39.436  22.907  1.00 31.45    0.037 C
ATOM   3790  CG  PRO A 252     -28.013  38.171  22.177  1.00 35.58    0.022 C
ATOM   3793  CD  PRO A 252     -27.158  37.093  22.795  1.00 27.24    0.127 C
ATOM   3796  N   ASN A 253     -26.500  39.193  25.794  1.00 30.06   -0.346 N
ATOM   3797  HN  ASN A 253     -26.876  38.259  25.629  1.00  0.00    0.163 HD
ATOM   3798  CA  ASN A 253     -26.450  39.709  27.158  1.00 27.14    0.185 C
ATOM   3800  C   ASN A 253     -25.285  39.209  27.977  1.00 31.17    0.241 C
ATOM   3801  O   ASN A 253     -25.051  39.782  29.054  1.00 34.26   -0.271 OA
ATOM   3802  CB  ASN A 253     -27.749  39.291  27.904  1.00 25.12    0.137 C
ATOM   3805  CG  ASN A 253     -28.960  39.959  27.279  1.00 37.67    0.217 C
ATOM   3806  ND2 ASN A 253     -29.877  39.202  26.688  1.00 30.87   -0.370 N
ATOM   3807 1HD2 ASN A 253     -30.691  39.651  26.268  1.00  0.00    0.159 HD
ATOM   3808 2HD2 ASN A 253     -29.838  38.183  26.662  1.00  0.00    0.159 HD
ATOM   3809  OD1 ASN A 253     -29.007  41.189  27.310  1.00 39.59   -0.274 OA
ATOM   3810  N   LYS A 254     -24.664  38.088  27.560  1.00 23.76   -0.346 N
ATOM   3811  HN  LYS A 254     -24.942  37.600  26.709  1.00  0.00    0.163 HD
ATOM   3812  CA  LYS A 254     -23.561  37.611  28.407  1.00 26.54    0.176 C
ATOM   3814  C   LYS A 254     -22.186  37.672  27.764  1.00 25.01    0.241 C
ATOM   3815  O   LYS A 254     -21.182  37.450  28.464  1.00 23.92   -0.271 OA
ATOM   3816  CB  LYS A 254     -23.892  36.185  28.868  1.00 27.45    0.035 C
ATOM   3819  CG  LYS A 254     -25.119  36.125  29.772  1.00 29.47    0.004 C
ATOM   3822  CD  LYS A 254     -25.246  34.761  30.428  1.00 34.95    0.027 C
ATOM   3825  CE  LYS A 254     -26.445  34.721  31.382  1.00 36.27    0.229 C
ATOM   3828  NZ  LYS A 254     -26.568  33.338  31.946  1.00 39.01   -0.079 N
ATOM   3829  HZ1 LYS A 254     -27.366  33.311  32.581  1.00  0.00    0.274 HD
ATOM   3830  HZ2 LYS A 254     -25.706  33.020  32.390  1.00  0.00    0.274 HD
ATOM   3831  HZ3 LYS A 254     -26.624  32.625  31.219  1.00  0.00    0.274 HD
ATOM   3832  N   ALA A 255     -22.099  37.895  26.455  1.00 20.88   -0.346 N
ATOM   3833  HN  ALA A 255     -22.958  37.998  25.914  1.00  0.00    0.163 HD
ATOM   3834  CA  ALA A 255     -20.819  37.997  25.770  1.00 21.07    0.172 C
ATOM   3836  C   ALA A 255     -19.942  39.053  26.438  1.00 24.35    0.240 C
ATOM   3837  O   ALA A 255     -20.475  40.110  26.776  1.00 25.34   -0.271 OA
ATOM   3838  CB  ALA A 255     -20.994  38.414  24.305  1.00 22.88    0.042 C
ATOM   3842  N   GLY A 256     -18.648  38.825  26.638  1.00 20.20   -0.351 N
ATOM   3843  HN  GLY A 256     -18.255  37.918  26.388  1.00  0.00    0.163 HD
ATOM   3844  CA  GLY A 256     -17.781  39.847  27.208  1.00 17.95    0.225 C
ATOM   3847  C   GLY A 256     -17.930  39.987  28.722  1.00 23.42    0.236 C
ATOM   3848  O   GLY A 256     -17.356  40.920  29.290  1.00 24.25   -0.272 OA
ATOM   3849  N   THR A 257     -18.701  39.149  29.402  1.00 20.18   -0.344 N
ATOM   3850  HN  THR A 257     -19.196  38.408  28.906  1.00  0.00    0.163 HD
ATOM   3851  CA  THR A 257     -18.852  39.271  30.852  1.00 24.84    0.205 C
ATOM   3853  C   THR A 257     -18.335  38.032  31.565  1.00 25.61    0.243 C
ATOM   3854  O   THR A 257     -18.329  36.893  31.050  1.00 21.86   -0.271 OA
ATOM   3855  CB  THR A 257     -20.332  39.469  31.255  1.00 30.26    0.146 C
ATOM   3857  CG2 THR A 257     -21.040  40.523  30.424  1.00 30.70    0.042 C
ATOM   3861  OG1 THR A 257     -21.072  38.245  31.147  1.00 33.76   -0.393 OA
ATOM   3862  HG1 THR A 257     -21.981  38.367  31.395  1.00  0.00    0.210 HD
ATOM   3863  N   HIS A 258     -18.063  38.137  32.874  1.00 21.40   -0.346 N
ATOM   3864  HN  HIS A 258     -18.188  39.021  33.368  1.00  0.00    0.163 HD
ATOM   3865  CA  HIS A 258     -17.575  36.929  33.580  1.00 23.15    0.182 C
ATOM   3867  C   HIS A 258     -18.691  35.925  33.824  1.00 20.54    0.241 C
ATOM   3868  O   HIS A 258     -18.485  34.724  34.098  1.00 24.43   -0.271 OA
ATOM   3869  CB  HIS A 258     -16.806  37.409  34.810  1.00 34.53    0.093 C
ATOM   3872  CG  HIS A 258     -17.750  37.870  35.876  1.00 45.31    0.028 A
ATOM   3873  CD2 HIS A 258     -17.983  37.392  37.119  1.00 52.44    0.114 A
ATOM   3875  ND1 HIS A 258     -18.610  38.924  35.693  1.00 54.42   -0.354 N
ATOM   3876  HD1 HIS A 258     -18.680  39.491  34.848  1.00  0.00    0.166 HD
ATOM   3877  CE1 HIS A 258     -19.337  39.088  36.792  1.00 53.40    0.180 A
ATOM   3879  NE2 HIS A 258     -18.977  38.170  37.667  1.00 54.06   -0.360 N
ATOM   3880  HE2 HIS A 258     -19.372  38.055  38.600  1.00  0.00    0.166 HD
ATOM   3881  N   ASP A 259     -19.947  36.307  33.527  1.00 23.06   -0.345 N
ATOM   3882  HN  ASP A 259     -20.098  37.272  33.232  1.00  0.00    0.163 HD
ATOM   3883  CA  ASP A 259     -21.096  35.430  33.602  1.00 25.72    0.186 C
ATOM   3885  C   ASP A 259     -21.090  34.321  32.555  1.00 28.86    0.241 C
ATOM   3886  O   ASP A 259     -21.620  33.230  32.812  1.00 28.72   -0.271 OA
ATOM   3887  CB  ASP A 259     -22.426  36.184  33.525  1.00 36.13    0.147 C
ATOM   3890  CG  ASP A 259     -22.494  37.249  34.613  1.00 51.54    0.175 C
ATOM   3891  OD1 ASP A 259     -22.225  36.939  35.795  1.00 54.08   -0.648 OA
ATOM   3892  OD2 ASP A 259     -22.784  38.408  34.258  1.00 56.34   -0.648 OA
ATOM   3893  N   ASP A 260     -20.409  34.509  31.422  1.00 22.71   -0.344 N
ATOM   3894  HN  ASP A 260     -19.914  35.386  31.259  1.00  0.00    0.163 HD
ATOM   3895  CA  ASP A 260     -20.379  33.443  30.414  1.00 21.23    0.200 C
ATOM   3897  C   SER A 260     -19.263  32.472  30.689  1.00 20.65    0.243 C
ATOM   3898  O   SER A 260     -19.117  31.460  30.005  1.00 18.37   -0.271 OA
ATOM   3899  CB  SER A 260     -20.234  34.075  28.999  1.00 22.04    0.199 C
ATOM   3902  OG  SER A 260     -18.951  34.721  28.978  1.00 28.76   -0.398 OA
ATOM   3903  HG  SER A 260     -18.862  35.107  28.114  1.00  0.00    0.209 HD
ATOM   3904  N   HIS A 261     -18.416  32.717  31.710  1.00 23.25   -0.346 N
ATOM   3905  HN  HIS A 261     -18.564  33.519  32.322  1.00  0.00    0.163 HD
ATOM   3906  CA  HIS A 261     -17.287  31.821  31.927  1.00 18.66    0.182 C
ATOM   3908  C   HIS A 261     -17.681  30.395  32.275  1.00 22.56    0.241 C
ATOM   3909  O   HIS A 261     -17.150  29.451  31.682  1.00 25.35   -0.271 OA
ATOM   3910  CB  HIS A 261     -16.383  32.349  33.081  1.00 19.28    0.093 C
ATOM   3913  CG  HIS A 261     -15.421  31.310  33.579  1.00 23.39    0.028 A
ATOM   3914  CD2 HIS A 261     -15.506  30.434  34.615  1.00 21.17    0.114 A
ATOM   3916  ND1 HIS A 261     -14.212  31.050  32.939  1.00 22.91   -0.354 N
ATOM   3917  HD1 HIS A 261     -13.856  31.551  32.125  1.00  0.00    0.166 HD
ATOM   3918  CE1 HIS A 261     -13.595  30.049  33.554  1.00 24.28    0.180 A
ATOM   3920  NE2 HIS A 261     -14.355  29.661  34.579  1.00 25.56   -0.360 N
ATOM   3921  HE2 HIS A 261     -14.126  28.913  35.234  1.00  0.00    0.166 HD
ATOM   3922  N   GLY A 262     -18.521  30.234  33.320  1.00 19.46   -0.351 N
ATOM   3923  HN  GLY A 262     -19.041  31.025  33.700  1.00  0.00    0.163 HD
ATOM   3924  CA  GLY A 262     -18.665  28.906  33.889  1.00 19.91    0.225 C
ATOM   3927  C   GLY A 262     -20.012  28.483  34.410  1.00 24.39    0.236 C
ATOM   3928  O   GLY A 262     -20.120  27.654  35.331  1.00 20.75   -0.272 OA
ATOM   3929  N   ALA A 263     -21.050  28.943  33.703  1.00 24.51   -0.347 N
ATOM   3930  HN  ALA A 263     -20.899  29.585  32.925  1.00  0.00    0.163 HD
ATOM   3931  CA  ALA A 263     -22.411  28.513  34.059  1.00 24.23    0.172 C
ATOM   3933  C   ALA A 263     -23.211  28.516  32.767  1.00 23.58    0.243 C
ATOM   3934  O   ALA A 263     -22.823  29.220  31.828  1.00 25.91   -0.271 OA
ATOM   3935  CB  ALA A 263     -23.011  29.472  35.081  1.00 21.67    0.042 C
ATOM   3939  N   PRO A 264     -24.231  27.685  32.688  1.00 26.47   -0.337 N
ATOM   3940  CA  PRO A 264     -25.054  27.592  31.486  1.00 25.06    0.179 C
ATOM   3942  C   PRO A 264     -25.600  28.976  31.171  1.00 23.22    0.241 C
ATOM   3943  O   PRO A 264     -25.830  29.756  32.100  1.00 24.16   -0.271 OA
ATOM   3944  CB  PRO A 264     -26.173  26.633  31.875  1.00 28.30    0.037 C
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ATOM   3947  CG  PRO A 264     -25.561  25.797  32.965  1.00 27.87     0.022 C
ATOM   3950  CD  PRO A 264     -24.678  26.741  33.737  1.00 28.13     0.127 C
ATOM   3953  N   LEU A 265     -25.834  29.271  29.904  1.00 23.39    -0.346 N
ATOM   3954  HN  LEU A 265     -25.616  28.584  29.182  1.00  0.00     0.163 HD
ATOM   3955  CA  LEU A 265     -26.397  30.556  29.518  1.00 24.72     0.177 C
ATOM   3957  C   LEU A 265     -27.877  30.688  29.870  1.00 26.81     0.240 C
ATOM   3958  O   LEU A 265     -28.321  31.815  30.137  1.00 30.52    -0.271 OA
ATOM   3959  CB  LEU A 265     -26.280  30.732  27.985  1.00 23.65     0.038 C
ATOM   3962  CG  LEU A 265     -24.821  30.713  27.491  1.00 30.48    -0.020 C
ATOM   3964  CD1 LEU A 265     -24.793  30.815  25.990  1.00 25.52     0.009 C
ATOM   3968  CD2 LEU A 265     -23.992  31.816  28.125  1.00 27.96     0.009 C
ATOM   3972  N   GLY A 266     -28.627  29.591  29.814  1.00 27.05    -0.351 N
ATOM   3973  HN  GLY A 266     -28.201  28.695  29.578  1.00  0.00     0.163 HD
ATOM   3974  CA  GLY A 266     -30.072  29.668  30.093  1.00 24.06     0.225 C
ATOM   3977  C   GLY A 266     -30.838  29.555  28.768  1.00 27.93     0.236 C
ATOM   3978  O   GLY A 266     -30.371  30.014  27.727  1.00 25.21    -0.272 OA
ATOM   3979  N   ASP A 267     -32.013  28.930  28.805  1.00 28.25    -0.346 N
ATOM   3980  HN  ASP A 267     -32.380  28.619  29.704  1.00  0.00     0.163 HD
ATOM   3981  CA  ASP A 267     -32.792  28.677  27.597  1.00 31.83     0.186 C
ATOM   3983  C   ASP A 267     -33.095  29.942  26.805  1.00 31.50     0.241 C
ATOM   3984  O   ASP A 267     -32.864  30.021  25.589  1.00 32.31    -0.271 OA
ATOM   3985  CB  ASP A 267     -34.102  27.953  27.925  1.00 41.24     0.147 C
ATOM   3988  CG  ASP A 267     -33.889  26.580  28.535  1.00 49.30     0.175 C
ATOM   3989  OD1 ASP A 267     -33.100  25.766  28.009  1.00 49.09    -0.648 OA
ATOM   3990  OD2 ASP A 267     -34.529  26.297  29.573  1.00 54.77    -0.648 OA
ATOM   3991  N   ALA A 268     -33.589  30.952  27.520  1.00 27.47    -0.346 N
ATOM   3992  HN  ALA A 268     -33.753  30.844  28.521  1.00  0.00     0.163 HD
ATOM   3993  CA  ALA A 268     -33.895  32.226  26.849  1.00 31.81     0.172 C
ATOM   3995  C   ALA A 268     -32.683  32.837  26.170  1.00 28.62     0.240 C
ATOM   3996  O   ALA A 268     -32.734  33.279  25.015  1.00 31.29    -0.271 OA
ATOM   3997  CB  ALA A 268     -34.477  33.202  27.868  1.00 31.74     0.042 C
ATOM   4001  N   GLU A 269     -31.550  32.850  26.883  1.00 26.22    -0.346 N
ATOM   4002  HN  GLU A 269     -31.539  32.477  27.832  1.00  0.00     0.163 HD
ATOM   4003  CA  GLU A 269     -30.324  33.402  26.296  1.00 24.40     0.177 C
ATOM   4005  C   GLU A 269     -29.875  32.585  25.089  1.00 25.09     0.241 C
ATOM   4006  O   GLU A 269     -29.438  33.109  24.058  1.00 24.45    -0.271 OA
ATOM   4007  CB  GLU A 269     -29.193  33.479  27.316  1.00 23.02     0.045 C
ATOM   4010  CG  GLU A 269     -27.976  34.268  26.840  1.00 27.69     0.116 C
ATOM   4013  CD  GLU A 269     -28.263  35.700  26.441  1.00 36.08     0.172 C
ATOM   4014  OE1 GLU A 269     -29.359  36.255  26.709  1.00 31.73    -0.648 OA
ATOM   4015  OE2 GLU A 269     -27.394  36.363  25.843  1.00 33.18    -0.648 OA
ATOM   4016  N   ILE A 270     -29.993  31.266  25.191  1.00 23.57    -0.346 N
ATOM   4017  HN  ILE A 270     -30.365  30.843  26.041  1.00  0.00     0.163 HD
ATOM   4018  CA  ILE A 270     -29.578  30.428  24.059  1.00 24.00     0.180 C
ATOM   4020  C   ILE A 270     -30.429  30.760  22.844  1.00 24.56     0.241 C
ATOM   4021  O   ILE A 270     -29.896  30.765  21.733  1.00 27.64    -0.271 OA
ATOM   4022  CB  ILE A 270     -29.639  28.938  24.385  1.00 26.50     0.013 C
ATOM   4024  CG1 ILE A 270     -28.365  28.556  25.169  1.00 22.90     0.002 C
ATOM   4027  CG2 ILE A 270     -29.751  28.088  23.119  1.00 26.26     0.012 C
ATOM   4031  CD1 ILE A 270     -28.487  27.212  25.859  1.00 25.01     0.005 C
ATOM   4035  N   ALA A 271     -31.733  30.980  23.065  1.00 24.71    -0.346 N
ATOM   4036  HN  ALA A 271     -32.121  30.916  24.006  1.00  0.00     0.163 HD
ATOM   4037  CA  ALA A 271     -32.585  31.314  21.926  1.00 25.39     0.172 C
ATOM   4039  C   ALA A 271     -32.107  32.619  21.298  1.00 24.20     0.240 C
ATOM   4040  O   ALA A 271     -32.032  32.644  20.068  1.00 28.90    -0.271 OA
ATOM   4041  CB  ALA A 271     -34.069  31.383  22.276  1.00 27.17     0.042 C
ATOM   4045  N   LEU A 272     -31.807  33.655  22.066  1.00 25.07    -0.346 N
ATOM   4046  HN  LEU A 272     -31.946  33.577  23.074  1.00  0.00     0.163 HD
ATOM   4047  CA  LEU A 272     -31.284  34.907  21.521  1.00 24.66     0.177 C
ATOM   4049  C   LEU A 272     -29.932  34.794  20.840  1.00 27.16     0.241 C
ATOM   4050  O   LEU A 272     -29.598  35.564  19.930  1.00 27.50    -0.271 OA
ATOM   4051  CB  LEU A 272     -31.136  35.943  22.667  1.00 32.34     0.038 C
ATOM   4054  CG  LEU A 272     -32.475  36.264  23.366  1.00 38.85    -0.020 C
ATOM   4056  CD1 LEU A 272     -32.266  37.063  24.651  1.00 41.31     0.009 C
ATOM   4060  CD2 LEU A 272     -33.380  37.018  22.398  1.00 36.38     0.009 C
ATOM   4064  N   THR A 273     -29.091  33.864  21.312  1.00 24.67    -0.344 N
ATOM   4065  HN  THR A 273     -29.387  33.295  22.105  1.00  0.00     0.163 HD
ATOM   4066  CA  THR A 273     -27.771  33.632  20.740  1.00 21.05     0.205 C
ATOM   4068  C   THR A 273     -27.918  32.979  19.378  1.00 22.84     0.243 C
ATOM   4069  O   THR A 273     -27.236  33.366  18.420  1.00 25.50    -0.271 OA
ATOM   4070  CB  THR A 273     -26.920  32.751  21.676  1.00 26.16     0.146 C
ATOM   4072  CG2 THR A 273     -25.552  32.430  21.092  1.00 24.32     0.042 C
ATOM   4076  OG1 THR A 273     -26.785  33.459  22.929  1.00 20.97    -0.393 OA
ATOM   4077  HG1 THR A 273     -27.639  33.659  23.294  1.00  0.00     0.210 HD
ATOM   4078  N   ARG A 274     -28.870  32.036  19.255  1.00 24.26    -0.346 N
ATOM   4079  HN  ARG A 274     -29.427  31.737  20.055  1.00  0.00     0.163 HD
ATOM   4080  CA  ARG A 274     -29.073  31.460  17.932  1.00 27.15     0.176 C
ATOM   4082  C   ARG A 274     -29.452  32.576  16.949  1.00 28.91     0.241 C
ATOM   4083  O   ARG A 274     -29.020  32.571  15.799  1.00 24.73    -0.271 OA
ATOM   4084  CB  ARG A 274     -30.127  30.364  17.898  1.00 23.31     0.036 C
ATOM   4087  CG  ARG A 274     -29.691  29.016  18.448  1.00 27.99     0.023 C
ATOM   4090  CD  ARG A 274     -30.896  28.049  18.552  1.00 23.49     0.138 C
ATOM   4093  NE  ARG A 274     -30.397  26.691  18.236  1.00 24.12    -0.227 N
ATOM   4094  HE  ARG A 274     -30.599  26.314  17.310  1.00  0.00     0.177 HD
ATOM   4095  CZ  ARG A 274     -29.705  25.930  19.075  1.00 26.01     0.665 C
ATOM   4096  NH1 ARG A 274     -29.471  26.378  20.306  1.00 27.17    -0.235 N
ATOM   4097 1HH1 ARG A 274     -29.790  27.309  20.572  1.00  0.00     0.174 HD
ATOM   4098 2HH1 ARG A 274     -28.939  25.793  20.951  1.00  0.00     0.174 HD
ATOM   4099  NH2 ARG A 274     -29.290  24.719  18.729  1.00 22.08    -0.235 N
ATOM   4100 1HH2 ARG A 274     -29.469  24.376  17.785  1.00  0.00     0.174 HD
ATOM   4101 2HH2 ARG A 274     -28.758  24.134  19.374  1.00  0.00     0.174 HD
ATOM   4102  N   GLU A 275     -30.319  33.484  17.405  1.00 27.70    -0.346 N
ATOM   4103  HN  GLU A 275     -30.643  33.431  18.371  1.00  0.00     0.163 HD
ATOM   4104  CA  GLU A 275     -30.809  34.553  16.536  1.00 31.94     0.177 C
ATOM   4106  C   GLU A 275     -29.672  35.478  16.155  1.00 30.08     0.241 C
ATOM   4107  O   GLU A 275     -29.563  35.883  14.989  1.00 25.76    -0.271 OA
ATOM   4108  CB  GLU A 275     -31.929  35.329  17.250  1.00 39.95     0.045 C
ATOM   4111  CG  GLU A 275     -32.325  36.644  16.621  1.00 67.08     0.116 C
ATOM   4114  CD  GLU A 275     -33.482  37.371  17.278  1.00 76.96     0.172 C
ATOM   4115  OE1 GLU A 275     -33.778  37.180  18.476  1.00 81.75    -0.648 OA
ATOM   4116  OE2 GLU A 275     -34.137  38.183  16.578  1.00 86.70    -0.648 OA
ATOM   4117  N   GLN A 276     -28.805  35.808  17.119  1.00 26.50    -0.346 N
ATOM   4118  HN  GLN A 276     -28.915  35.443  18.065  1.00  0.00     0.163 HD
ATOM   4119  CA  GLN A 276     -27.696  36.704  16.788  1.00 29.58     0.177 C
ATOM   4121  C   GLN A 276     -26.699  36.078  15.829  1.00 32.22     0.241 C
ATOM   4122  O   GLN A 276     -26.142  36.718  14.904  1.00 30.31    -0.271 OA
ATOM   4123  CB  GLN A 276     -26.990  37.189  18.075  1.00 40.15     0.044 C
ATOM   4126  CG  GLN A 276     -26.568  38.649  17.986  1.00 62.56     0.105 C
ATOM   4129  CD  GLN A 276     -25.283  38.993  18.698  1.00 74.17     0.215 C
ATOM   4130  NE2 GLN A 276     -24.143  38.864  18.018  1.00 82.87    -0.370 N
ATOM   4131 1HE2 GLN A 276     -23.274  39.097  18.499  1.00  0.00     0.159 HD
ATOM   4132 2HE2 GLN A 276     -24.150  38.536  17.052  1.00  0.00     0.159 HD
ATOM   4133  OE1 GLN A 276     -25.274  39.391  19.869  1.00 80.15    -0.274 OA
ATOM   4134  N   LEU A 277     -26.423  34.785  16.028  1.00 31.05    -0.346 N
ATOM   4135  HN  LEU A 277     -26.888  34.284  16.785  1.00  0.00     0.163 HD
ATOM   4136  CA  LEU A 277     -25.470  34.078  15.183  1.00 28.15     0.177 C
ATOM   4138  C   LEU A 277     -26.069  33.670  13.836  1.00 29.48     0.240 C
ATOM   4139  O   LEU A 277     -25.294  33.257  12.974  1.00 29.57    -0.271 OA
ATOM   4140  CB  LEU A 277     -25.020  32.797  15.906  1.00 25.23     0.038 C
ATOM   4143  CG  LEU A 277     -24.039  32.981  17.070  1.00 22.55    -0.020 C
ATOM   4145  CD1 LEU A 277     -23.750  31.627  17.728  1.00 30.18     0.009 C
ATOM   4149  CD2 LEU A 277     -22.729  33.582  16.563  1.00 20.01     0.009 C
ATOM   4153  N   GLY A 278     -27.400  33.598  13.722  1.00 28.95    -0.351 N
ATOM   4154  HN  GLY A 278     -27.998  33.856  14.507  1.00  0.00     0.163 HD
ATOM   4155  CA  GLY A 278     -27.996  33.144  12.455  1.00 30.96     0.225 C
ATOM   4158  C   GLY A 278     -27.936  31.624  12.350  1.00 32.99     0.236 C
ATOM   4159  O   GLY A 278     -27.882  31.058  11.265  1.00 34.43    -0.272 OA
ATOM   4160  N   TRP A 279     -27.919  30.954  13.510  1.00 28.89    -0.346 N
ATOM   4161  HN  TRP A 279     -27.972  31.486  14.378  1.00  0.00     0.163 HD
ATOM   4162  CA  TRP A 279     -27.829  29.510  13.591  1.00 30.20     0.181 C
ATOM   4164  C   TRP A 279     -29.244  28.972  13.714  1.00 30.03     0.241 C
ATOM   4165  O   TRP A 279     -29.874  29.117  14.749  1.00 34.03    -0.271 OA
ATOM   4166  CB  TRP A 279     -27.012  29.059  14.803  1.00 28.07     0.075 C
ATOM   4169  CG  TRP A 279     -26.871  27.561  14.838  1.00 18.61    -0.028 A
ATOM   4170  CD1 TRP A 279     -27.531  26.661  15.617  1.00 21.73     0.096 A
ATOM   4172  CD2 TRP A 279     -25.960  26.807  14.043  1.00 18.46    -0.002 A
ATOM   4173  CE2 TRP A 279     -26.130  25.451  14.377  1.00 17.20     0.042 A
ATOM   4174  CE3 TRP A 279     -25.003  27.168  13.087  1.00 26.95     0.014 A
ATOM   4176  NE1 TRP A 279     -27.108  25.373  15.353  1.00 17.21    -0.365 N
ATOM   4177  HE1 TRP A 279     -27.453  24.521  15.796  1.00  0.00     0.165 HD
ATOM   4178  CZ2 TRP A 279     -25.380  24.441  13.786  1.00 20.84     0.030 A
ATOM   4180  CZ3 TRP A 279     -24.271  26.154  12.495  1.00 25.43     0.001 A
ATOM   4182  CH2 TRP A 279     -24.456  24.809  12.843  1.00 23.88     0.002 A
ATOM   4184  N   LYS A 280     -29.715  28.261  12.708  1.00 34.11    -0.346 N
ATOM   4185  HN  LYS A 280     -29.088  28.016  11.942  1.00  0.00     0.163 HD
ATOM   4186  CA  LYS A 280     -31.088  27.818  12.654  1.00 38.35     0.176 C
ATOM   4188  C   LYS A 280     -31.396  26.427  13.153  1.00 39.60     0.241 C
ATOM   4189  O   LYS A 280     -32.588  26.099  13.180  1.00 42.89    -0.271 OA
ATOM   4190  CB  LYS A 280     -31.535  27.851  11.165  1.00 54.05     0.035 C
ATOM   4193  CG  LYS A 280     -30.410  28.097  10.179  1.00 68.10     0.004 C
ATOM   4196  CD  LYS A 280     -30.821  27.881   8.737  1.00 77.94     0.027 C
ATOM   4199  CE  LYS A 280     -29.655  28.036   7.777  1.00 85.48     0.229 C
ATOM   4202  NZ  LYS A 280     -29.563  29.414   7.221  1.00 91.73    -0.079 N
ATOM   4203  HZ1 LYS A 280     -28.780  29.518   6.576  1.00  0.00     0.274 HD
ATOM   4204  HZ2 LYS A 280     -29.523  30.110   7.965  1.00  0.00     0.274 HD
ATOM   4205  HZ3 LYS A 280     -30.441  29.695   6.784  1.00  0.00     0.274 HD
ATOM   4206  N   TYR A 281     -30.391  25.613  13.444  1.00 29.87    -0.346 N
ATOM   4207  HN  TYR A 281     -29.432  25.962  13.452  1.00  0.00     0.163 HD
ATOM   4208  CA  TYR A 281     -30.668  24.214  13.753  1.00 26.66     0.180 C
ATOM   4210  C   TYR A 281     -30.991  23.949  15.199  1.00 28.57     0.241 C
ATOM   4211  O   TYR A 281     -30.596  24.729  16.068  1.00 30.55    -0.271 OA
ATOM   4212  CB  TYR A 281     -29.448  23.418  13.258  1.00 26.85     0.073 C
ATOM   4215  CG  TYR A 281     -29.217  23.748  11.790  1.00 27.23    -0.056 A
ATOM   4216  CD1 TYR A 281     -30.044  23.228  10.800  1.00 32.46     0.010 A
ATOM   4218  CD2 TYR A 281     -28.184  24.585  11.424  1.00 30.09     0.010 A
ATOM   4220  CE1 TYR A 281     -29.817  23.539   9.459  1.00 34.90     0.037 A
ATOM   4222  CE2 TYR A 281     -27.953  24.910  10.100  1.00 34.01     0.037 A
ATOM   4224  CZ  TYR A 281     -28.771  24.368   9.125  1.00 38.41     0.065 A
ATOM   4225  OH  TYR A 281     -28.521  24.691   7.811  1.00 45.55    -0.361 OA
ATOM   4226  HH  TYR A 281     -27.799  25.263   7.580  1.00  0.00     0.217 HD
ATOM   4227  N   ALA A 282     -31.745  22.880  15.445  1.00 26.84    -0.346 N
ATOM   4228  HN  ALA A 282     -32.053  22.277  14.682  1.00  0.00     0.163 HD
ATOM   4229  CA  ALA A 282     -32.126  22.583  16.831  1.00 29.70     0.172 C
ATOM   4231  C   ALA A 282     -30.901  21.986  17.544  1.00 24.62     0.243 C
ATOM   4232  O   ALA A 282     -29.896  21.656  16.932  1.00 23.43    -0.271 OA
ATOM   4233  CB  ALA A 282     -33.287  21.599  16.889  1.00 29.35     0.042 C
ATOM   4237  N   PRO A 283     -31.017  21.857  18.841  1.00 24.50    -0.337 N
ATOM   4238  CA  PRO A 283     -29.913  21.324  19.642  1.00 24.23     0.179 C
ATOM   4240  C   PRO A 283     -29.504  19.979  19.118  1.00 26.95     0.241 C
ATOM   4241  O   PRO A 283     -30.296  19.074  18.820  1.00 26.31    -0.271 OA
ATOM   4242  CB  PRO A 283     -30.488  21.268  21.051  1.00 27.39     0.037 C
ATOM   4245  CG  PRO A 283     -31.442  22.428  21.069  1.00 27.90     0.022 C
ATOM   4248  CD  PRO A 283     -32.125  22.339  19.705  1.00 25.69     0.127 C
ATOM   4251  N   PHE A 284     -28.185  19.783  19.003  1.00 23.16    -0.346 N
ATOM   4252  HN  PHE A 284     -27.566  20.567  19.210  1.00  0.00     0.163 HD
ATOM   4253  CA  PHE A 284     -27.578  18.525  18.602  1.00 21.54     0.180 C
ATOM   4255  C   PHE A 284     -27.950  18.155  17.176  1.00 23.31     0.241 C
ATOM   4256  O   PHE A 284     -27.813  16.989  16.792  1.00 24.17    -0.271 OA
ATOM   4257  CB  PHE A 284     -27.937  17.392  19.604  1.00 19.26     0.073 C
ATOM   4260  CG  PHE A 284     -27.545  17.795  21.017  1.00 26.31    -0.056 A
ATOM   4261  CD1 PHE A 284     -26.209  17.820  21.391  1.00 23.00     0.007 A
ATOM   4263  CD2 PHE A 284     -28.507  18.170  21.930  1.00 18.96     0.007 A
ATOM   4265  CE1 PHE A 284     -25.854  18.204  22.674  1.00 21.18     0.001 A
ATOM   4267  CE2 PHE A 284     -28.154  18.579  23.206  1.00 24.43     0.001 A
ATOM   4269  CZ  PHE A 284     -26.823  18.589  23.570  1.00 21.40     0.000 A
ATOM   4271  N   GLU A 285     -28.302  19.147  16.363  1.00 23.78    -0.346 N
ATOM   4272  HN  GLU A 285     -28.339  20.095  16.738  1.00  0.00     0.163 HD
ATOM   4273  CA  GLU A 285     -28.638  18.940  14.957  1.00 23.86     0.177 C
ATOM   4275  C   GLU A 285     -27.614  19.678  14.114  1.00 23.00     0.241 C
ATOM   4276  O   GLU A 285     -27.454  20.901  14.233  1.00 25.25    -0.271 OA
ATOM   4277  CB  GLU A 285     -30.066  19.466  14.676  1.00 28.88     0.045 C
ATOM   4280  CG  GLU A 285     -30.340  19.693  13.211  1.00 40.84     0.116 C
ATOM   4283  CD  GLU A 285     -31.592  20.377  12.737  1.00 53.01     0.172 C
ATOM   4284  OE1 GLU A 285     -32.123  21.360  13.305  1.00 47.98    -0.648 OA
ATOM   4285  OE2 GLU A 285     -32.094  19.915  11.671  1.00 54.98    -0.648 OA
ATOM   4286  N   ILE A 286     -26.872  18.906  13.322  1.00 21.82    -0.346 N
ATOM   4287  HN  ILE A 286     -26.998  17.895  13.365  1.00  0.00     0.163 HD
ATOM   4288  CA  ILE A 286     -25.890  19.447  12.399  1.00 22.24     0.180 C
ATOM   4290  C   ILE A 286     -26.269  18.946  11.001  1.00 21.26     0.243 C
ATOM   4291  O   ILE A 286     -26.305  17.722  10.860  1.00 22.39    -0.271 OA
ATOM   4292  CB  ILE A 286     -24.474  18.913  12.731  1.00 24.15     0.013 C
ATOM   4294  CG1 ILE A 286     -24.080  19.256  14.182  1.00 20.14     0.002 C
ATOM   4297  CG2 ILE A 286     -23.462  19.462  11.739  1.00 22.93     0.012 C
ATOM   4301  CD1 ILE A 286     -23.837  20.722  14.436  1.00 19.11     0.005 C
ATOM   4305  N   PRO A 287     -26.436  19.806  10.029  1.00 24.66    -0.337 N
ATOM   4306  CA  PRO A 287     -26.790  19.360   8.676  1.00 24.85     0.179 C
ATOM   4308  C   PRO A 287     -25.631  18.663   8.002  1.00 28.11     0.241 C
ATOM   4309  O   PRO A 287     -24.441  18.975   8.184  1.00 24.78    -0.271 OA
ATOM   4310  CB  PRO A 287     -27.214  20.617   7.959  1.00 25.82     0.037 C
ATOM   4313  CG  PRO A 287     -26.443  21.710   8.644  1.00 30.02     0.022 C
ATOM   4316  CD  PRO A 287     -26.388  21.280  10.109  1.00 25.93     0.127 C
ATOM   4319  N   SER A 288     -25.968  17.716   7.112  1.00 25.60    -0.344 N
ATOM   4320  HN  SER A 288     -26.957  17.527   6.949  1.00  0.00     0.163 HD
ATOM   4321  CA  SER A 288     -24.985  16.953   6.376  1.00 27.04     0.200 C
ATOM   4323  C   SER A 288     -23.988  17.815   5.625  1.00 21.74     0.243 C
ATOM   4324  O   SER A 288     -22.826  17.400   5.555  1.00 24.42    -0.271 OA
ATOM   4325  CB  SER A 288     -25.689  15.973   5.411  1.00 37.26     0.199 C
ATOM   4328  OG  SER A 288     -26.563  16.734   4.581  1.00 41.54    -0.398 OA
ATOM   4329  HG  SER A 288     -26.996  16.131   3.988  1.00  0.00     0.209 HD
ATOM   4330  N   GLU A 289     -24.332  18.981   5.117  1.00 22.34    -0.346 N
ATOM   4331  HN  GLU A 289     -25.289  19.313   5.238  1.00  0.00     0.163 HD
ATOM   4332  CA  GLU A 289     -23.379  19.809   4.385  1.00 25.93     0.177 C
ATOM   4334  C   GLU A 289     -22.313  20.402   5.305  1.00 23.51     0.241 C
ATOM   4335  O   GLU A 289     -21.197  20.667   4.846  1.00 24.75    -0.271 OA
ATOM   4336  CB  GLU A 289     -24.145  20.897   3.633  1.00 39.37     0.045 C
ATOM   4339  CG  GLU A 289     -24.317  22.228   4.312  1.00 47.55     0.116 C
ATOM   4342  CD  GLU A 289     -25.733  22.619   4.688  1.00 70.84     0.172 C
ATOM   4343  OE1 GLU A 289     -26.633  21.746   4.722  1.00 75.77    -0.648 OA
ATOM   4344  OE2 GLU A 289     -25.968  23.826   4.966  1.00 70.55    -0.648 OA
ATOM   4345  N   ILE A 290     -22.621  20.603   6.579  1.00 23.19    -0.346 N
ATOM   4346  HN  ILE A 290     -23.560  20.384   6.912  1.00  0.00     0.163 HD
ATOM   4347  CA  ILE A 290     -21.615  21.142   7.525  1.00 23.04     0.180 C
ATOM   4349  C   ILE A 290     -20.644  20.036   7.893  1.00 19.42     0.241 C
ATOM   4350  O   ILE A 290     -19.410  20.208   7.891  1.00 19.11    -0.271 OA
ATOM   4351  CB  ILE A 290     -22.306  21.779   8.744  1.00 19.82     0.013 C
ATOM   4353  CG1 ILE A 290     -22.898  23.116   8.268  1.00 25.91     0.002 C
ATOM   4356  CG2 ILE A 290     -21.326  21.985   9.899  1.00 17.79     0.012 C
ATOM   4360  CD1 ILE A 290     -23.497  23.978   9.340  1.00 31.18     0.005 C
ATOM   4364  N   TYR A 291     -21.170  18.822   8.076  1.00 20.64    -0.346 N
ATOM   4365  HN  TYR A 291     -22.182  18.696   8.056  1.00  0.00     0.163 HD
ATOM   4366  CA  TYR A 291     -20.297  17.678   8.304  1.00 19.86     0.180 C
ATOM   4368  C   TYR A 291     -19.325  17.441   7.155  1.00 20.67     0.241 C
ATOM   4369  O   TYR A 291     -18.135  17.144   7.280  1.00 17.40    -0.271 OA
ATOM   4370  CB  TYR A 291     -21.108  16.395   8.475  1.00 21.45     0.073 C
ATOM   4373  CG  TYR A 291     -21.612  16.146   9.865  1.00 20.78    -0.056 A
ATOM   4374  CD1 TYR A 291     -20.741  15.973  10.937  1.00 22.28     0.010 A
ATOM   4376  CD2 TYR A 291     -22.968  16.044  10.121  1.00 20.11     0.010 A
ATOM   4378  CE1 TYR A 291     -21.212  15.700  12.211  1.00 19.47     0.037 A
ATOM   4380  CE2 TYR A 291     -23.467  15.780  11.401  1.00 21.11     0.037 A
ATOM   4382  CZ  TYR A 291     -22.569  15.613  12.435  1.00 22.35     0.065 A
ATOM   4383  OH  TYR A 291     -23.064  15.388  13.711  1.00 17.62    -0.361 OA
ATOM   4384  HH  TYR A 291     -22.446  15.273  14.423  1.00  0.00     0.217 HD
ATOM   4385  N   ALA A 292     -19.825  17.629   5.919  1.00 20.67    -0.346 N
ATOM   4386  HN  ALA A 292     -20.798  17.917   5.814  1.00  0.00     0.163 HD
ATOM   4387  CA  ALA A 292     -19.015  17.432   4.734  1.00 20.20     0.172 C
ATOM   4389  C   ALA A 292     -17.832  18.393   4.673  1.00 19.14     0.240 C
ATOM   4390  O   ALA A 292     -16.771  17.977   4.191  1.00 19.63    -0.271 OA
ATOM   4391  CB  ALA A 292     -19.833  17.655   3.442  1.00 25.45     0.042 C
ATOM   4395  N   GLN A 293     -17.993  19.615   5.154  1.00 15.06    -0.346 N
ATOM   4396  HN  GLN A 293     -18.901  19.886   5.530  1.00  0.00     0.163 HD
ATOM   4397  CA  GLN A 293     -16.915  20.572   5.159  1.00 18.16     0.177 C
ATOM   4399  C   GLN A 293     -15.951  20.372   6.343  1.00 18.30     0.241 C
ATOM   4400  O   GLN A 293     -14.778  20.743   6.213  1.00 18.36    -0.271 OA
ATOM   4401  CB  GLN A 293     -17.505  21.981   5.150  1.00 25.16     0.044 C
ATOM   4404  CG  GLN A 293     -18.090  22.273   3.740  1.00 31.85     0.105 C
ATOM   4407  CD  GLN A 293     -18.799  23.616   3.779  1.00 32.96     0.215 C
ATOM   4408  NE2 GLN A 293     -20.061  23.550   4.188  1.00 33.70    -0.370 N
ATOM   4409 1HE2 GLN A 293     -20.537  24.452   4.214  1.00  0.00     0.159 HD
ATOM   4410 2HE2 GLN A 293     -20.562  22.696   4.434  1.00  0.00     0.159 HD
ATOM   4411  OE1 GLN A 293     -18.195  24.646   3.482  1.00 43.42    -0.274 OA
ATOM   4412  N   TRP A 294     -16.424  19.777   7.419  1.00 19.03    -0.346 N
ATOM   4413  HN  TRP A 294     -17.399  19.480   7.452  1.00  0.00     0.163 HD
ATOM   4414  CA  TRP A 294     -15.541  19.541   8.575  1.00 16.78     0.181 C
ATOM   4416  C   TRP A 294     -14.857  18.195   8.570  1.00 20.86     0.241 C
ATOM   4417  O   TRP A 294     -13.767  18.037   9.146  1.00 17.54    -0.271 OA
ATOM   4418  CB  TRP A 294     -16.412  19.620   9.821  1.00 12.23     0.075 C
ATOM   4421  CG  TRP A 294     -16.505  20.962  10.453  1.00 18.04    -0.028 A
ATOM   4422  CD1 TRP A 294     -17.589  21.787  10.499  1.00 17.25     0.096 A
ATOM   4424  CD2 TRP A 294     -15.472  21.600  11.221  1.00 16.28    -0.002 A
ATOM   4425  CE2 TRP A 294     -16.008  22.801  11.719  1.00 19.12     0.042 A
ATOM   4426  CE3 TRP A 294     -14.166  21.216  11.573  1.00 15.88     0.014 A
ATOM   4428  NE1 TRP A 294     -17.302  22.909  11.246  1.00 16.92    -0.365 N
ATOM   4429  HE1 TRP A 294     -17.937  23.688  11.420  1.00  0.00     0.165 HD
ATOM   4430  CZ2 TRP A 294     -15.269  23.681  12.518  1.00 15.72     0.030 A
ATOM   4432  CZ3 TRP A 294     -13.451  22.079  12.393  1.00 15.05     0.001 A
ATOM   4434  CH2 TRP A 294     -13.989  23.294  12.823  1.00 14.67     0.002 A
ATOM   4436  N   ASP A 295     -15.462  17.185   7.913  1.00 16.77    -0.345 N
ATOM   4437  HN  ASP A 295     -16.316  17.351   7.380  1.00  0.00     0.163 HD
ATOM   4438  CA  ASP A 295     -14.872  15.844   7.978  1.00 13.73     0.186 C
ATOM   4440  C   ASP A 295     -13.449  15.817   7.469  1.00 16.18     0.241 C
ATOM   4441  O   ASP A 295     -13.146  16.358   6.392  1.00 17.69    -0.271 OA
ATOM   4442  CB  ASP A 295     -15.686  14.811   7.181  1.00 21.49     0.147 C
ATOM   4445  CG  ASP A 295     -15.346  13.395   7.622  1.00 21.27     0.175 C
ATOM   4446  OD1 ASP A 295     -15.814  12.885   8.664  1.00 26.04    -0.648 OA
ATOM   4447  OD2 ASP A 295     -14.549  12.796   6.886  1.00 19.55    -0.648 OA
ATOM   4448  N   ALA A 296     -12.562  15.100   8.176  1.00 14.65    -0.346 N
ATOM   4449  HN  ALA A 296     -12.863  14.592   9.008  1.00  0.00     0.163 HD
ATOM   4450  CA  ALA A 296     -11.159  15.048   7.750  1.00 13.03     0.172 C
ATOM   4452  C   ALA A 296     -10.692  13.616   7.524  1.00 15.02     0.240 C
ATOM   4453  O   ALA A 296      -9.484  13.366   7.496  1.00 16.66    -0.271 OA
ATOM   4454  CB  ALA A 296     -10.306  15.652   8.904  1.00 15.40     0.042 C
ATOM   4458  N   LYS A 297     -11.621  12.669   7.401  1.00 15.30    -0.346 N
ATOM   4459  HN  LYS A 297     -12.609  12.921   7.398  1.00  0.00     0.163 HD
ATOM   4460  CA  LYS A 297     -11.221  11.267   7.270  1.00 19.07     0.176 C
ATOM   4462  C   LYS A 297     -10.501  10.973   5.969  1.00 20.76     0.241 C
ATOM   4463  O   LYS A 297      -9.541  10.205   5.963  1.00 20.48    -0.271 OA
ATOM   4464  CB  LYS A 297     -12.436  10.332   7.390  1.00 22.31     0.035 C
ATOM   4467  CG  LYS A 297     -12.958  10.284   8.817  1.00 21.49     0.004 C
ATOM   4470  CD  LYS A 297     -13.952   9.163   9.032  1.00 27.68     0.027 C
ATOM   4473  CE  LYS A 297     -15.282   9.404   8.330  1.00 37.64     0.229 C
ATOM   4476  NZ  LYS A 297     -16.200  10.288   9.105  1.00 39.22    -0.079 N
ATOM   4477  HZ1 LYS A 297     -17.091  10.449   8.635  1.00  0.00     0.274 HD
ATOM   4478  HZ2 LYS A 297     -15.745  11.171   9.336  1.00  0.00     0.274 HD
ATOM   4479  HZ3 LYS A 297     -16.346   9.924  10.047  1.00  0.00     0.274 HD
ATOM   4480  N   GLU A 298     -10.933  11.552   4.859  1.00 20.73    -0.346 N
ATOM   4481  HN  GLU A 298     -11.715  12.205   4.914  1.00  0.00     0.163 HD
ATOM   4482  CA  GLU A 298     -10.329  11.287   3.567  1.00 25.17     0.177 C
ATOM   4484  C   GLU A 298      -8.939  11.880   3.473  1.00 21.50     0.241 C
ATOM   4485  O   GLU A 298      -7.986  11.211   3.087  1.00 17.94    -0.271 OA
ATOM   4486  CB  GLU A 298     -11.230  11.889   2.477  1.00 36.97     0.045 C
ATOM   4489  CG  GLU A 298     -10.998  11.351   1.085  1.00 55.98     0.116 C
ATOM   4492  CD  GLU A 298     -11.743  12.158   0.034  1.00 69.06     0.172 C
ATOM   4493  OE1 GLU A 298     -12.837  12.689   0.315  1.00 74.69    -0.648 OA
ATOM   4494  OE2 GLU A 298     -11.202  12.260  -1.087  1.00 77.50    -0.648 OA
ATOM   4495  N   ALA A 299      -8.819  13.152   3.850  1.00 21.08    -0.346 N
ATOM   4496  HN  ALA A 299      -9.648  13.675   4.131  1.00  0.00     0.163 HD
ATOM   4497  CA  ALA A 299      -7.511  13.806   3.866  1.00 20.82     0.172 C
ATOM   4499  C   ALA A 299      -6.611  13.140   4.918  1.00 18.85     0.240 C
ATOM   4500  O   ALA A 299      -5.418  13.012   4.629  1.00 17.62    -0.271 OA
ATOM   4501  CB  ALA A 299      -7.618  15.297   4.202  1.00 21.63     0.042 C
ATOM   4505  N   GLY A 300      -7.140  12.762   6.086  1.00 14.39    -0.351 N
ATOM   4506  HN  GLY A 300      -8.138  12.857   6.272  1.00  0.00     0.163 HD
ATOM   4507  CA  GLY A 300      -6.216  12.198   7.101  1.00 15.44     0.225 C
ATOM   4510  C   GLY A 300      -5.639  10.862   6.648  1.00 15.92     0.236 C
ATOM   4511  O   GLY A 300      -4.452  10.521   6.772  1.00 15.66    -0.272 OA
ATOM   4512  N   GLN A 301      -6.496  10.021   6.050  1.00 15.05    -0.346 N
ATOM   4513  HN  GLN A 301      -7.478  10.269   5.927  1.00  0.00     0.163 HD
ATOM   4514  CA  GLN A 301      -5.974   8.726   5.576  1.00 14.20     0.177 C
ATOM   4516  C   GLN A 301      -4.945   8.902   4.474  1.00 16.27     0.241 C
ATOM   4517  O   GLN A 301      -3.947   8.172   4.327  1.00 19.10    -0.271 OA
ATOM   4518  CB  GLN A 301      -7.195   7.986   5.017  1.00 32.20     0.044 C
ATOM   4521  CG  GLN A 301      -6.849   6.603   4.487  1.00 59.22     0.105 C
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ATOM   4524  CD  GLN A 301      -8.099   5.835   4.083  1.00 77.58      0.215 C
ATOM   4525  NE2 GLN A 301      -7.896   4.575   3.702  1.00 86.51     -0.370 N
ATOM   4526 1HE2 GLN A 301      -6.964   4.161   3.686  1.00  0.00      0.159 HD
ATOM   4527 2HE2 GLN A 301      -8.734   4.060   3.431  1.00  0.00      0.159 HD
ATOM   4528  OE1 GLN A 301      -9.228   6.337   4.102  1.00 84.61     -0.274 OA
ATOM   4529  N   ALA A 302      -5.143   9.863   3.575  1.00 13.81     -0.346 N
ATOM   4530  HN  ALA A 302      -5.991  10.427   3.634  1.00  0.00      0.163 HD
ATOM   4531  CA  ALA A 302      -4.179  10.137   2.501  1.00 18.59      0.172 C
ATOM   4533  C   ALA A 302      -2.833  10.557   3.063  1.00 16.71      0.240 C
ATOM   4534  O   ALA A 302      -1.772  10.069   2.640  1.00 15.84     -0.271 OA
ATOM   4535  CB  ALA A 302      -4.675  11.224   1.557  1.00 18.09      0.042 C
ATOM   4539  N   LYS A 303      -2.832  11.486   4.050  1.00 10.77     -0.346 N
ATOM   4540  HN  LYS A 303      -3.703  11.892   4.391  1.00  0.00      0.163 HD
ATOM   4541  CA  LYS A 303      -1.544  11.887   4.610  1.00 13.78      0.176 C
ATOM   4543  C   LYS A 303      -0.890  10.746   5.411  1.00  9.86      0.241 C
ATOM   4544  O   LYS A 303       0.331  10.639   5.365  1.00 13.44     -0.271 OA
ATOM   4545  CB  LYS A 303      -1.763  13.057   5.594  1.00 14.95      0.035 C
ATOM   4548  CG  LYS A 303      -2.169  14.339   4.863  1.00 25.36      0.004 C
ATOM   4551  CD  LYS A 303      -2.544  15.395   5.903  1.00 38.00      0.027 C
ATOM   4554  CE  LYS A 303      -3.394  16.517   5.303  1.00 39.98      0.229 C
ATOM   4557  NZ  LYS A 303      -4.074  17.328   6.355  1.00 31.96     -0.079 N
ATOM   4558  HZ1 LYS A 303      -4.641  18.076   5.955  1.00  0.00      0.274 HD
ATOM   4559  HZ2 LYS A 303      -3.404  17.693   7.032  1.00  0.00      0.274 HD
ATOM   4560  HZ3 LYS A 303      -4.626  16.738   6.978  1.00  0.00      0.274 HD
ATOM   4561  N   GLU A 304      -1.655   9.953   6.124  1.00  8.84     -0.346 N
ATOM   4562  HN  GLU A 304      -2.668  10.067   6.151  1.00  0.00      0.163 HD
ATOM   4563  CA  GLU A 304      -0.958   8.864   6.901  1.00 11.72      0.177 C
ATOM   4565  C   GLU A 304      -0.433   7.809   5.969  1.00 12.64      0.241 C
ATOM   4566  O   GLU A 304       0.638   7.213   6.130  1.00 15.44     -0.271 OA
ATOM   4567  CB  GLU A 304      -1.947   8.232   7.917  1.00  7.07      0.045 C
ATOM   4570  CG  GLU A 304      -1.189   7.188   8.766  1.00  7.49      0.116 C
ATOM   4573  CD  GLU A 304      -2.035   6.690   9.941  1.00 16.93      0.172 C
ATOM   4574  OE1 GLU A 304      -3.035   7.333  10.300  1.00 21.10     -0.648 OA
ATOM   4575  OE2 GLU A 304      -1.677   5.675  10.524  1.00 17.59     -0.648 OA
ATOM   4576  N   SER A 305      -1.229   7.515   4.886  1.00 13.63     -0.344 N
ATOM   4577  HN  SER A 305      -2.135   7.974   4.788  1.00  0.00      0.163 HD
ATOM   4578  CA  SER A 305      -0.797   6.558   3.877  1.00 16.89      0.200 C
ATOM   4580  C   SER A 305       0.527   6.941   3.247  1.00 13.23      0.243 C
ATOM   4581  O   SER A 305       1.432   6.110   3.115  1.00 12.77     -0.271 OA
ATOM   4582  CB  SER A 305      -1.802   6.379   2.685  1.00 15.43      0.199 C
ATOM   4585  OG  SER A 305      -2.878   5.646   3.226  1.00 34.64     -0.398 OA
ATOM   4586  HG  SER A 305      -3.486   5.538   2.504  1.00  0.00      0.209 HD
ATOM   4587  N   ALA A 306       0.704   8.245   2.992  1.00 13.30     -0.346 N
ATOM   4588  HN  ALA A 306      -0.052   8.905   3.174  1.00  0.00      0.163 HD
ATOM   4589  CA  ALA A 306       1.968   8.723   2.457  1.00 15.41      0.172 C
ATOM   4591  C   ALA A 306       3.071   8.563   3.505  1.00 17.23      0.240 C
ATOM   4592  O   ALA A 306       4.200   8.204   3.160  1.00 12.90     -0.271 OA
ATOM   4593  CB  ALA A 306       1.819  10.197   2.065  1.00 14.64      0.042 C
ATOM   4597  N   TRP A 307       2.796   8.809   4.790  1.00 11.18     -0.346 N
ATOM   4598  HN  TRP A 307       1.868   9.134   5.061  1.00  0.00      0.163 HD
ATOM   4599  CA  TRP A 307       3.824   8.612   5.801  1.00 11.62      0.181 C
ATOM   4601  C   TRP A 307       4.189   7.124   5.882  1.00  7.02      0.241 C
ATOM   4602  O   TRP A 307       5.362   6.809   6.123  1.00  8.76     -0.271 OA
ATOM   4603  CB  TRP A 307       3.325   9.131   7.181  1.00  8.68      0.075 C
ATOM   4606  CG  TRP A 307       4.426   9.065   8.224  1.00 10.27     -0.028 A
ATOM   4607  CD1 TRP A 307       5.383   9.989   8.477  1.00 11.23      0.096 A
ATOM   4609  CD2 TRP A 307       4.683   7.978   9.128  1.00 13.89     -0.002 A
ATOM   4610  CE2 TRP A 307       5.809   8.304   9.892  1.00 11.33      0.042 A
ATOM   4611  CE3 TRP A 307       4.044   6.757   9.371  1.00 11.90      0.014 A
ATOM   4613  NE1 TRP A 307       6.222   9.540   9.497  1.00 11.68     -0.365 N
ATOM   4614  HE1 TRP A 307       7.014  10.053   9.883  1.00  0.00      0.165 HD
ATOM   4615  CZ2 TRP A 307       6.334   7.477  10.891  1.00 14.26      0.030 A
ATOM   4617  CZ3 TRP A 307       4.574   5.929  10.368  1.00 14.34      0.001 A
ATOM   4619  CH2 TRP A 307       5.712   6.281  11.100  1.00 15.06      0.002 A
ATOM   4621  N   ASN A 308       3.183   6.236   5.837  1.00  9.72     -0.346 N
ATOM   4622  HN  ASN A 308       2.219   6.555   5.738  1.00  0.00      0.163 HD
ATOM   4623  CA  ASN A 308       3.483   4.801   5.931  1.00 11.09      0.185 C
ATOM   4625  C   ASN A 308       4.483   4.348   4.876  1.00 11.39      0.241 C
ATOM   4626  O   ASN A 308       5.360   3.539   5.121  1.00 10.85     -0.271 OA
ATOM   4627  CB  ASN A 308       2.177   3.992   5.787  1.00 11.06      0.137 C
ATOM   4630  CG  ASN A 308       1.300   4.007   7.026  1.00 14.71      0.217 C
ATOM   4631  ND2 ASN A 308       0.013   3.650   6.949  1.00 14.50     -0.370 N
ATOM   4632 1HD2 ASN A 308      -0.421   3.317   6.088  1.00  0.00      0.159 HD
ATOM   4633 2HD2 ASN A 308      -0.576   3.660   7.782  1.00  0.00      0.159 HD
ATOM   4634  OD1 ASN A 308       1.826   4.410   8.069  1.00 11.31     -0.274 OA
ATOM   4635  N   GLU A 309       4.294   4.818   3.637  1.00 11.22     -0.346 N
ATOM   4636  HN  GLU A 309       3.506   5.435   3.440  1.00  0.00      0.163 HD
ATOM   4637  CA  GLU A 309       5.228   4.442   2.555  1.00 13.95      0.177 C
ATOM   4639  C   GLU A 309       6.589   5.029   2.795  1.00 14.15      0.241 C
ATOM   4640  O   GLU A 309       7.599   4.404   2.518  1.00 14.00     -0.271 OA
ATOM   4641  CB  GLU A 309       4.725   5.026   1.213  1.00 19.96      0.045 C
ATOM   4644  CG  GLU A 309       3.415   4.456   0.749  1.00 27.54      0.116 C
ATOM   4647  CD  GLU A 309       2.977   5.010  -0.607  1.00 42.19      0.172 C
ATOM   4648  OE1 GLU A 309       3.329   6.137  -1.001  1.00 42.55     -0.648 OA
ATOM   4649  OE2 GLU A 309       2.216   4.290  -1.289  1.00 50.85     -0.648 OA
ATOM   4650  N   LYS A 310       6.697   6.238   3.357  1.00 13.98     -0.346 N
ATOM   4651  HN  LYS A 310       5.848   6.776   3.529  1.00  0.00      0.163 HD
ATOM   4652  CA  LYS A 310       7.966   6.809   3.728  1.00 11.98      0.176 C
ATOM   4654  C   LYS A 310       8.692   6.001   4.803  1.00 14.42      0.241 C
ATOM   4655  O   LYS A 310       9.915   5.858   4.792  1.00 14.11     -0.271 OA
ATOM   4656  CB  LYS A 310       7.815   8.209   4.354  1.00 20.86      0.035 C
ATOM   4659  CG  LYS A 310       7.689   9.335   3.353  1.00 32.44      0.004 C
ATOM   4662  CD  LYS A 310       7.242  10.623   4.035  1.00 43.48      0.027 C
ATOM   4665  CE  LYS A 310       8.244  11.100   5.071  1.00 44.40      0.229 C
ATOM   4668  NZ  LYS A 310       8.234  12.597   5.138  1.00 59.95     -0.079 N
ATOM   4669  HZ1 LYS A 310       8.907  12.917   5.834  1.00  0.00      0.274 HD
ATOM   4670  HZ2 LYS A 310       7.299  12.966   5.311  1.00  0.00      0.274 HD
ATOM   4671  HZ3 LYS A 310       8.395  13.022   4.225  1.00  0.00      0.274 HD
ATOM   4672  N   PHE A 311       7.896   5.473   5.750  1.00 12.83     -0.346 N
ATOM   4673  HN  PHE A 311       6.884   5.601   5.721  1.00  0.00      0.163 HD
ATOM   4674  CA  PHE A 311       8.532   4.710   6.822  1.00 11.77      0.180 C
ATOM   4676  C   PHE A 311       9.057   3.400   6.247  1.00  9.68      0.241 C
ATOM   4677  O   PHE A 311      10.114   2.891   6.605  1.00 10.93     -0.271 OA
ATOM   4678  CB  PHE A 311       7.475   4.459   7.931  1.00  8.50      0.073 C
ATOM   4681  CG  PHE A 311       8.164   3.715   9.067  1.00  9.76     -0.056 A
ATOM   4682  CD1 PHE A 311       8.957   4.382   9.971  1.00 14.09      0.007 A
ATOM   4684  CD2 PHE A 311       8.036   2.329   9.162  1.00 16.81      0.007 A
ATOM   4686  CE1 PHE A 311       9.631   3.701  10.982  1.00 16.16      0.001 A
ATOM   4688  CE2 PHE A 311       8.708   1.650  10.163  1.00 18.26      0.001 A
ATOM   4690  CZ  PHE A 311       9.495   2.331  11.075  1.00 18.11      0.000 A
ATOM   4692  N   ALA A 312       8.309   2.803   5.328  1.00 11.97     -0.346 N
ATOM   4693  HN  ALA A 312       7.419   3.206   5.034  1.00  0.00      0.163 HD
ATOM   4694  CA  ALA A 312       8.800   1.538   4.742  1.00 13.32      0.172 C
ATOM   4696  C   ALA A 312      10.090   1.770   3.977  1.00 11.41      0.240 C
ATOM   4697  O   ALA A 312      11.034   0.973   4.043  1.00 13.62     -0.271 OA
ATOM   4698  CB  ALA A 312       7.724   0.925   3.882  1.00 13.48      0.042 C
ATOM   4702  N   ALA A 313      10.164   2.873   3.204  1.00 11.67     -0.346 N
ATOM   4703  HN  ALA A 313       9.367   3.505   3.162  1.00  0.00      0.163 HD
ATOM   4704  CA  ALA A 313      11.420   3.163   2.518  1.00 14.31      0.172 C
ATOM   4706  C   ALA A 313      12.549   3.403   3.494  1.00 14.75      0.240 C
ATOM   4707  O   ALA A 313      13.735   3.274   3.169  1.00 14.13     -0.271 OA
ATOM   4708  CB  ALA A 313      11.193   4.392   1.630  1.00 15.20      0.042 C
ATOM   4712  N   TYR A 314      12.265   4.086   4.617  1.00 10.64     -0.346 N
ATOM   4713  HN  TYR A 314      11.309   4.413   4.758  1.00  0.00      0.163 HD
ATOM   4714  CA  TYR A 314      13.258   4.380   5.641  1.00 11.07      0.180 C
ATOM   4716  C   TYR A 314      13.789   3.075   6.201  1.00 12.63      0.241 C
ATOM   4717  O   TYR A 314      15.012   2.959   6.362  1.00 14.20     -0.271 OA
ATOM   4718  CB  TYR A 314      12.643   5.269   6.755  1.00 11.47      0.073 C
ATOM   4721  CG  TYR A 314      13.495   5.541   7.969  1.00 14.92     -0.056 A
ATOM   4722  CD1 TYR A 314      14.451   6.543   7.958  1.00 13.83      0.010 A
ATOM   4724  CD2 TYR A 314      13.348   4.802   9.149  1.00 18.11      0.010 A
ATOM   4726  CE1 TYR A 314      15.220   6.818   9.095  1.00 15.24      0.037 A
ATOM   4728  CE2 TYR A 314      14.117   5.065  10.277  1.00 17.61      0.037 A
ATOM   4730  CZ  TYR A 314      15.045   6.091  10.245  1.00 18.91      0.065 A
ATOM   4731  OH  TYR A 314      15.846   6.427  11.336  1.00 17.61     -0.361 OA
ATOM   4732  HH  TYR A 314      16.483   7.131  11.314  1.00  0.00      0.217 HD
ATOM   4733  N   ALA A 315      12.884   2.128   6.526  1.00 14.96     -0.346 N
ATOM   4734  HN  ALA A 315      11.892   2.308   6.373  1.00  0.00      0.163 HD
ATOM   4735  CA  ALA A 315      13.304   0.848   7.094  1.00 17.87      0.172 C
ATOM   4737  C   ALA A 315      14.162   0.025   6.119  1.00 16.29      0.240 C
ATOM   4738  O   ALA A 315      15.025  -0.727   6.529  1.00 14.83     -0.271 OA
ATOM   4739  CB  ALA A 315      12.129  -0.023   7.514  1.00 13.04      0.042 C
ATOM   4743  N   LYS A 316      13.984   0.210   4.829  1.00 15.02     -0.346 N
ATOM   4744  HN  LYS A 316      13.236   0.824   4.506  1.00  0.00      0.163 HD
ATOM   4745  CA  LYS A 316      14.853  -0.459   3.844  1.00 16.81      0.176 C
ATOM   4747  C   LYS A 316      16.237   0.161   3.869  1.00 18.02      0.241 C
ATOM   4748  O   LYS A 316      17.261  -0.527   3.800  1.00 18.88     -0.271 OA
ATOM   4749  CB  LYS A 316      14.249  -0.310   2.434  1.00 15.26      0.035 C
ATOM   4752  CG  LYS A 316      13.116  -1.287   2.194  1.00 15.19      0.004 C
ATOM   4755  CD  LYS A 316      13.174  -1.778   0.748  1.00 44.21      0.027 C
ATOM   4758  CE  LYS A 316      12.320  -0.904  -0.153  1.00 56.23      0.229 C
ATOM   4761  NZ  LYS A 316      12.474  -1.234  -1.600  1.00 51.58     -0.079 N
ATOM   4762  HZ1 LYS A 316      11.900  -0.647  -2.205  1.00  0.00      0.274 HD
ATOM   4763  HZ2 LYS A 316      12.289  -2.223  -1.770  1.00  0.00      0.274 HD
ATOM   4764  HZ3 LYS A 316      13.454  -1.197  -1.880  1.00  0.00      0.274 HD
ATOM   4765  N   ALA A 317      16.339   1.478   4.051  1.00 14.75     -0.346 N
ATOM   4766  HN  ALA A 317      15.502   2.042   4.198  1.00  0.00      0.163 HD
ATOM   4767  CA  ALA A 317      17.661   2.111   4.038  1.00 14.87      0.172 C
ATOM   4769  C   ALA A 317      18.351   2.062   5.373  1.00 21.67      0.240 C
ATOM   4770  O   ALA A 317      19.589   2.077   5.416  1.00 19.48     -0.271 OA
ATOM   4771  CB  ALA A 317      17.486   3.534   3.503  1.00 16.91      0.042 C
ATOM   4775  N   TYR A 318      17.619   2.095   6.501  1.00 15.39     -0.346 N
ATOM   4776  HN  TYR A 318      16.603   2.067   6.410  1.00  0.00      0.163 HD
ATOM   4777  CA  TYR A 318      18.189   2.169   7.858  1.00 14.10      0.181 C
ATOM   4779  C   TYR A 318      17.424   1.180   8.729  1.00 17.11      0.243 C
ATOM   4780  O   TYR A 318      16.606   1.533   9.585  1.00 16.65     -0.271 OA
ATOM   4781  CB  TYR A 318      17.957   3.599   8.448  1.00 14.02      0.073 C
ATOM   4784  CG  TYR A 318      18.676   4.656   7.627  1.00 16.73     -0.056 A
ATOM   4785  CD1 TYR A 318      20.031   4.880   7.885  1.00 16.53      0.010 A
ATOM   4787  CD2 TYR A 318      18.057   5.378   6.611  1.00 16.44      0.010 A
ATOM   4789  CE1 TYR A 318      20.747   5.809   7.152  1.00 18.52      0.037 A
ATOM   4791  CE2 TYR A 318      18.788   6.318   5.889  1.00 14.42      0.037 A
ATOM   4793  CZ  TYR A 318      20.110   6.500   6.152  1.00 18.22      0.065 A
ATOM   4794  OH  TYR A 318      20.853   7.434   5.436  1.00 21.80     -0.361 OA
ATOM   4795  HH  TYR A 318      20.412   7.912   4.744  1.00  0.00      0.217 HD
ATOM   4796  N   PRO A 319      17.667  -0.118   8.552  1.00 16.64     -0.337 N
ATOM   4797  CA  PRO A 319      16.970  -1.171   9.236  1.00 16.54      0.179 A
ATOM   4799  C   PRO A 319      17.157  -1.208  10.747  1.00 13.98      0.241 C
ATOM   4800  O   PRO A 319      16.151  -1.433  11.436  1.00 16.73     -0.271 OA
ATOM   4801  CB  PRO A 319      17.461  -2.473   8.606  1.00 18.78      0.037 A
ATOM   4804  CG  PRO A 319      18.540  -2.125   7.667  1.00 18.63      0.022 A
ATOM   4807  CD  PRO A 319      18.661  -0.640   7.560  1.00 19.74      0.127 A
ATOM   4810  N   GLN A 320      18.341  -0.930  11.245  1.00 13.52     -0.346 N
ATOM   4811  HN  GLN A 320      19.119  -0.734  10.615  1.00  0.00      0.163 HD
ATOM   4812  CA  GLN A 320      18.556  -0.899  12.688  1.00 18.30      0.177 C
ATOM   4814  C   GLN A 320      17.817   0.266  13.362  1.00 18.48      0.241 C
ATOM   4815  O   GLN A 320      17.205   0.071  14.410  1.00 15.20     -0.271 OA
ATOM   4816  CB  GLN A 320      20.032  -0.733  12.995  1.00 21.18      0.044 C
ATOM   4819  CG  GLN A 320      20.663  -2.060  13.407  1.00 62.68      0.105 C
ATOM   4822  CD  GLN A 320      22.040  -2.219  12.781  1.00 71.94      0.215 C
ATOM   4823  NE2 GLN A 320      22.313  -3.403  12.242  1.00 79.46     -0.370 N
ATOM   4824 1HE2 GLN A 320      21.652  -4.179  12.241  1.00  0.00      0.159 HD
ATOM   4825 2HE2 GLN A 320      23.236  -3.510  11.822  1.00  0.00      0.159 HD
ATOM   4826  OE1 GLN A 320      22.840  -1.280  12.782  1.00 79.99     -0.274 OA
ATOM   4827  N   GLU A 321      17.903   1.440  12.750  1.00 13.17     -0.346 N
ATOM   4828  HN  GLU A 321      18.464   1.528  11.903  1.00  0.00      0.163 HD
ATOM   4829  CA  GLU A 321      17.203   2.608  13.277  1.00 15.40      0.177 C
ATOM   4831  C   GLU A 321      15.697   2.461  13.188  1.00 16.83      0.241 C
ATOM   4832  O   GLU A 321      14.958   2.856  14.118  1.00 14.55     -0.271 OA
ATOM   4833  CB  GLU A 321      17.557   3.878  12.472  1.00 15.44      0.045 C
ATOM   4836  CG  GLU A 321      19.008   4.289  12.664  1.00 27.68      0.116 C
ATOM   4839  CD  GLU A 321      20.025   3.638  11.743  1.00 27.31      0.172 C
ATOM   4840  OE1 GLU A 321      19.782   2.648  11.032  1.00 26.40     -0.648 OA
ATOM   4841  OE2 GLU A 321      21.158   4.172  11.716  1.00 43.38     -0.648 OA
ATOM   4842  N   ALA A 322      15.161   1.847  12.116  1.00 11.03     -0.346 N
ATOM   4843  HN  ALA A 322      15.777   1.524  11.370  1.00  0.00      0.163 HD
ATOM   4844  CA  ALA A 322      13.735   1.632  11.993  1.00 12.62      0.172 C
ATOM   4846  C   ALA A 322      13.216   0.713  13.098  1.00 14.78      0.240 C
ATOM   4847  O   ALA A 322      12.129   0.906  13.635  1.00 11.67     -0.271 OA
ATOM   4848  CB  ALA A 322      13.279   1.045  10.635  1.00 15.07      0.042 C
ATOM   4852  N   ALA A 323      14.001  -0.316  13.432  1.00 13.37     -0.346 N
ATOM   4853  HN  ALA A 323      14.898  -0.445  12.965  1.00  0.00      0.163 HD
ATOM   4854  CA  ALA A 323      13.577  -1.252  14.461  1.00 14.91      0.172 C
ATOM   4856  C   ALA A 323      13.610  -0.499  15.814  1.00 12.45      0.240 C
ATOM   4857  O   ALA A 323      12.728  -0.768  16.623  1.00 12.79     -0.271 OA
ATOM   4858  CB  ALA A 323      14.525  -2.447  14.509  1.00 18.58      0.042 C
ATOM   4862  N   GLU A 324      14.649   0.325  16.019  1.00 12.67     -0.346 N
ATOM   4863  HN  GLU A 324      15.392   0.454  15.333  1.00  0.00      0.163 HD
ATOM   4864  CA  GLU A 324      14.632   1.034  17.323  1.00 10.63      0.177 C
ATOM   4866  C   GLU A 324      13.491   2.033  17.404  1.00 10.51      0.241 C
ATOM   4867  O   GLU A 324      12.916   2.218  18.481  1.00 13.48     -0.271 OA
ATOM   4868  CB  GLU A 324      15.958   1.813  17.440  1.00 13.79      0.045 C
ATOM   4871  CG  GLU A 324      17.050   0.900  17.990  1.00 17.96      0.116 C
ATOM   4874  CD  GLU A 324      16.701   0.505  19.423  1.00 29.50      0.172 C
ATOM   4875  OE1 GLU A 324      16.763   1.411  20.287  1.00 23.31     -0.648 OA
ATOM   4876  OE2 GLU A 324      16.313  -0.657  19.688  1.00 21.00     -0.648 OA
ATOM   4877  N   PHE A 325      13.169   2.749  16.324  1.00 10.19     -0.346 N
ATOM   4878  HN  PHE A 325      13.726   2.642  15.476  1.00  0.00      0.163 HD
ATOM   4879  CA  PHE A 325      12.041   3.683  16.320  1.00 13.49      0.180 C
ATOM   4881  C   PHE A 325      10.753   2.971  16.708  1.00 14.79      0.241 C
ATOM   4882  O   PHE A 325       9.977   3.421  17.583  1.00 14.56     -0.271 OA
ATOM   4883  CB  PHE A 325      11.853   4.292  14.931  1.00 11.72      0.073 C
ATOM   4886  CG  PHE A 325      10.802   5.381  14.813  1.00 12.25     -0.056 A
ATOM   4887  CD1 PHE A 325      11.093   6.693  15.114  1.00 15.73      0.007 A
ATOM   4889  CD2 PHE A 325       9.530   5.069  14.360  1.00 15.01      0.007 A
ATOM   4891  CE1 PHE A 325      10.114   7.686  15.004  1.00 13.97      0.001 A
ATOM   4893  CE2 PHE A 325       8.548   6.036  14.245  1.00 16.02      0.001 A
ATOM   4895  CZ  PHE A 325       8.845   7.346  14.555  1.00 11.98      0.000 A
ATOM   4897  N   THR A 326      10.522   1.806  16.095  1.00 12.62     -0.344 N
ATOM   4898  HN  THR A 326      11.194   1.463  15.408  1.00  0.00      0.163 HD
ATOM   4899  CA  THR A 326       9.337   1.017  16.384  1.00 12.18      0.205 C
ATOM   4901  C   THR A 326       9.296   0.550  17.837  1.00  7.43      0.243 C
ATOM   4902  O   THR A 326       8.244   0.655  18.489  1.00 12.29     -0.271 OA
ATOM   4903  CB  THR A 326       9.309  -0.188  15.399  1.00 17.90      0.146 C
ATOM   4905  CG2 THR A 326       8.181  -1.123  15.748  1.00 21.50      0.042 C
ATOM   4909  OG1 THR A 326       9.074   0.379  14.086  1.00 19.83     -0.393 OA
ATOM   4910  HG1 THR A 326       9.785   0.969  13.866  1.00  0.00      0.210 HD
ATOM   4911  N   ARG A 327      10.382   0.043  18.366  1.00  8.62     -0.346 N
ATOM   4912  HN  ARG A 327      11.225  -0.027  17.795  1.00  0.00      0.163 HD
ATOM   4913  CA  ARG A 327      10.421  -0.424  19.747  1.00 10.92      0.176 C
ATOM   4915  C   ARG A 327      10.147   0.758  20.709  1.00 10.34      0.241 C
ATOM   4916  O   ARG A 327       9.315   0.674  21.597  1.00 11.59     -0.271 OA
ATOM   4917  CB  ARG A 327      11.810  -1.001  20.011  1.00 12.81      0.036 C
ATOM   4920  CG  ARG A 327      11.870  -1.553  21.450  1.00 13.16      0.023 C
ATOM   4923  CD  ARG A 327      13.286  -1.869  21.884  1.00 12.48      0.138 C
ATOM   4926  NE  ARG A 327      14.307  -0.840  21.845  1.00 14.15     -0.227 N
ATOM   4927  HE  ARG A 327      14.910  -0.759  21.026  1.00  0.00      0.177 HD
ATOM   4928  CZ  ARG A 327      14.467   0.005  22.872  1.00 14.65      0.665 C
ATOM   4929  NH1 ARG A 327      13.628  -0.078  23.905  1.00 11.35     -0.235 N
ATOM   4930 1HH1 ARG A 327      12.868  -0.755  23.964  1.00  0.00      0.174 HD
ATOM   4931 2HH1 ARG A 327      13.750   0.565  24.687  1.00  0.00      0.174 HD
ATOM   4932  NH2 ARG A 327      15.455   0.885  22.795  1.00 10.66     -0.235 N
ATOM   4933 1HH2 ARG A 327      16.097   0.948  22.005  1.00  0.00      0.174 HD
ATOM   4934 2HH2 ARG A 327      15.577   1.528  23.577  1.00  0.00      0.174 HD
ATOM   4935  N   ARG A 328      10.817   1.893  20.469  1.00 13.05     -0.346 N
ATOM   4936  HN  ARG A 328      11.439   1.956  19.663  1.00  0.00      0.163 HD
ATOM   4937  CA  ARG A 328      10.658   3.050  21.366  1.00 10.55      0.176 C
ATOM   4939  C   ARG A 328       9.287   3.649  21.294  1.00 13.85      0.241 C
ATOM   4940  O   ARG A 328       8.751   4.019  22.363  1.00 14.99     -0.271 OA
ATOM   4941  CB  ARG A 328      11.790   4.072  21.086  1.00  8.59      0.036 C
ATOM   4944  CG  ARG A 328      13.138   3.509  21.483  1.00  6.22      0.023 C
ATOM   4947  CD  ARG A 328      14.285   4.441  21.017  1.00 10.23      0.138 C
ATOM   4950  NE  ARG A 328      14.039   5.851  21.426  1.00  9.11     -0.227 N
ATOM   4951  HE  ARG A 328      13.155   6.085  21.878  1.00  0.00      0.177 HD
ATOM   4952  CZ  ARG A 328      14.930   6.817  21.223  1.00  9.18      0.665 C
ATOM   4953  NH1 ARG A 328      16.118   6.514  20.676  1.00  9.45     -0.235 N
ATOM   4954 1HH1 ARG A 328      16.329   5.555  20.400  1.00  0.00      0.174 HD
ATOM   4955 2HH1 ARG A 328      16.801   7.255  20.520  1.00  0.00      0.174 HD
ATOM   4956  NH2 ARG A 328      14.656   8.062  21.581  1.00 10.54     -0.235 N
ATOM   4957 1HH2 ARG A 328      13.753   8.292  21.997  1.00  0.00      0.174 HD
ATOM   4958 2HH2 ARG A 328      15.339   8.803  21.425  1.00  0.00      0.174 HD
ATOM   4959  N   MET A 329       8.645   3.718  20.132  1.00  9.40     -0.346 N
ATOM   4960  HN  MET A 329       9.107   3.382  19.287  1.00  0.00      0.163 HD
ATOM   4961  CA  MET A 329       7.298   4.262  20.036  1.00 12.35      0.177 C
ATOM   4963  C   MET A 329       6.289   3.337  20.712  1.00 15.91      0.241 C
ATOM   4964  O   MET A 329       5.256   3.800  21.208  1.00 16.25     -0.271 OA
ATOM   4965  CB  MET A 329       6.832   4.482  18.590  1.00 15.52      0.045 C
ATOM   4968  CG  MET A 329       7.577   5.600  17.898  1.00 18.52      0.076 C
ATOM   4971  SD  MET A 329       7.564   7.200  18.808  1.00 27.68     -0.173 SA
ATOM   4972  CE  MET A 329       5.834   7.543  18.668  1.00 22.32      0.089 C
ATOM   4976  N   LYS A 330       6.538   2.035  20.719  1.00 13.62     -0.346 N
ATOM   4977  HN  LYS A 330       7.349   1.669  20.220  1.00  0.00      0.163 HD
ATOM   4978  CA  LYS A 330       5.651   1.121  21.441  1.00 15.25      0.176 C
ATOM   4980  C   LYS A 330       5.907   1.224  22.952  1.00 17.57      0.240 C
ATOM   4981  O   LYS A 330       5.078   0.700  23.694  1.00 20.97     -0.271 OA
ATOM   4982  CB  LYS A 330       5.967  -0.351  21.144  1.00 20.01      0.035 C
ATOM   4985  CG  LYS A 330       5.555  -0.932  19.825  1.00 32.79      0.004 C
ATOM   4988  CD  LYS A 330       5.510  -2.468  19.908  1.00 39.64      0.027 C
ATOM   4991  CE  LYS A 330       6.504  -3.031  18.905  1.00 42.95      0.229 C
ATOM   4994  NZ  LYS A 330       6.740  -4.488  19.081  1.00 51.82     -0.079 N
ATOM   4995  HZ1 LYS A 330       7.407  -4.866  18.408  1.00  0.00      0.274 HD
ATOM   4996  HZ2 LYS A 330       5.862  -5.006  19.054  1.00  0.00      0.274 HD
ATOM   4997  HZ3 LYS A 330       7.027  -4.698  20.037  1.00  0.00      0.274 HD
ATOM   4998  N   GLY A 331       7.056   1.674  23.423  1.00 16.11     -0.351 N
ATOM   4999  HN  GLY A 331       7.760   2.000  22.761  1.00  0.00      0.163 HD
ATOM   5000  CA  GLY A 331       7.363   1.725  24.851  1.00 16.41      0.225 C
ATOM   5003  C   GLY A 331       7.868   0.359  25.327  1.00 23.34      0.236 C
ATOM   5004  O   GLY A 331       7.862   0.147  26.544  1.00 19.87     -0.272 OA
ATOM   5005  N   GLU A 332       8.366  -0.509  24.444  1.00 17.27     -0.346 N
ATOM   5006  HN  GLU A 332       8.423  -0.249  23.459  1.00  0.00      0.163 HD
ATOM   5007  CA  GLU A 332       8.830  -1.825  24.870  1.00 20.85      0.177 C
ATOM   5009  C   GLU A 332      10.293  -1.826  25.324  1.00 17.31      0.241 C
ATOM   5010  O   GLU A 332      11.094  -1.045  24.812  1.00 17.88     -0.271 OA
ATOM   5011  CB  GLU A 332       8.789  -2.804  23.682  1.00 27.43      0.045 C
ATOM   5014  CG  GLU A 332       7.499  -3.493  23.329  1.00 48.43      0.116 C
ATOM   5017  CD  GLU A 332       7.695  -4.491  22.186  1.00 57.41      0.172 C
ATOM   5018  OE1 GLU A 332       8.799  -4.626  21.611  1.00 50.64     -0.648 OA
ATOM   5019  OE2 GLU A 332       6.685  -5.166  21.875  1.00 70.82     -0.648 OA
ATOM   5020  N   MET A 333      10.662  -2.751  26.214  1.00 16.87     -0.346 N
ATOM   5021  HN  MET A 333       9.977  -3.405  26.593  1.00  0.00      0.163 HD
ATOM   5022  CA  MET A 333      12.059  -2.816  26.639  1.00 19.38      0.177 C
ATOM   5024  C   MET A 333      12.862  -3.585  25.597  1.00 17.61      0.243 C
ATOM   5025  O   MET A 333      12.270  -4.482  24.980  1.00 16.20     -0.271 OA
ATOM   5026  CB  MET A 333      12.149  -3.636  27.939  1.00 20.01      0.045 C
ATOM   5029  CG  MET A 333      11.269  -3.127  29.060  1.00 29.52      0.076 C
ATOM   5032  SD  MET A 333      11.446  -1.360  29.325  1.00 46.40     -0.173 SA
ATOM   5033  CE  MET A 333      13.142  -1.282  29.799  1.00 13.63      0.089 C
ATOM   5037  N   PRO A 334      14.155  -3.367  25.523  1.00 16.61     -0.337 N
ATOM   5038  CA  PRO A 334      15.027  -4.159  24.660  1.00 18.11      0.179 C
ATOM   5040  C   PRO A 334      14.927  -5.608  25.125  1.00 22.37      0.241 C
ATOM   5041  O   PRO A 334      14.789  -5.839  26.335  1.00 17.78     -0.271 OA
ATOM   5042  CB  PRO A 334      16.421  -3.627  24.939  1.00 18.77      0.037 C
ATOM   5045  CG  PRO A 334      16.221  -2.268  25.526  1.00 21.70      0.022 C
ATOM   5048  CD  PRO A 334      14.932  -2.374  26.315  1.00 19.62      0.127 C
ATOM   5051  N   SER A 335      15.001  -6.595  24.242  1.00 20.49     -0.344 N
ATOM   5052  HN  SER A 335      15.179  -6.383  23.260  1.00  0.00      0.163 HD
ATOM   5053  CA  SER A 335      14.830  -7.982  24.665  1.00 24.61      0.200 C
ATOM   5055  CB  SER A 335      15.900  -8.472  25.633  1.00 20.70      0.243 C
ATOM   5056  O   SER A 335      15.608  -9.421  26.351  1.00 23.91     -0.271 OA
ATOM   5057  CB  SER A 335      14.805  -8.917  23.436  1.00 29.96      0.199 C
ATOM   5060  OG  SER A 335      16.097  -8.923  22.837  1.00 42.43     -0.398 OA
ATOM   5061  HG  SER A 335      16.082  -9.498  22.081  1.00  0.00      0.209 HD
ATOM   5062  N   ASP A 336      17.094  -7.885  25.696  1.00 22.80     -0.345 N
ATOM   5063  HN  ASP A 336      17.328  -7.092  25.099  1.00  0.00      0.163 HD
ATOM   5064  CA  ASP A 336      18.063  -8.429  26.664  1.00 24.25      0.186 C
ATOM   5066  C   ASP A 336      18.159  -7.620  27.958  1.00 25.40      0.241 C
ATOM   5067  O   ASP A 336      18.998  -7.893  28.819  1.00 22.74     -0.271 OA
ATOM   5068  CB  ASP A 336      19.442  -8.538  26.034  1.00 32.50      0.147 C
ATOM   5071  CG  ASP A 336      19.953  -7.269  25.406  1.00 40.34      0.175 C
ATOM   5072  OD1 ASP A 336      19.248  -6.237  25.411  1.00 47.80     -0.648 OA
ATOM   5073  OD2 ASP A 336      21.090  -7.338  24.880  1.00 53.43     -0.648 OA
ATOM   5074  N   PHE A 337      17.292  -6.620  28.115  1.00 19.84     -0.346 N
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ATOM   5075  HN  PHE A 337      16.568  -6.453  27.417  1.00  0.00      0.163 HD
ATOM   5076  CA  PHE A 337      17.388  -5.770  29.290  1.00 14.16      0.180 C
ATOM   5078  C   PHE A 337      17.202  -6.550  30.592  1.00 18.92      0.241 C
ATOM   5079  O   PHE A 337      17.986  -6.384  31.538  1.00 20.80     -0.271 OA
ATOM   5080  CB  PHE A 337      16.363  -4.621  29.175  1.00 21.29      0.073 C
ATOM   5083  CG  PHE A 337      16.378  -3.791  30.438  1.00 15.89     -0.056 A
ATOM   5084  CD1 PHE A 337      17.340  -2.831  30.651  1.00 20.28      0.007 A
ATOM   5086  CD2 PHE A 337      15.425  -4.030  31.408  1.00 13.91      0.007 A
ATOM   5088  CE1 PHE A 337      17.347  -2.104  31.832  1.00 17.77      0.001 A
ATOM   5090  CE2 PHE A 337      15.426  -3.312  32.600  1.00 18.89      0.001 A
ATOM   5092  CZ  PHE A 337      16.387  -2.339  32.795  1.00 20.67      0.000 A
ATOM   5094  N   ASP A 338      16.177  -7.393  30.671  1.00 15.88     -0.345 N
ATOM   5095  HN  ASP A 338      15.596  -7.570  29.852  1.00  0.00      0.163 HD
ATOM   5096  CA  ASP A 338      15.884  -8.068  31.941  1.00 19.01      0.186 C
ATOM   5098  C   ASP A 338      17.050  -8.902  32.428  1.00 21.98      0.241 C
ATOM   5099  O   ASP A 338      17.480  -8.829  33.577  1.00 18.93     -0.271 OA
ATOM   5100  CB  ASP A 338      14.599  -8.882  31.804  1.00 24.81      0.147 C
ATOM   5103  CG  ASP A 338      14.281  -9.711  33.026  1.00 21.40      0.175 C
ATOM   5104  OD1 ASP A 338      13.788  -9.193  34.043  1.00 27.39     -0.648 OA
ATOM   5105  OD2 ASP A 338      14.545 -10.932  32.986  1.00 37.20     -0.648 OA
ATOM   5106  N   ALA A 339      17.574  -9.714  31.525  1.00 22.62     -0.346 N
ATOM   5107  HN  ALA A 339      17.159  -9.743  30.594  1.00  0.00      0.163 HD
ATOM   5108  CA  ALA A 339      18.717 -10.566  31.807  1.00 26.00      0.172 C
ATOM   5110  C   ALA A 339      19.938  -9.746  32.197  1.00 23.56      0.240 C
ATOM   5111  O   ALA A 339      20.519 -10.034  33.234  1.00 21.22     -0.271 OA
ATOM   5112  CB  ALA A 339      19.034 -11.407  30.565  1.00 23.61      0.042 C
ATOM   5116  N   LYS A 340      20.247  -8.660  31.486  1.00 15.76     -0.346 N
ATOM   5117  HN  LYS A 340      19.665  -8.390  30.693  1.00  0.00      0.163 HD
ATOM   5118  CA  LYS A 340      21.404  -7.864  31.835  1.00 15.82      0.176 C
ATOM   5120  C   LYS A 340      21.228  -7.139  33.172  1.00 16.68      0.241 C
ATOM   5121  O   LYS A 340      22.180  -7.058  33.956  1.00 28.38     -0.271 OA
ATOM   5122  CB  LYS A 340      21.676  -6.862  30.729  1.00 19.28      0.035 C
ATOM   5125  CG  LYS A 340      22.359  -7.553  29.542  1.00 33.54      0.004 C
ATOM   5128  CD  LYS A 340      22.451  -6.596  28.368  1.00 49.88      0.027 C
ATOM   5131  CE  LYS A 340      23.658  -6.922  27.497  1.00 56.92      0.229 C
ATOM   5134  NZ  LYS A 340      23.532  -8.272  26.889  1.00 56.32     -0.079 N
ATOM   5135  HZ1 LYS A 340      24.340  -8.490  26.306  1.00  0.00      0.274 HD
ATOM   5136  HZ2 LYS A 340      22.658  -8.370  26.372  1.00  0.00      0.274 HD
ATOM   5137  HZ3 LYS A 340      23.376  -8.989  27.597  1.00  0.00      0.274 HD
ATOM   5138  N   ALA A 341      20.000  -6.688  33.426  1.00 16.17     -0.346 N
ATOM   5139  HN  ALA A 341      19.244  -6.831  32.756  1.00  0.00      0.163 HD
ATOM   5140  CA  ALA A 341      19.755  -5.978  34.695  1.00 16.66      0.172 C
ATOM   5142  C   ALA A 341      19.836  -6.985  35.824  1.00 16.09      0.240 C
ATOM   5143  O   ALA A 341      20.387  -6.646  36.877  1.00 17.11     -0.271 OA
ATOM   5144  CB  ALA A 341      18.400  -5.269  34.665  1.00 15.86      0.042 C
ATOM   5148  N   LYS A 342      19.344  -8.215  35.594  1.00 16.01     -0.346 N
ATOM   5149  HN  LYS A 342      18.905  -8.451  34.704  1.00  0.00      0.163 HD
ATOM   5150  CA  LYS A 342      19.462  -9.210  36.676  1.00 21.24      0.176 C
ATOM   5152  C   LYS A 342      20.892  -9.582  37.013  1.00 21.83      0.241 C
ATOM   5153  O   LYS A 342      21.260  -9.783  38.186  1.00 17.73     -0.271 OA
ATOM   5154  CB  LYS A 342      18.678 -10.499  36.370  1.00 24.04      0.035 C
ATOM   5157  CG  LYS A 342      17.183 -10.240  36.397  1.00 34.79      0.004 C
ATOM   5160  CD  LYS A 342      16.380 -11.504  36.141  1.00 44.46      0.027 C
ATOM   5163  CE  LYS A 342      14.889 -11.217  36.330  1.00 57.43      0.229 C
ATOM   5166  NZ  LYS A 342      14.091 -11.989  35.331  1.00 59.38     -0.079 N
ATOM   5167  HZ1 LYS A 342      13.097 -11.798  35.457  1.00  0.00      0.274 HD
ATOM   5168  HZ2 LYS A 342      14.296 -12.988  35.367  1.00  0.00      0.274 HD
ATOM   5169  HZ3 LYS A 342      14.397 -11.809  34.375  1.00  0.00      0.274 HD
ATOM   5170  N   GLU A 343      21.727  -9.670  35.994  1.00 24.07     -0.346 N
ATOM   5171  HN  GLU A 343      21.363  -9.548  35.049  1.00  0.00      0.163 HD
ATOM   5172  CA  GLU A 343      23.152  -9.936  36.169  1.00 21.57      0.177 C
ATOM   5174  C   GLU A 343      23.831  -8.809  36.934  1.00 19.88      0.241 C
ATOM   5175  O   GLU A 343      24.678  -9.036  37.803  1.00 16.78     -0.271 OA
ATOM   5176  CB  GLU A 343      23.713 -10.095  34.767  1.00 27.50      0.045 C
ATOM   5179  CG  GLU A 343      24.965 -10.846  34.434  1.00 51.50      0.116 C
ATOM   5182  CD  GLU A 343      25.187 -10.793  32.914  1.00 56.71      0.172 C
ATOM   5183  OE1 GLU A 343      24.577 -11.625  32.203  1.00 61.26     -0.648 OA
ATOM   5184  OE2 GLU A 343      25.930  -9.888  32.478  1.00 55.86     -0.648 OA
ATOM   5185  N   PHE A 344      23.504  -7.551  36.633  1.00 14.77     -0.346 N
ATOM   5186  HN  PHE A 344      22.836  -7.377  35.882  1.00  0.00      0.163 HD
ATOM   5187  CA  PHE A 344      24.082  -6.413  37.355  1.00 14.92      0.180 C
ATOM   5189  C   PHE A 344      23.669  -6.437  38.833  1.00 14.38      0.241 C
ATOM   5190  O   PHE A 344      24.474  -6.181  39.730  1.00 15.02     -0.271 OA
ATOM   5191  CB  PHE A 344      23.563  -5.125  36.690  1.00 17.25      0.073 C
ATOM   5194  CG  PHE A 344      23.915  -3.830  37.359  1.00 18.97     -0.056 A
ATOM   5195  CD1 PHE A 344      25.235  -3.419  37.443  1.00 15.62      0.007 A
ATOM   5197  CD2 PHE A 344      22.915  -3.014  37.879  1.00 19.33      0.007 A
ATOM   5199  CE1 PHE A 344      25.552  -2.219  38.054  1.00 17.22      0.001 A
ATOM   5201  CE2 PHE A 344      23.247  -1.826  38.508  1.00 16.31      0.001 A
ATOM   5203  CZ  PHE A 344      24.555  -1.417  38.586  1.00 14.39      0.000 A
ATOM   5205  N   ILE A 345      22.394  -6.680  39.100  1.00 15.57     -0.346 N
ATOM   5206  HN  ILE A 345      21.745  -6.802  38.323  1.00  0.00      0.163 HD
ATOM   5207  CA  ILE A 345      21.884  -6.779  40.480  1.00 17.97      0.180 C
ATOM   5209  C   ILE A 345      22.609  -7.886  41.240  1.00 17.24      0.241 C
ATOM   5210  O   ILE A 345      23.007  -7.749  42.397  1.00 14.60     -0.271 OA
ATOM   5211  CB  ILE A 345      20.363  -6.997  40.470  1.00 14.50      0.013 C
ATOM   5213  CG1 ILE A 345      19.669  -5.659  40.077  1.00 13.45      0.002 C
ATOM   5216  CG2 ILE A 345      19.775  -7.393  41.848  1.00 16.76      0.012 C
ATOM   5220  CD1 ILE A 345      18.278  -5.935  39.502  1.00 14.52      0.005 C
ATOM   5224  N   ALA A 346      22.715  -9.075  40.646  1.00 14.29     -0.346 N
ATOM   5225  HN  ALA A 346      22.328  -9.226  39.714  1.00  0.00      0.163 HD
ATOM   5226  CA  ALA A 346      23.403 -10.172  41.361  1.00 17.88      0.172 C
ATOM   5228  C   ALA A 346      24.855  -9.855  41.623  1.00 17.07      0.240 C
ATOM   5229  O   ALA A 346      25.404 -10.188  42.689  1.00 16.35     -0.271 OA
ATOM   5230  CB  ALA A 346      23.281 -11.474  40.579  1.00 19.21      0.042 C
ATOM   5234  N   LYS A 347      25.504  -9.172  40.677  1.00 14.76     -0.346 N
ATOM   5235  HN  LYS A 347      25.023  -8.948  39.806  1.00  0.00      0.163 HD
ATOM   5236  CA  LYS A 347      26.888  -8.738  40.860  1.00 15.04      0.176 C
ATOM   5238  C   LYS A 347      27.005  -7.792  42.037  1.00 17.52      0.241 C
ATOM   5239  O   LYS A 347      27.968  -7.841  42.814  1.00 21.04     -0.271 OA
ATOM   5240  CB  LYS A 347      27.419  -8.058  39.590  1.00 21.09      0.035 C
ATOM   5243  CG  LYS A 347      28.850  -7.587  39.656  1.00 34.45      0.004 C
ATOM   5246  CD  LYS A 347      29.140  -6.359  38.803  1.00 47.67      0.027 C
ATOM   5249  CE  LYS A 347      28.522  -5.101  39.376  1.00 61.06      0.229 C
ATOM   5252  NZ  LYS A 347      29.189  -3.832  38.966  1.00 61.24     -0.079 N
ATOM   5253  HZ1 LYS A 347      28.773  -2.985  39.352  1.00  0.00      0.274 HD
ATOM   5254  HZ2 LYS A 347      29.236  -3.771  37.949  1.00  0.00      0.274 HD
ATOM   5255  HZ3 LYS A 347      30.184  -3.869  39.187  1.00  0.00      0.274 HD
ATOM   5256  N   LEU A 348      26.066  -6.845  42.184  1.00 12.99     -0.346 N
ATOM   5257  HN  LEU A 348      25.317  -6.752  41.498  1.00  0.00      0.163 HD
ATOM   5258  CA  LEU A 348      26.126  -5.945  43.339  1.00 10.14      0.177 C
ATOM   5260  C   LEU A 348      25.946  -6.713  44.656  1.00 16.66      0.241 C
ATOM   5261  O   LEU A 348      26.606  -6.386  45.650  1.00 13.45     -0.271 OA
ATOM   5262  CB  LEU A 348      25.009  -4.900  43.256  1.00 12.56      0.038 C
ATOM   5265  CG  LEU A 348      25.083  -3.913  42.063  1.00 12.89     -0.020 C
ATOM   5267  CD1 LEU A 348      23.976  -2.860  42.237  1.00 17.46      0.009 C
ATOM   5271  CD2 LEU A 348      26.435  -3.216  41.995  1.00 11.51      0.009 C
ATOM   5275  N   GLN A 349      25.065  -7.693  44.678  1.00  9.99     -0.346 N
ATOM   5276  HN  GLN A 349      24.538  -7.945  43.842  1.00  0.00      0.163 HD
ATOM   5277  CA  GLN A 349      24.862  -8.420  45.958  1.00 16.37      0.177 C
ATOM   5279  C   GLN A 349      26.114  -9.205  46.337  1.00 19.41      0.241 C
ATOM   5280  O   GLN A 349      26.452  -9.386  47.523  1.00 14.54     -0.271 OA
ATOM   5281  CB  GLN A 349      23.666  -9.358  45.812  1.00 13.58      0.044 C
ATOM   5284  CG  GLN A 349      23.230 -10.101  47.086  1.00 12.91      0.105 C
ATOM   5287  CD  GLN A 349      22.935  -9.151  48.241  1.00 21.62      0.215 C
ATOM   5288  NE2 GLN A 349      23.713  -9.115  49.328  1.00 14.17     -0.370 N
ATOM   5289 1HE2 GLN A 349      23.516  -8.479  50.101  1.00  0.00      0.159 HD
ATOM   5290 2HE2 GLN A 349      24.545  -9.694  49.440  1.00  0.00      0.159 HD
ATOM   5291  OE1 GLN A 349      21.935  -8.455  48.107  1.00 14.54     -0.274 OA
ATOM   5292  N   ALA A 350      26.836  -9.683  45.327  1.00 16.34     -0.346 N
ATOM   5293  HN  ALA A 350      26.512  -9.538  44.371  1.00  0.00      0.163 HD
ATOM   5294  CA  ALA A 350      28.089 -10.415  45.558  1.00 18.16      0.172 C
ATOM   5296  C   ALA A 350      29.264  -9.521  45.883  1.00 21.82      0.240 C
ATOM   5297  O   ALA A 350      30.276 -10.024  46.399  1.00 23.56     -0.271 OA
ATOM   5298  CB  ALA A 350      28.415 -11.253  44.304  1.00 15.80      0.042 C
ATOM   5302  N   ASN A 351      29.280  -8.211  45.634  1.00 16.52     -0.346 N
ATOM   5303  HN  ASN A 351      28.429  -7.804  45.245  1.00  0.00      0.163 HD
ATOM   5304  CA  ASN A 351      30.390  -7.312  45.864  1.00 18.70      0.185 C
ATOM   5306  C   ASN A 351      29.921  -6.083  46.630  1.00 18.79      0.243 C
ATOM   5307  O   ASN A 351      29.646  -5.044  46.021  1.00 19.73     -0.271 OA
ATOM   5308  CB  ASN A 351      30.971  -6.778  44.510  1.00 23.83      0.137 C
ATOM   5311  CG  ASN A 351      31.542  -7.944  43.721  1.00 33.62      0.217 C
ATOM   5312  ND2 ASN A 351      30.860  -8.486  42.723  1.00 25.60     -0.370 N
ATOM   5313 1HD2 ASN A 351      29.961  -8.107  42.426  1.00  0.00      0.159 HD
ATOM   5314 2HD2 ASN A 351      31.243  -9.269  42.241  1.00  0.00      0.159 HD
ATOM   5315  OD1 ASN A 351      32.633  -8.404  44.082  1.00 29.05     -0.274 OA
ATOM   5316  N   PRO A 352      29.758  -6.220  47.931  1.00 17.82     -0.337 N
ATOM   5317  CA  PRO A 352      29.202  -5.161  48.737  1.00 19.82      0.179 A
ATOM   5319  C   PRO A 352      29.976  -3.862  48.722  1.00 11.49      0.241 C
ATOM   5320  O   PRO A 352      31.198  -3.874  48.676  1.00 19.17     -0.271 OA
ATOM   5321  CB  PRO A 352      29.196  -5.696  50.152  1.00 20.26      0.037 A
ATOM   5324  CG  PRO A 352      29.734  -7.071  50.129  1.00 23.80      0.022 A
ATOM   5327  CD  PRO A 352      30.050  -7.442  48.708  1.00 24.05      0.127 A
ATOM   5330  N   ALA A 353      29.268  -2.738  48.848  1.00 17.01     -0.346 N
ATOM   5331  HN  ALA A 353      28.252  -2.803  48.906  1.00  0.00      0.163 HD
ATOM   5332  CA  ALA A 353      29.887  -1.425  48.906  1.00 18.16      0.172 C
ATOM   5334  C   ALA A 353      28.959  -0.558  49.778  1.00 18.94      0.240 C
ATOM   5335  O   ALA A 353      27.731  -0.681  49.728  1.00 14.67     -0.271 OA
ATOM   5336  CB  ALA A 353      30.048  -0.798  47.520  1.00 17.44      0.042 C
ATOM   5340  N   LYS A 354      29.581   0.224  50.629  1.00 19.21     -0.346 N
ATOM   5341  HN  LYS A 354      30.601   0.215  50.656  1.00  0.00      0.163 HD
ATOM   5342  CA  LYS A 354      28.854  1.109  51.541  1.00 18.93      0.176 C
ATOM   5344  C   LYS A 354      28.843  2.470  50.865  1.00 19.56      0.241 C
ATOM   5345  O   LYS A 354      29.844  3.169  50.932  1.00 16.41     -0.271 OA
ATOM   5346  CB  LYS A 354      29.552  1.114  52.906  1.00 26.19      0.035 C
ATOM   5349  CG  LYS A 354      28.896  2.083  53.877  1.00 21.51      0.004 C
ATOM   5352  CD  LYS A 354      29.286  1.767  55.332  1.00 31.26      0.027 C
ATOM   5355  CE  LYS A 354      28.452  2.690  56.209  1.00 38.67      0.229 C
ATOM   5358  NZ  LYS A 354      29.133  3.135  57.450  1.00 50.17     -0.079 N
ATOM   5359  HZ1 LYS A 354      28.574  3.754  58.038  1.00  0.00      0.274 HD
ATOM   5360  HZ2 LYS A 354      30.029  3.568  57.228  1.00  0.00      0.274 HD
ATOM   5361  HZ3 LYS A 354      29.456  2.330  57.987  1.00  0.00      0.274 HD
ATOM   5362  N   ILE A 355      27.810  2.816  50.099  1.00 16.30     -0.346 N
ATOM   5363  HN  ILE A 355      27.010  2.186  50.047  1.00  0.00      0.163 HD
ATOM   5364  CA  ILE A 355      27.772  4.059  49.329  1.00 14.24      0.180 C
ATOM   5366  C   ILE A 355      26.387  4.663  49.508  1.00 15.15      0.241 C
ATOM   5367  O   ILE A 355      25.457  3.986  49.950  1.00 14.56     -0.271 OA
ATOM   5368  CB  ILE A 355      28.049  3.871  47.817  1.00 14.63      0.013 C
ATOM   5370  CG1 ILE A 355      27.035  2.896  47.190  1.00 16.48      0.002 C
ATOM   5373  CG2 ILE A 355      29.471  3.371  47.550  1.00 21.19      0.012 C
ATOM   5377  CD1 ILE A 355      27.167  2.742  45.668  1.00 18.86      0.005 C
ATOM   5381  N   ALA A 356      26.232  5.954  49.250  1.00 13.49     -0.346 N
ATOM   5382  HN  ALA A 356      27.039  6.503  48.953  1.00  0.00      0.163 HD
ATOM   5383  CA  ALA A 356      24.935  6.607  49.381  1.00 12.95      0.172 C
ATOM   5385  C   ALA A 356      24.034  6.011  48.299  1.00 14.59      0.240 C
ATOM   5386  O   ALA A 356      24.550  5.666  47.226  1.00 12.29     -0.271 OA
ATOM   5387  CB  ALA A 356      25.073  8.138  49.178  1.00 13.17      0.042 C
ATOM   5391  N   SER A 357      22.711  5.965  48.530  1.00 12.01     -0.344 N
ATOM   5392  HN  SER A 357      22.321  6.291  49.414  1.00  0.00      0.163 HD
ATOM   5393  CA  SER A 357      21.839  5.429  47.468  1.00 13.21      0.200 C
ATOM   5395  C   SER A 357      21.753  6.452  46.325  1.00 10.74      0.243 C
ATOM   5396  O   SER A 357      21.452  6.006  45.224  1.00 12.49     -0.271 OA
ATOM   5397  CB  SER A 357      20.442  4.983  47.914  1.00  9.04      0.199 C
ATOM   5400  OG  SER A 357      19.800  5.990  48.705  1.00 11.28     -0.398 OA
ATOM   5401  HG  SER A 357      18.934  5.714  48.981  1.00  0.00      0.209 HD
ATOM   5402  N   ARG A 358      22.110  7.724  46.514  1.00 11.36     -0.346 N
ATOM   5403  HN  ARG A 358      22.333  8.072  47.447  1.00  0.00      0.163 HD
ATOM   5404  CA  ARG A 358      22.174  8.619  45.333  1.00 12.81      0.176 C
ATOM   5406  C   ARG A 358      23.310  8.179  44.419  1.00 10.80      0.241 C
ATOM   5407  O   ARG A 358      23.178  8.263  43.177  1.00 11.82     -0.271 OA
ATOM   5408  CB  ARG A 358      22.373 10.096  45.669  1.00 13.91      0.036 C
ATOM   5411  CG  ARG A 358      23.645 10.402  46.473  1.00 16.31      0.023 C
ATOM   5414  CD  ARG A 358      23.882 11.901  46.540  1.00 17.50      0.138 C
ATOM   5417  NE  ARG A 358      25.059 12.240  47.343  1.00 17.99     -0.227 N
ATOM   5418  HE  ARG A 358      25.455 11.484  47.902  1.00  0.00      0.177 HD
ATOM   5419  CZ  ARG A 358      25.669 13.411  47.429  1.00 28.20      0.665 C
ATOM   5420  NH1 ARG A 358      25.247 14.460  46.755  1.00 19.46     -0.235 N
ATOM   5421 1HH1 ARG A 358      25.717 15.363  46.821  1.00  0.00      0.174 HD
ATOM   5422 2HH1 ARG A 358      24.455 14.349  46.121  1.00  0.00      0.174 HD
ATOM   5423  NH2 ARG A 358      26.716 13.558  48.267  1.00 19.61     -0.235 N
ATOM   5424 1HH2 ARG A 358      27.186 14.461  48.333  1.00  0.00      0.174 HD
ATOM   5425 2HH2 ARG A 358      27.043 12.745  48.789  1.00  0.00      0.174 HD
ATOM   5426  N   LYS A 359      24.424  7.681  44.984  1.00 12.33     -0.346 N
ATOM   5427  HN  LYS A 359      24.503  7.661  46.001  1.00  0.00      0.163 HD
ATOM   5428  CA  LYS A 359      25.532  7.164  44.162  1.00 14.07      0.176 C
ATOM   5430  C   LYS A 359      25.190  5.817  43.541  1.00 11.65      0.241 C
ATOM   5431  O   LYS A 359      25.506  5.514  42.369  1.00 11.54     -0.271 OA
ATOM   5432  CB  LYS A 359      26.802  7.033  45.001  1.00 20.67      0.035 C
ATOM   5435  CG  LYS A 359      28.028  6.479  44.246  1.00 23.08      0.004 C
ATOM   5438  CD  LYS A 359      28.465  7.486  43.201  1.00 36.10      0.027 C
ATOM   5441  CE  LYS A 359      29.782  7.078  42.541  1.00 49.60      0.229 C
ATOM   5444  NZ  LYS A 359      29.624  7.041  41.054  1.00 40.98     -0.079 N
ATOM   5445  HZ1 LYS A 359      30.503  6.769  40.614  1.00  0.00      0.274 HD
ATOM   5446  HZ2 LYS A 359      29.271  7.924  40.686  1.00  0.00      0.274 HD
ATOM   5447  HZ3 LYS A 359      28.852  6.440  40.768  1.00  0.00      0.274 HD
ATOM   5448  N   ALA A 360      24.435  4.967  44.261  1.00 12.24     -0.346 N
ATOM   5449  HN  ALA A 360      24.171  5.221  45.213  1.00  0.00      0.163 HD
ATOM   5450  CA  ALA A 360      23.984  3.688  43.714  1.00 11.57      0.172 C
ATOM   5452  C   ALA A 360      22.999  3.919  42.568  1.00 13.85      0.240 C
ATOM   5453  O   ALA A 360      22.920  3.171  41.567  1.00 11.57     -0.271 OA
ATOM   5454  CB  ALA A 360      23.327  2.837  44.820  1.00 13.63      0.042 C
ATOM   5458  N   SER A 361      22.232  5.020  42.669  1.00 10.41     -0.344 N
ATOM   5459  HN  SER A 361      22.276  5.585  43.517  1.00  0.00      0.163 HD
ATOM   5460  CA  SER A 361      21.335  5.423  41.584  1.00 13.28      0.200 C
ATOM   5462  C   SER A 361      22.137  5.845  40.342  1.00 13.60      0.243 C
ATOM   5463  O   SER A 361      21.795  5.377  39.237  1.00 12.40     -0.271 OA
ATOM   5464  CB  SER A 361      20.413  6.566  42.071  1.00  9.50      0.199 C
ATOM   5467  OG  SER A 361      19.719  7.130  40.936  1.00 11.31     -0.398 OA
ATOM   5468  HG  SER A 361      19.153  7.832  41.235  1.00  0.00      0.209 HD
ATOM   5469  N   GLN A 362      23.170  6.671  40.495  1.00 11.40     -0.346 N
ATOM   5470  HN  GLN A 362      23.364  7.067  41.415  1.00  0.00      0.163 HD
ATOM   5471  CA  GLN A 362      24.037  7.022  39.357  1.00 12.21      0.177 C
ATOM   5473  C   GLN A 362      24.689  5.784  38.730  1.00 13.04      0.241 C
ATOM   5474  O   GLN A 362      24.792  5.655  37.519  1.00 11.93     -0.271 OA
ATOM   5475  CB  GLN A 362      25.210  7.938  39.777  1.00 14.43      0.044 C
ATOM   5478  CG  GLN A 362      25.903  8.517  38.493  1.00 15.09      0.105 C
ATOM   5481  CD  GLN A 362      26.962  9.501  38.951  1.00 31.20      0.215 C
ATOM   5482  NE2 GLN A 362      27.090 10.635  38.277  1.00 20.44     -0.370 N
ATOM   5483 1HE2 GLN A 362      26.543 10.855  37.445  1.00  0.00      0.159 HD
ATOM   5484 2HE2 GLN A 362      27.802 11.297  38.585  1.00  0.00      0.159 HD
ATOM   5485  OE1 GLN A 362      27.627  9.234  39.962  1.00 23.13     -0.274 OA
ATOM   5486  N   ASN A 363      25.110  4.812  39.550  1.00 11.84     -0.346 N
ATOM   5487  HN  ASN A 363      25.031  4.953  40.557  1.00  0.00      0.163 HD
ATOM   5488  CA  ASN A 363      25.675  3.565  39.064  1.00 12.78      0.185 C
ATOM   5490  C   ASN A 363      24.663  2.762  38.260  1.00 12.62      0.241 C
ATOM   5491  O   ASN A 363      25.089  2.159  37.256  1.00 14.03     -0.271 OA
ATOM   5492  CB  ASN A 363      26.145  2.676  40.226  1.00 12.44      0.137 C
ATOM   5495  CG  ASN A 363      27.415  3.201  40.858  1.00 23.17      0.217 C
ATOM   5496  ND2 ASN A 363      27.754  2.681  42.038  1.00 18.19     -0.370 N
ATOM   5497 1HD2 ASN A 363      28.610  3.035  42.464  1.00  0.00      0.159 HD
ATOM   5498 2HD2 ASN A 363      27.193  1.961  42.493  1.00  0.00      0.159 HD
ATOM   5499  OD1 ASN A 363      28.098  4.077  40.304  1.00 18.68     -0.274 OA
ATOM   5500  N   ALA A 364      23.380  2.737  38.638  1.00 11.65     -0.346 N
ATOM   5501  HN  ALA A 364      23.098  3.209  39.497  1.00  0.00      0.163 HD
ATOM   5502  CA  ALA A 364      22.388  2.047  37.840  1.00 11.41      0.172 C
ATOM   5504  C   ALA A 364      22.177  2.788  36.510  1.00 12.95      0.240 C
ATOM   5505  O   ALA A 364      21.923  2.175  35.453  1.00 13.91     -0.271 OA
ATOM   5506  CB  ALA A 364      21.005  1.928  38.535  1.00 12.05      0.042 C
ATOM   5510  N   ILE A 365      22.183  4.137  36.533  1.00 12.47     -0.346 N
ATOM   5511  HN  ILE A 365      22.307  4.632  37.416  1.00  0.00      0.163 HD
ATOM   5512  CA  ILE A 365      22.010  4.893  35.282  1.00 12.80      0.180 C
ATOM   5514  C   ILE A 365      23.155  4.539  34.317  1.00 15.63      0.241 C
ATOM   5515  O   ILE A 365      22.973  4.399  33.094  1.00 15.20     -0.271 OA
ATOM   5516  CB  ILE A 365      21.975  6.425  35.511  1.00 11.56      0.013 C
ATOM   5518  CG1 ILE A 365      20.734  6.770  36.377  1.00 13.34      0.002 C
ATOM   5521  CG2 ILE A 365      21.907  7.120  34.147  1.00 16.26      0.012 C
ATOM   5525  CD1 ILE A 365      20.650  8.258  36.792  1.00  9.30      0.005 C
ATOM   5529  N   GLU A 366      24.338  4.414  34.886  1.00 13.95     -0.346 N
ATOM   5530  HN  GLU A 366      24.434  4.562  35.891  1.00  0.00      0.163 HD
ATOM   5531  CA  GLU A 366      25.525  4.062  34.082  1.00 15.11      0.177 C
ATOM   5533  C   GLU A 366      25.410  2.660  33.516  1.00 18.26      0.241 C
ATOM   5534  O   GLU A 366      25.830  2.445  32.386  1.00 13.52     -0.271 OA
ATOM   5535  CB  GLU A 366      26.798  4.212  34.959  1.00 22.75      0.045 C
ATOM   5538  CG  GLU A 366      28.111  3.983  34.253  1.00 25.64      0.116 C
ATOM   5541  CD  GLU A 366      28.465  5.075  33.241  1.00 20.82      0.172 C
ATOM   5542  OE1 GLU A 366      28.318  6.275  33.530  1.00 18.92     -0.648 OA
ATOM   5543  OE2 GLU A 366      28.922  4.733  32.124  1.00 28.94     -0.648 OA
ATOM   5544  N   ALA A 367      24.860  1.699  34.242  1.00 15.92     -0.346 N
ATOM   5545  HN  ALA A 367      24.536  1.904  35.187  1.00  0.00      0.163 HD
ATOM   5546  CA  ALA A 367      24.711  0.342  33.701  1.00 16.94      0.172 C
ATOM   5548  C   ALA A 367      23.564  0.262  32.719  1.00 19.44      0.240 C
ATOM   5549  O   ALA A 367      23.636 -0.541  31.792  1.00 18.03     -0.271 OA
ATOM   5550  CB  ALA A 367      24.495 -0.652  34.836  1.00 17.24      0.042 C
ATOM   5554  N   PHE A 368      22.424  0.938  32.913  1.00 10.51     -0.346 N
ATOM   5555  HN  PHE A 368      22.371  1.567  33.714  1.00  0.00      0.163 HD
ATOM   5556  CA  PHE A 368      21.268  0.832  32.061  1.00 12.26      0.180 C
ATOM   5558  C   PHE A 368      21.343  1.776  30.850  1.00 13.61      0.241 C
ATOM   5559  O   PHE A 368      20.786  1.478  29.796  1.00 17.74     -0.271 OA
ATOM   5560  CB  PHE A 368      19.954  1.180  32.799  1.00 13.68      0.073 C
ATOM   5563  CG  PHE A 368      19.588  0.243  33.928  1.00 14.35     -0.056 A
ATOM   5564  CD1 PHE A 368      20.303 -0.894  34.189  1.00 19.92      0.007 A
ATOM   5566  CD2 PHE A 368      18.484  0.537  34.723  1.00 23.58      0.007 A
ATOM   5568  CE1 PHE A 368      19.974 -1.746  35.238  1.00 27.39      0.001 A
ATOM   5570  CE2 PHE A 368      18.139 -0.309  35.766  1.00 24.27      0.001 A
ATOM   5572  CZ  PHE A 368      18.881 -1.430  36.019  1.00 26.35      0.000 A
ATOM   5574  N   GLY A 369      22.085  2.849  30.957  1.00 14.81     -0.351 N
ATOM   5575  HN  GLY A 369      22.583  2.991  31.836  1.00  0.00      0.163 HD
ATOM   5576  CA  GLY A 369      22.255  3.858  29.916  1.00 16.53      0.225 C
ATOM   5579  C   GLY A 369      20.953  4.508  29.492  1.00 17.62     -0.238 C
ATOM   5580  O   GLY A 369      21.859  3.639  27.560  1.00 16.95     -0.272 OA
ATOM   5581  N   PRO A 370      23.527  2.435  28.392  1.00 18.28     -0.337 N
ATOM   5582  CA  PRO A 370      23.859  1.842  27.092  1.00 16.51      0.179 C
ATOM   5584  C   PRO A 370      22.774  0.932  26.565  1.00 19.48      0.241 C
ATOM   5585  O   PRO A 370      22.654  0.651  25.370  1.00 22.50     -0.271 OA
ATOM   5586  CB  PRO A 370      25.118  1.020  27.387  1.00 19.21      0.037 C
ATOM   5589  CG  PRO A 370      25.719  1.683  28.587  1.00 19.85      0.022 C
ATOM   5592  CD  PRO A 370      24.522  2.043  29.439  1.00 19.34      0.127 C
ATOM   5595  N   LEU A 371      21.873  0.435  27.398  1.00 14.02     -0.346 N
ATOM   5596  HN  LEU A 371      21.930  0.696  28.382  1.00  0.00      0.163 HD
ATOM   5597  CA  LEU A 371      20.805 -0.465  26.984  1.00 15.79      0.177 C
ATOM   5599  C   LEU A 371      19.537  0.255  26.625  1.00 16.21      0.241 C
ATOM   5600  O   LEU A 371      18.680 -0.322  25.953  1.00 14.49     -0.271 OA
ATOM   5601  CB  LEU A 371      20.457 -1.400  28.158  1.00 17.97      0.038 C
ATOM   5604  CG  LEU A 371      21.688 -2.162  28.697  1.00 26.08     -0.020 C
ATOM   5606  CD1 LEU A 371      21.247 -3.075  29.829  1.00 27.60      0.009 C
ATOM   5610  CD2 LEU A 371      22.330 -2.958  27.563  1.00 30.56      0.009 C
ATOM   5614  N   LEU A 372      19.392  1.477  27.152  1.00 11.02     -0.346 N
ATOM   5615  HN  LEU A 372      20.144  1.876  27.714  1.00  0.00      0.163 HD
ATOM   5616  CA  LEU A 372      18.171  2.246  26.933  1.00 12.42      0.177 C
ATOM   5618  C   LEU A 372      18.438  3.598  26.296  1.00 13.76      0.243 C
ATOM   5619  O   LEU A 372      18.429  4.668  26.927  1.00 12.92     -0.271 OA
ATOM   5620  CB  LEU A 372      17.523  2.513  28.329  1.00  9.98      0.038 C
ATOM   5623  CG  LEU A 372      17.100  1.257  29.109  1.00 17.16     -0.020 C
ATOM   5625  CD1 LEU A 372      16.617  1.677  30.501  1.00 17.71      0.009 C
ATOM   5629  CD2 LEU A 372      16.033  0.483  28.359  1.00 12.87      0.009 C
ATOM   5633  N   PRO A 373      18.634  3.652  24.978  1.00 12.67     -0.337 N
ATOM   5634  CA  PRO A 373      18.828  4.856  24.230  1.00 12.37      0.179 C
ATOM   5636  C   PRO A 373      17.641  5.801  24.320  1.00 12.42      0.241 C
ATOM   5637  O   PRO A 373      17.767  6.991  24.012  1.00 11.12     -0.271 OA
ATOM   5638  CB  PRO A 373      19.050  4.384  22.768  1.00 14.08      0.037 C
ATOM   5641  CG  PRO A 373      18.450  3.002  22.737  1.00 13.89      0.022 C
ATOM   5644  CD  PRO A 373      18.726  2.409  24.102  1.00 13.40      0.127 C
ATOM   5647  N   GLU A 374      16.470  5.326  24.747  1.00  8.96     -0.346 N
ATOM   5648  HN  GLU A 374      16.397  4.330  24.955  1.00  0.00      0.163 HD
ATOM   5649  CA  GLU A 374      15.286  6.163  24.931  1.00 12.52      0.177 C
ATOM   5651  C   GLU A 374      15.378  7.057  26.166  1.00 12.10      0.241 C
ATOM   5652  O   GLU A 374      14.485  7.901  26.325  1.00  9.97     -0.271 OA
ATOM   5653  CB  GLU A 374      14.018  5.287  25.045  1.00 10.23      0.045 C
ATOM   5656  CG  GLU A 374      14.097  4.255  26.171  1.00 15.07      0.116 C
ATOM   5659  CD  GLU A 374      14.437  2.867  25.626  1.00 15.28      0.172 C
ATOM   5660  OE1 GLU A 374      15.480  2.755  24.943  1.00 10.55     -0.648 OA
ATOM   5661  OE2 GLU A 374      13.680  1.901  25.856  1.00 15.43     -0.648 OA
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ATOM   5662  N   PHE A 375      16.351   6.886  27.060  1.00  9.08    -0.346 N
ATOM   5663  HN  PHE A 375      17.028   6.129  26.970  1.00  0.00     0.163 HD
ATOM   5664  CA  PHE A 375      16.408   7.843  28.191  1.00  8.01     0.180 C
ATOM   5666  C   PHE A 375      16.460   9.298  27.751  1.00 11.26     0.241 C
ATOM   5667  O   PHE A 375      17.137   9.700  26.796  1.00  8.85    -0.271 OA
ATOM   5668  CB  PHE A 375      17.736   7.613  28.941  1.00 11.04     0.073 C
ATOM   5671  CG  PHE A 375      17.697   6.665  30.094  1.00 16.40    -0.056 A
ATOM   5672  CD1 PHE A 375      16.545   6.364  30.774  1.00 18.34     0.007 A
ATOM   5674  CD2 PHE A 375      18.927   6.105  30.509  1.00 19.28     0.007 A
ATOM   5676  CE1 PHE A 375      16.574   5.489  31.860  1.00 22.81     0.001 A
ATOM   5678  CE2 PHE A 375      18.954   5.248  31.604  1.00 19.37     0.001 A
ATOM   5680  CZ  PHE A 375      17.773   4.921  32.246  1.00 16.69     0.000 A
ATOM   5682  N   LEU A 376      15.650  10.139  28.423  1.00  7.94    -0.346 N
ATOM   5683  HN  LEU A 376      14.963   9.777  29.084  1.00  0.00     0.163 HD
ATOM   5684  CA  LEU A 376      15.770  11.592  28.190  1.00 10.88     0.177 C
ATOM   5686  C   LEU A 376      15.727  12.170  29.611  1.00 13.32     0.240 C
ATOM   5687  O   LEU A 376      14.623  12.286  30.128  1.00 11.26    -0.271 OA
ATOM   5688  CB  LEU A 376      14.652  12.092  27.276  1.00 11.91     0.038 C
ATOM   5691  CG  LEU A 376      14.686  13.570  26.890  1.00 18.47    -0.020 C
ATOM   5693  CD1 LEU A 376      16.093  14.012  26.504  1.00 16.22     0.009 C
ATOM   5697  CD2 LEU A 376      13.716  13.847  25.735  1.00 13.52     0.009 C
ATOM   5701  N   GLY A 377      16.860  12.312  30.294  1.00 10.18    -0.351 N
ATOM   5702  HN  GLY A 377      17.753  12.182  29.819  1.00  0.00     0.163 HD
ATOM   5703  CA  GLY A 377      16.843  12.650  31.706  1.00 11.95     0.225 C
ATOM   5706  C   GLY A 377      17.254  14.050  32.032  1.00 10.06     0.235 C
ATOM   5707  O   GLY A 377      17.620  14.828  31.151  1.00 12.56    -0.272 OA
ATOM   5708  N   GLY A 378      17.171  14.443  33.323  1.00  9.75    -0.351 N
ATOM   5709  HN  GLY A 378      16.853  13.814  34.061  1.00  0.00     0.163 HD
ATOM   5710  CA  GLY A 378      17.565  15.826  33.598  1.00 10.03     0.225 C
ATOM   5713  C   GLY A 378      17.406  16.085  35.095  1.00 11.81     0.236 C
ATOM   5714  O   GLY A 378      16.943  15.231  35.835  1.00 12.53    -0.272 OA
ATOM   5715  N   SER A 379      17.911  17.237  35.492  1.00  8.19    -0.344 N
ATOM   5716  HN  SER A 379      18.350  17.871  34.825  1.00  0.00     0.163 HD
ATOM   5717  CA  SER A 379      17.827  17.586  36.916  1.00  6.20     0.200 C
ATOM   5719  C   SER A 379      17.536  19.099  36.910  1.00  7.95     0.243 C
ATOM   5720  O   SER A 379      18.004  19.807  36.014  1.00  8.76    -0.271 OA
ATOM   5721  CB  SER A 379      19.171  17.359  37.613  1.00 11.99     0.199 C
ATOM   5724  OG  SER A 379      19.162  18.014  38.890  1.00 13.92    -0.398 OA
ATOM   5725  HG  SER A 379      19.996  17.873  39.323  1.00  0.00     0.209 HD
ATOM   5726  N   ALA A 380      16.885  19.544  37.976  1.00  6.24    -0.346 N
ATOM   5727  HN  ALA A 380      16.586  18.884  38.694  1.00  0.00     0.163 HD
ATOM   5728  CA  ALA A 380      16.592  20.953  38.136  1.00  7.22     0.172 C
ATOM   5730  C   ALA A 380      17.762  21.684  38.818  1.00 11.92     0.240 C
ATOM   5731  O   ALA A 380      17.625  22.120  39.958  1.00 10.04    -0.271 OA
ATOM   5732  CB  ALA A 380      15.278  21.194  38.882  1.00  4.08     0.042 C
ATOM   5736  N   ASP A 381      18.820  21.879  38.033  1.00  8.59    -0.346 N
ATOM   5737  HN  ASP A 381      18.791  21.495  37.088  1.00  0.00     0.163 HD
ATOM   5738  CA  ASP A 381      20.013  22.603  38.435  1.00  6.53     0.186 C
ATOM   5740  C   ASP A 381      20.700  21.935  39.630  1.00 13.52     0.241 C
ATOM   5741  O   ASP A 381      21.352  22.626  40.414  1.00 14.79    -0.271 OA
ATOM   5742  CB  ASP A 381      19.744  24.074  38.801  1.00 13.72     0.147 C
ATOM   5745  CG  ASP A 381      21.029  24.919  38.755  1.00 20.88     0.175 C
ATOM   5746  OD1 ASP A 381      21.861  24.804  37.835  1.00 16.89    -0.648 OA
ATOM   5747  OD2 ASP A 381      21.266  25.707  39.696  1.00 15.35    -0.648 OA
ATOM   5748  N   LEU A 382      20.611  20.608  39.775  1.00 14.14    -0.346 N
ATOM   5749  HN  LEU A 382      20.053  20.077  39.106  1.00  0.00     0.163 HD
ATOM   5750  CA  LEU A 382      21.278  19.896  40.848  1.00 13.47     0.177 C
ATOM   5752  C   LEU A 382      22.015  18.671  40.313  1.00 13.68     0.241 C
ATOM   5753  O   LEU A 382      22.172  17.673  41.034  1.00 14.40    -0.271 OA
ATOM   5754  CB  LEU A 382      20.280  19.447  41.932  1.00 10.71     0.038 C
ATOM   5757  CG  LEU A 382      19.747  20.639  42.777  1.00 12.84    -0.020 C
ATOM   5759  CD1 LEU A 382      18.539  20.207  43.575  1.00 11.95     0.009 C
ATOM   5763  CD2 LEU A 382      20.894  21.132  43.671  1.00 22.16     0.009 C
ATOM   5767  N   ALA A 383      22.524  18.702  39.081  1.00 15.06    -0.346 N
ATOM   5768  HN  ALA A 383      22.424  19.549  38.522  1.00  0.00     0.163 HD
ATOM   5769  CA  ALA A 383      23.226  17.542  38.510  1.00 18.29     0.172 C
ATOM   5771  C   ALA A 383      24.363  16.983  39.349  1.00 16.96     0.240 C
ATOM   5772  O   ALA A 383      24.451  15.743  39.510  1.00 17.26    -0.271 OA
ATOM   5773  CB  ALA A 383      23.812  17.849  37.110  1.00 10.31     0.042 C
ATOM   5777  N   PRO A 384      25.214  17.811  39.942  1.00 17.17    -0.337 N
ATOM   5778  CA  PRO A 384      26.349  17.335  40.734  1.00 20.92     0.179 C
ATOM   5780  C   PRO A 384      25.946  16.838  42.121  1.00 19.91     0.241 C
ATOM   5781  O   PRO A 384      26.778  16.131  42.739  1.00 17.43    -0.271 OA
ATOM   5782  CB  PRO A 384      27.308  18.510  40.876  1.00 22.18     0.037 C
ATOM   5785  CG  PRO A 384      26.486  19.718  40.567  1.00 26.51     0.022 C
ATOM   5788  CD  PRO A 384      25.315  19.267  39.751  1.00 22.79     0.127 C
ATOM   5791  N   SER A 385      24.738  17.176  42.575  1.00 16.28    -0.344 N
ATOM   5792  HN  SER A 385      24.135  17.781  42.017  1.00  0.00     0.163 HD
ATOM   5793  CA  SER A 385      24.276  16.678  43.875  1.00 17.86     0.200 C
ATOM   5795  C   SER A 385      23.313  15.504  43.707  1.00 19.50     0.243 C
ATOM   5796  O   SER A 385      23.301  14.584  44.529  1.00 17.22    -0.271 OA
ATOM   5797  CB  SER A 385      23.483  17.752  44.647  1.00 18.04     0.199 C
ATOM   5800  OG  SER A 385      24.353  18.856  44.818  1.00 29.62    -0.398 OA
ATOM   5801  HG  SER A 385      23.865  19.518  45.294  1.00  0.00     0.209 HD
ATOM   5802  N   ASN A 386      22.442  15.614  42.689  1.00 15.34    -0.345 N
ATOM   5803  HN  ASN A 386      22.426  16.451  42.106  1.00  0.00     0.163 HD
ATOM   5804  CA  ASN A 386      21.513  14.505  42.432  1.00 15.91     0.185 C
ATOM   5806  C   ASN A 386      22.208  13.337  41.711  1.00 12.22     0.241 C
ATOM   5807  O   ASN A 386      21.677  12.212  41.790  1.00 15.20    -0.271 OA
ATOM   5808  CB  ASN A 386      20.303  14.868  41.580  1.00 13.27     0.137 C
ATOM   5811  CG  ASN A 386      19.357  15.884  42.148  1.00 17.30     0.217 C
ATOM   5812  ND2 ASN A 386      19.178  15.981  43.464  1.00 12.08    -0.370 N
ATOM   5813  1HD2 ASN A 386      18.535  16.672  43.850  1.00  0.00     0.159 HD
ATOM   5814  2HD2 ASN A 386      19.647  15.363  44.126  1.00  0.00     0.159 HD
ATOM   5815  OD1 ASN A 386      18.790  16.631  41.348  1.00 13.11    -0.274 OA
ATOM   5816  N   LEU A 387      23.290  13.565  41.002  1.00 11.79    -0.346 N
ATOM   5817  HN  LEU A 387      23.601  14.533  40.921  1.00  0.00     0.163 HD
ATOM   5818  CA  LEU A 387      24.086  12.544  40.318  1.00 11.84     0.177 C
ATOM   5820  C   LEU A 387      23.304  11.884  39.177  1.00 15.40     0.241 C
ATOM   5821  O   LEU A 387      23.193  10.658  39.112  1.00 14.76    -0.271 OA
ATOM   5822  CB  LEU A 387      24.637  11.471  41.279  1.00 11.94     0.038 C
ATOM   5825  CG  LEU A 387      25.418  12.040  42.475  1.00 16.27    -0.020 C
ATOM   5827  CD1 LEU A 387      25.847  10.962  43.465  1.00 17.23     0.009 C
ATOM   5831  CD2 LEU A 387      26.668  12.791  42.016  1.00 13.63     0.009 C
ATOM   5835  N   THR A 388      22.781  12.732  38.306  1.00 13.62    -0.344 N
ATOM   5836  HN  THR A 388      22.976  13.726  38.427  1.00  0.00     0.163 HD
ATOM   5837  CA  THR A 388      21.938  12.328  37.178  1.00 11.56     0.205 C
ATOM   5839  C   THR A 388      22.704  12.225  35.868  1.00 11.01     0.243 C
ATOM   5840  O   THR A 388      22.111  11.753  34.896  1.00 14.82    -0.271 OA
ATOM   5841  CB  THR A 388      20.840  13.366  36.949  1.00 16.09     0.146 C
ATOM   5843  CG2 THR A 388      19.701  13.139  37.919  1.00 15.14     0.042 C
ATOM   5847  OG1 THR A 388      21.386  14.688  37.173  1.00 12.62    -0.393 OA
ATOM   5848  HG1 THR A 388      20.703  15.333  37.031  1.00  0.00     0.210 HD
ATOM   5849  N   LEU A 389      23.955  12.662  35.825  1.00 14.39    -0.346 N
ATOM   5850  HN  LEU A 389      24.379  13.111  36.637  1.00  0.00     0.163 HD
ATOM   5851  CA  LEU A 389      24.724  12.483  34.571  1.00 16.13     0.177 C
ATOM   5853  C   LEU A 389      25.438  11.126  34.553  1.00 12.60     0.241 C
ATOM   5854  O   LEU A 389      25.911  10.630  35.578  1.00 18.55    -0.271 OA
ATOM   5855  CB  LEU A 389      25.775  13.564  34.445  1.00 17.77     0.038 C
ATOM   5858  CG  LEU A 389      25.243  15.010  34.321  1.00 16.51    -0.020 C
ATOM   5860  CD1 LEU A 389      26.309  15.989  34.817  1.00 14.48     0.009 C
ATOM   5864  CD2 LEU A 389      24.881  15.246  32.868  1.00 19.40     0.009 C
ATOM   5868  N   TRP A 390      25.491  10.467  33.397  1.00 18.00    -0.346 N
ATOM   5869  HN  TRP A 390      24.980  10.826  32.591  1.00  0.00     0.163 HD
ATOM   5870  CA  TRP A 390      26.273   9.233  33.264  1.00 11.97     0.181 C
ATOM   5872  C   TRP A 390      27.309   9.510  32.168  1.00 16.03     0.241 C
ATOM   5873  O   TRP A 390      27.281  10.569  31.512  1.00 14.27    -0.271 OA
ATOM   5874  CB  TRP A 390      25.446   7.989  33.065  1.00 18.56     0.075 C
ATOM   5877  CG  TRP A 390      24.651   7.976  31.788  1.00 17.36    -0.028 A
ATOM   5878  CD1 TRP A 390      23.533   8.742  31.532  1.00 20.76     0.096 A
ATOM   5880  CD2 TRP A 390      24.890   7.187  30.636  1.00 18.05    -0.002 A
ATOM   5881  CE2 TRP A 390      23.885   7.493  29.689  1.00 19.20     0.042 A
ATOM   5882  CE3 TRP A 390      25.857   6.220  30.301  1.00 12.62     0.014 A
ATOM   5884  NE1 TRP A 390      23.092   8.459  30.251  1.00 18.06    -0.365 N
ATOM   5885  HE1 TRP A 390      22.296   8.903  29.794  1.00  0.00     0.165 HD
ATOM   5886  CZ2 TRP A 390      23.837   6.904  28.421  1.00 19.31     0.030 A
ATOM   5888  CZ3 TRP A 390      25.788   5.618  29.061  1.00 14.43     0.001 A
ATOM   5890  CH2 TRP A 390      24.812   5.993  28.105  1.00 22.30     0.002 A
ATOM   5892  N   SER A 391      28.222   8.577  31.907  1.00 16.29    -0.344 N
ATOM   5893  HN  SER A 391      28.178   7.675  32.381  1.00  0.00     0.163 HD
ATOM   5894  CA  SER A 391      29.293   8.846  30.937  1.00 11.93     0.200 C
ATOM   5896  C   SER A 391      28.731   9.115  29.552  1.00 19.19     0.242 C
ATOM   5897  O   SER A 391      29.421   9.820  28.818  1.00 20.22    -0.271 OA
ATOM   5898  CB  SER A 391      30.291   7.681  30.943  1.00 21.31     0.199 C
ATOM   5901  OG  SER A 391      29.648   6.493  30.465  1.00 16.28    -0.398 OA
ATOM   5902  HG  SER A 391      30.266   5.772  30.469  1.00  0.00     0.209 HD
ATOM   5903  N   GLY A 392      27.573   8.586  29.155  1.00 19.55    -0.350 N
ATOM   5904  HN  GLY A 392      27.047   7.977  29.782  1.00  0.00     0.163 HD
ATOM   5905  CA  GLY A 392      27.056   8.884  27.810  1.00 15.48     0.225 C
ATOM   5908  C   GLY A 392      26.022  10.011  27.773  1.00 18.67     0.236 C
ATOM   5909  O   GLY A 392      25.294  10.150  26.774  1.00 16.36    -0.272 OA
ATOM   5910  N   SER A 393      25.833  10.799  28.823  1.00 16.78    -0.344 N
ATOM   5911  HN  SER A 393      26.377  10.630  29.659  1.00  0.00     0.163 HD
ATOM   5912  CA  SER A 393      24.877  11.896  28.812  1.00 13.15     0.200 C
ATOM   5914  C   SER A 393      25.348  12.961  27.809  1.00 14.68     0.243 C
ATOM   5915  O   SER A 393      26.527  13.322  27.891  1.00 16.64    -0.271 OA
ATOM   5916  CB  SER A 393      24.811  12.717  30.139  1.00  9.89     0.199 C
ATOM   5919  OG  SER A 393      24.163  11.862  31.084  1.00 14.34    -0.398 OA
ATOM   5920  HG  SER A 393      24.123  12.361  31.891  1.00  0.00     0.209 HD
ATOM   5921  N   LYS A 394      24.463  13.466  26.985  1.00 13.19    -0.346 N
ATOM   5922  HN  LYS A 394      23.517  13.085  26.979  1.00  0.00     0.163 HD
ATOM   5923  CA  LYS A 394      24.798  14.570  26.066  1.00 11.94     0.176 C
ATOM   5925  C   LYS A 394      23.648  15.571  26.188  1.00 11.08     0.241 C
ATOM   5926  O   LYS A 394      22.503  15.191  25.962  1.00 12.13    -0.271 OA
ATOM   5927  CB  LYS A 394      24.931  14.130  24.615  1.00 19.69     0.035 C
ATOM   5930  CG  LYS A 394      25.861  12.990  24.427  1.00 34.27     0.004 C
ATOM   5933  CD  LYS A 394      25.499  12.215  23.033  1.00 51.61     0.027 C
ATOM   5936  CE  LYS A 394      24.206  11.431  23.137  1.00 51.33     0.229 C
ATOM   5939  NZ  LYS A 394      24.218  10.132  22.410  1.00 55.65    -0.079 N
ATOM   5940  HZ1 LYS A 394      23.348   9.604  22.480  1.00  0.00     0.274 HD
ATOM   5941  HZ2 LYS A 394      25.007   9.561  22.714  1.00  0.00     0.274 HD
ATOM   5942  HZ3 LYS A 394      24.472  10.273  21.432  1.00  0.00     0.274 HD
ATOM   5943  N   ALA A 395      23.948  16.794  26.659  1.00 10.86    -0.346 N
ATOM   5944  HN  ALA A 395      24.907  17.061  26.882  1.00  0.00     0.163 HD
ATOM   5945  CA  ALA A 395      22.827  17.729  26.838  1.00  9.01     0.172 C
ATOM   5947  C   ALA A 395      22.243  18.231  25.540  1.00 10.62     0.240 C
ATOM   5948  O   ALA A 395      22.969  18.663  24.600  1.00 14.15    -0.271 OA
ATOM   5949  CB  ALA A 395      23.336  18.860  27.748  1.00 11.44     0.042 C
ATOM   5953  N   ILE A 396      20.904  18.365  25.453  1.00 10.51    -0.346 N
ATOM   5954  HN  ILE A 396      20.324  18.165  26.267  1.00  0.00     0.163 HD
ATOM   5955  CA  ILE A 396      20.273  18.795  24.203  1.00  9.21     0.180 C
ATOM   5957  C   ILE A 396      20.436  20.277  23.922  1.00 13.68     0.241 C
ATOM   5958  O   ILE A 396      20.167  20.619  22.775  1.00 15.08    -0.271 OA
ATOM   5959  CB  ILE A 396      18.771  18.455  24.078  1.00 11.13     0.013 C
ATOM   5961  CG1 ILE A 396      17.915  19.190  25.123  1.00 12.35     0.002 C
ATOM   5964  CG2 ILE A 396      18.679  16.932  24.236  1.00 12.82     0.012 C
ATOM   5968  CD1 ILE A 396      16.402  18.988  24.841  1.00 15.44     0.005 C
ATOM   5972  N   ASN A 397      20.902  21.096  24.843  1.00 14.59    -0.346 N
ATOM   5973  HN  ASN A 397      21.062  20.790  25.803  1.00  0.00     0.163 HD
ATOM   5974  CA  ASN A 397      21.180  22.478  24.412  1.00 20.86     0.185 C
ATOM   5976  C   ASN A 397      22.497  22.490  23.615  1.00 23.56     0.241 C
ATOM   5977  O   ASN A 397      22.754  23.467  22.927  1.00 25.16    -0.271 OA
ATOM   5978  CB  ASN A 397      21.290  23.442  25.586  1.00 17.06     0.137 C
ATOM   5981  CG  ASN A 397      22.312  22.949  26.591  1.00 26.07     0.217 C
ATOM   5982  ND2 ASN A 397      23.373  23.726  26.716  1.00 26.04    -0.370 N
ATOM   5983  1HD2 ASN A 397      24.061  23.394  27.392  1.00  0.00     0.159 HD
ATOM   5984  2HD2 ASN A 397      23.515  24.582  26.179  1.00  0.00     0.159 HD
ATOM   5985  OD1 ASN A 397      22.141  21.916  27.239  1.00 22.95    -0.274 OA
ATOM   5986  N   GLU A 398      23.361  21.488  23.720  1.00 18.01    -0.346 N
ATOM   5987  HN  GLU A 398      23.152  20.733  24.373  1.00  0.00     0.163 HD
ATOM   5988  CA  GLU A 398      24.587  21.414  22.952  1.00 21.75     0.177 C
ATOM   5990  C   GLU A 398      24.443  20.537  21.714  1.00 24.98     0.241 C
ATOM   5991  O   GLU A 398      25.067  20.810  20.682  1.00 22.79    -0.271 OA
ATOM   5992  CB  GLU A 398      25.737  20.901  23.834  1.00 21.42     0.045 C
ATOM   5995  CG  GLU A 398      25.968  21.912  24.975  1.00 41.19     0.116 C
ATOM   5998  CD  GLU A 398      26.727  21.324  26.149  1.00 52.18     0.172 C
ATOM   5999  OE1 GLU A 398      27.438  20.311  25.969  1.00 51.03    -0.648 OA
ATOM   6000  OE2 GLU A 398      26.628  21.842  27.286  1.00 63.09    -0.648 OA
ATOM   6001  N   ASP A 399      23.699  19.440  21.827  1.00 17.89    -0.346 N
ATOM   6002  HN  ASP A 399      23.220  19.250  22.708  1.00  0.00     0.163 HD
ATOM   6003  CA  ASP A 399      23.552  18.498  20.713  1.00 15.30     0.186 C
ATOM   6005  C   ASP A 399      22.085  18.081  20.696  1.00 13.54     0.241 C
ATOM   6006  O   ASP A 399      21.641  17.400  21.608  1.00 13.40    -0.271 OA
ATOM   6007  CB  ASP A 399      24.405  17.260  21.030  1.00 19.56     0.147 C
ATOM   6010  CG  ASP A 399      24.236  16.135  20.024  1.00 27.76     0.175 C
ATOM   6011  OD1 ASP A 399      23.416  16.201  19.081  1.00 23.54    -0.648 OA
ATOM   6012  OD2 ASP A 399      24.943  15.117  20.240  1.00 38.18    -0.648 OA
ATOM   6013  N   ALA A 400      21.360  18.454  19.650  1.00 11.43    -0.346 N
ATOM   6014  HN  ALA A 400      21.811  18.935  18.872  1.00  0.00     0.163 HD
ATOM   6015  CA  ALA A 400      19.927  18.186  19.597  1.00 16.07     0.172 C
ATOM   6017  C   ALA A 400      19.586  16.709  19.600  1.00 11.77     0.240 C
ATOM   6018  O   ALA A 400      18.422  16.376  19.920  1.00 13.63    -0.271 OA
ATOM   6019  CB  ALA A 400      19.297  18.920  18.399  1.00 14.57     0.042 C
ATOM   6023  N   ALA A 401      20.511  15.818  19.239  1.00  9.44    -0.346 N
ATOM   6024  HN  ALA A 401      21.417  16.155  18.912  1.00  0.00     0.163 HD
ATOM   6025  CA  ALA A 401      20.276  14.387  19.294  1.00  9.36     0.172 C
ATOM   6027  C   ALA A 401      20.646  13.822  20.673  1.00 15.23     0.240 C
ATOM   6028  O   ALA A 401      20.671  12.599  20.778  1.00 10.98    -0.271 OA
ATOM   6029  CB  ALA A 401      21.047  13.630  18.216  1.00 17.61     0.042 C
ATOM   6033  N   GLY A 402      20.851  14.655  21.696  1.00 13.19    -0.351 N
ATOM   6034  HN  GLY A 402      20.696  15.654  21.563  1.00  0.00     0.163 HD
ATOM   6035  CA  GLY A 402      21.292  14.170  23.000  1.00 11.08     0.225 C
ATOM   6038  C   GLY A 402      20.186  13.524  23.822  1.00 14.84     0.236 C
ATOM   6039  O   GLY A 402      19.078  13.253  23.346  1.00 13.72    -0.272 OA
ATOM   6040  N   ASN A 403      20.450  13.340  25.124  1.00 11.09    -0.346 N
ATOM   6041  HN  ASN A 403      21.301  13.749  25.509  1.00  0.00     0.163 HD
ATOM   6042  CA  ASN A 403      19.588  12.591  26.006  1.00  9.17     0.185 C
ATOM   6044  C   ASN A 403      19.561  13.152  27.441  1.00  9.41     0.241 C
ATOM   6045  O   ASN A 403      19.237  12.416  28.378  1.00 11.22    -0.271 OA
ATOM   6046  CB  ASN A 403      20.094  11.142  26.125  1.00  9.89     0.137 C
ATOM   6049  CG  ASN A 403      21.549  11.104  26.530  1.00 15.09     0.217 C
ATOM   6050  ND2 ASN A 403      22.320  10.086  26.121  1.00 16.34    -0.370 N
ATOM   6051  1HD2 ASN A 403      23.302  10.060  26.394  1.00  0.00     0.159 HD
ATOM   6052  2HD2 ASN A 403      21.919   9.319  25.581  1.00  0.00     0.159 HD
ATOM   6053  OD1 ASN A 403      22.032  12.028  27.180  1.00 12.20    -0.274 OA
ATOM   6054  N   TYR A 404      19.909  14.427  27.538  1.00 10.45    -0.346 N
ATOM   6055  HN  TYR A 404      20.148  14.980  26.715  1.00  0.00     0.163 HD
ATOM   6056  CA  TYR A 404      19.935  15.013  28.907  1.00  9.62     0.180 C
ATOM   6058  C   TYR A 404      19.399  16.425  28.810  1.00 13.39     0.241 C
ATOM   6059  O   TYR A 404      19.760  17.104  27.822  1.00 10.57    -0.271 OA
ATOM   6060  CB  TYR A 404      21.370  15.020  29.425  1.00  9.80     0.073 C
ATOM   6063  CG  TYR A 404      21.361  15.410  30.907  1.00  9.34    -0.056 A
ATOM   6064  CD1 TYR A 404      21.149  14.436  31.872  1.00 10.95     0.010 A
ATOM   6066  CD2 TYR A 404      21.551  16.734  31.250  1.00  9.77     0.010 A
ATOM   6068  CE1 TYR A 404      21.111  14.822  33.220  1.00 12.45     0.037 A
ATOM   6070  CE2 TYR A 404      21.513  17.115  32.585  1.00 12.42     0.037 A
ATOM   6072  CZ  TYR A 404      21.281  16.152  33.536  1.00 14.61     0.065 A
ATOM   6073  OH  TYR A 404      21.224  16.531  34.876  1.00 17.40    -0.361 OA
ATOM   6074  HH  TYR A 404      21.341  17.448  35.094  1.00  0.00     0.217 HD
ATOM   6075  N   ILE A 405      18.643  16.909  29.787  1.00  8.60    -0.346 N
ATOM   6076  HN  ILE A 405      18.397  16.308  30.574  1.00  0.00     0.163 HD
ATOM   6077  CA  ILE A 405      18.159  18.280  29.757  1.00  8.55     0.180 C
ATOM   6079  C   ILE A 405      18.568  18.984  31.062  1.00 11.25     0.241 C
ATOM   6080  O   ILE A 405      18.285  18.534  32.193  1.00  8.61    -0.271 OA
ATOM   6081  CB  ILE A 405      16.601  18.344  29.668  1.00  9.00     0.013 C
ATOM   6083  CG1 ILE A 405      16.067  17.627  28.428  1.00 11.07     0.002 C
ATOM   6086  CG2 ILE A 405      16.198  19.812  29.681  1.00  9.88     0.012 C
ATOM   6090  CD1 ILE A 405      14.555  17.513  28.366  1.00 16.64     0.005 C
ATOM   6094  N   HIS A 406      19.293  20.083  30.936  1.00  7.88    -0.346 N
ATOM   6095  HN  HIS A 406      19.686  20.305  30.021  1.00  0.00     0.163 HD
ATOM   6096  CA  HIS A 406      19.558  20.996  32.049  1.00 11.86     0.182 C
ATOM   6098  C   HIS A 406      18.299  21.850  32.235  1.00 10.46     0.241 C
ATOM   6099  O   HIS A 406      18.078  22.819  31.489  1.00  8.72    -0.271 OA
ATOM   6100  CB  HIS A 406      20.725  21.927  31.709  1.00 13.67     0.093 C
ATOM   6103  CG  HIS A 406      22.044  21.240  31.794  1.00 18.94     0.028 A
ATOM   6104  CD2 HIS A 406      22.860  20.874  30.751  1.00 17.12     0.114 A
ATOM   6106  ND1 HIS A 406      22.667  20.868  32.967  1.00 17.27    -0.354 N
ATOM   6107  HD1 HIS A 406      22.309  21.015  33.911  1.00  0.00     0.166 HD
ATOM   6108  CE1 HIS A 406      23.830  20.277  32.643  1.00 19.43     0.180 A
ATOM   6110  NE2 HIS A 406      23.947  20.278  31.306  1.00 17.94    -0.360 N
ATOM   6111  HE2 HIS A 406      24.733  19.890  30.785  1.00  0.00     0.166 HD
ATOM   6112  N   TYR A 407      17.428  21.502  33.168  1.00  8.09    -0.346 N
ATOM   6113  HN  TYR A 407      17.652  20.736  33.803  1.00  0.00     0.163 HD
ATOM   6114  CA  TYR A 407      16.154  22.196  33.302  1.00  7.70     0.180 C
ATOM   6116  C   TYR A 407      16.225  23.530  34.017  1.00  9.97     0.241 C
ATOM   6117  O   TYR A 407      15.215  24.272  34.001  1.00 10.25    -0.271 OA
ATOM   6118  CB  TYR A 407      15.180  21.285  34.115  1.00  6.70     0.073 C
ATOM   6121  CG  TYR A 407      14.552  20.160  33.323  1.00  9.83    -0.056 A
ATOM   6122  CD1 TYR A 407      13.485  20.414  32.483  1.00  7.44     0.010 A
ATOM   6124  CD2 TYR A 407      15.015  18.847  33.457  1.00  9.75     0.010 A
ATOM   6126  CE1 TYR A 407      12.872  19.392  31.744  1.00  9.71     0.037 A
ATOM   6128  CE2 TYR A 407      14.376  17.807  32.769  1.00 10.47     0.037 A
ATOM   6130  CZ  TYR A 407      13.332  18.096  31.923  1.00 13.23     0.065 A
ATOM   6131  OH  TYR A 407      12.691  17.052  31.248  1.00 10.06    -0.361 OA
ATOM   6132  HH  TYR A 407      13.006  16.164  31.371  1.00  0.00     0.217 HD
ATOM   6133  N   GLY A 408      17.348  23.826  34.670  1.00  7.45    -0.351 N
ATOM   6134  HN  GLY A 408      18.166  23.217  34.640  1.00  0.00     0.163 HD
ATOM   6135  CA  GLY A 408      17.340  25.096  35.446  1.00  6.94     0.225 C
ATOM   6138  C   GLY A 408      16.591  24.914  36.757  1.00 10.55     0.236 C
ATOM   6139  O   GLY A 408      16.115  23.807  37.093  1.00  7.41    -0.272 OA
ATOM   6140  N   VAL A 409      16.375  26.029  37.486  1.00  9.35    -0.346 N
ATOM   6141  HN  VAL A 409      16.650  26.948  37.138  1.00  0.00     0.163 HD
ATOM   6142  CA  VAL A 409      15.721  25.872  38.817  1.00  9.18     0.180 C
ATOM   6144  C   VAL A 409      14.220  25.984  38.621  1.00  9.18     0.241 C
ATOM   6145  O   VAL A 409      13.618  27.045  38.849  1.00  7.15    -0.271 OA
ATOM   6146  CB  VAL A 409      16.230  26.989  39.773  1.00 10.04     0.009 C
ATOM   6148  CG1 VAL A 409      15.735  26.721  41.194  1.00 14.17     0.012 C
ATOM   6152  CG2 VAL A 409      17.762  26.989  39.767  1.00 11.19     0.012 C
ATOM   6156  N   ARG A 410      13.625  24.928  38.046  1.00  6.99    -0.346 N
ATOM   6157  HN  ARG A 410      14.166  24.075  37.909  1.00  0.00     0.163 HD
ATOM   6158  CA  ARG A 410      12.221  24.954  37.606  1.00  6.18     0.176 C
ATOM   6160  C   ARG A 410      11.614  23.590  37.903  1.00  8.96     0.241 C
ATOM   6161  O   ARG A 410      11.390  22.800  36.988  1.00  7.17    -0.271 OA
ATOM   6162  CB  ARG A 410      12.254  25.172  36.074  1.00  6.94     0.036 C
ATOM   6165  CG  ARG A 410      12.765  26.514  35.563  1.00  9.68     0.023 C
ATOM   6168  CD  ARG A 410      12.827  26.525  34.036  1.00 10.11     0.138 C
ATOM   6171  NE  ARG A 410      13.387  27.785  33.481  1.00 12.75    -0.227 N
ATOM   6172  HE  ARG A 410      12.811  28.623  33.560  1.00  0.00     0.177 HD
ATOM   6173  CZ  ARG A 410      14.559  27.918  32.897  1.00 12.64     0.665 C
ATOM   6174  NH1 ARG A 410      15.424  26.885  32.827  1.00  8.05    -0.235 N
ATOM   6175  1HH1 ARG A 410      15.182  25.974  33.217  1.00  0.00     0.174 HD
ATOM   6176  2HH1 ARG A 410      16.332  26.988  32.374  1.00  0.00     0.174 HD
ATOM   6177  NH2 ARG A 410      14.882  29.131  32.377  1.00  9.90    -0.235 N
ATOM   6178  1HH2 ARG A 410      14.228  29.912  32.430  1.00  0.00     0.174 HD
ATOM   6179  2HH2 ARG A 410      15.790  29.234  31.924  1.00  0.00     0.174 HD
ATOM   6180  N   GLU A 411      11.350  23.243  39.168  1.00  6.54    -0.346 N
ATOM   6181  HN  GLU A 411      11.437  23.918  39.928  1.00  0.00     0.163 HD
ATOM   6182  CA  GLU A 411      10.929  21.854  39.429  1.00  6.18     0.177 C
ATOM   6184  C   GLU A 411       9.569  21.503  38.849  1.00  4.24     0.241 C
ATOM   6185  O   GLU A 411       9.372  20.375  38.393  1.00  7.65    -0.271 OA
ATOM   6186  CB  GLU A 411      10.842  21.690  40.970  1.00  8.49     0.045 C
ATOM   6189  CG  GLU A 411      12.267  21.770  41.552  1.00  9.02     0.116 C
ATOM   6192  CD  GLU A 411      12.641  23.179  41.978  1.00 10.69     0.172 C
ATOM   6193  OE1 GLU A 411      11.894  24.165  41.817  1.00  9.21    -0.648 OA
ATOM   6194  OE2 GLU A 411      13.781  23.367  42.453  1.00 12.67    -0.648 OA
ATOM   6195  N   PHE A 412       8.631  22.466  38.990  1.00  3.87    -0.346 N
ATOM   6196  HN  PHE A 412       8.849  23.364  39.421  1.00  0.00     0.163 HD
ATOM   6197  CA  PHE A 412       7.277  22.158  38.491  1.00  5.38     0.180 C
ATOM   6199  C   PHE A 412       7.216  22.100  36.967  1.00  6.39     0.241 C
ATOM   6200  O   PHE A 412       6.640  21.141  36.447  1.00  6.98    -0.271 OA
ATOM   6201  CB  PHE A 412       6.296  23.254  38.999  1.00  8.83     0.073 C
ATOM   6204  CG  PHE A 412       4.799  23.087  38.871  1.00  8.64    -0.056 A
ATOM   6205  CD1 PHE A 412       4.187  21.896  38.514  1.00  6.52     0.007 A
ATOM   6207  CD2 PHE A 412       3.983  24.192  39.163  1.00  6.14     0.007 A
ATOM   6209  CE1 PHE A 412       2.803  21.774  38.409  1.00  8.14     0.001 A
ATOM   6211  CE2 PHE A 412       2.593  24.099  39.118  1.00  6.90     0.001 A
ATOM   6213  CZ  PHE A 412       1.997  22.881  38.732  1.00  9.35     0.000 A
ATOM   6215  N   GLY A 413       7.906  23.034  36.311  1.00  5.06    -0.351 N
ATOM   6216  HN  GLY A 413       8.434  23.746  36.815  1.00  0.00     0.163 HD
ATOM   6217  CA  GLY A 413       7.884  23.008  34.807  1.00  7.25     0.225 C
ATOM   6220  C   GLY A 413       8.630  21.743  34.344  1.00  7.02     0.236 C
ATOM   6221  O   GLY A 413       8.179  21.061  33.417  1.00  7.57    -0.272 OA
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ATOM   6222  N   MET A 414       9.710  21.390  35.047  1.00  4.76   -0.346 N
ATOM   6223  HN  MET A 414       9.988  21.953  35.850  1.00  0.00    0.163 HD
ATOM   6224  CA  MET A 414      10.500  20.217  34.691  1.00  6.80    0.177 C
ATOM   6226  C   MET A 414       9.609  18.967  34.709  1.00  8.43    0.241 C
ATOM   6227  O   MET A 414       9.670  18.131  33.815  1.00  5.40   -0.271 OA
ATOM   6228  CB  MET A 414      11.640  19.998  35.728  1.00  7.87    0.045 C
ATOM   6231  CG  MET A 414      12.270  18.599  35.646  1.00  9.94    0.076 C
ATOM   6234  SD  MET A 414      13.625  18.310  36.794  1.00 10.94   -0.173 SA
ATOM   6235  CE  MET A 414      12.726  18.170  38.356  1.00 11.22    0.089 C
ATOM   6239  N   THR A 415       8.818  18.811  35.775  1.00  6.06   -0.344 N
ATOM   6240  HN  THR A 415       8.787  19.546  36.481  1.00  0.00    0.163 HD
ATOM   6241  CA  THR A 415       7.993  17.611  35.957  1.00  6.04    0.205 C
ATOM   6243  C   THR A 415       6.836  17.542  34.977  1.00  7.40    0.243 C
ATOM   6244  O   THR A 415       6.556  16.468  34.398  1.00  7.87   -0.271 OA
ATOM   6245  CB  THR A 415       7.499  17.511  37.423  1.00  6.82    0.146 C
ATOM   6247  CG2 THR A 415       6.945  16.108  37.710  1.00  5.85    0.042 C
ATOM   6251  OG1 THR A 415       8.643  17.562  38.289  1.00  7.81   -0.393 OA
ATOM   6252  HG1 THR A 415       8.986  18.430  38.111  1.00  0.00    0.210 HD
ATOM   6253  N   ALA A 416       6.159  18.658  34.690  1.00  6.04   -0.346 N
ATOM   6254  HN  ALA A 416       6.397  19.524  35.174  1.00  0.00    0.163 HD
ATOM   6255  CA  ALA A 416       5.082  18.666  33.695  1.00  7.97    0.172 C
ATOM   6257  C   ALA A 416       5.614  18.658  32.262  1.00  6.70    0.240 C
ATOM   6258  O   ALA A 416       4.932  18.108  31.399  1.00  6.41   -0.271 OA
ATOM   6259  CB  ALA A 416       4.264  19.939  33.967  1.00  6.89    0.042 C
ATOM   6263  N   ILE A 417       6.842  19.133  32.016  1.00  5.74   -0.346 N
ATOM   6264  HN  ILE A 417       7.350  19.630  32.748  1.00  0.00    0.163 HD
ATOM   6265  CA  ILE A 417       7.464  18.941  30.693  1.00  4.66    0.180 C
ATOM   6267  C   ILE A 417       7.725  17.457  30.500  1.00  7.34    0.241 C
ATOM   6268  O   ILE A 417       7.442  16.890  29.421  1.00  7.55   -0.271 OA
ATOM   6269  CB  ILE A 417       8.758  19.760  30.549  1.00  6.77    0.013 C
ATOM   6271  CG1 ILE A 417       8.416  21.256  30.295  1.00  6.20    0.002 C
ATOM   6274  CG2 ILE A 417       9.725  19.205  29.481  1.00  4.39    0.012 C
ATOM   6278  CD1 ILE A 417       9.689  22.081  30.525  1.00  8.48    0.005 C
ATOM   6282  N   ALA A 418       8.270  16.790  31.516  1.00  6.30   -0.346 N
ATOM   6283  HN  ALA A 418       8.506  17.269  32.385  1.00  0.00    0.163 HD
ATOM   6284  CA  ALA A 418       8.526  15.344  31.360  1.00  6.42    0.172 C
ATOM   6286  C   ALA A 418       7.260  14.550  31.129  1.00  8.24    0.240 C
ATOM   6287  O   ALA A 418       7.258  13.491  30.462  1.00  9.00   -0.271 OA
ATOM   6288  CB  ALA A 418       9.280  14.862  32.593  1.00  6.77    0.042 C
ATOM   6292  N   ASN A 419       6.126  14.969  31.735  1.00  6.71   -0.346 N
ATOM   6293  HN  ASN A 419       6.175  15.724  32.420  1.00  0.00    0.163 HD
ATOM   6294  CA  ASN A 419       4.847  14.369  31.432  1.00  9.12    0.185 C
ATOM   6296  C   ASN A 419       4.514  14.504  29.924  1.00 10.50    0.241 C
ATOM   6297  O   ASN A 419       4.003  13.551  29.326  1.00  8.11   -0.271 OA
ATOM   6298  CB  ASN A 419       3.703  15.046  32.215  1.00  3.70    0.137 C
ATOM   6301  CG  ASN A 419       3.700  14.670  33.688  1.00  9.55    0.217 C
ATOM   6302  ND2 ASN A 419       2.943  15.414  34.518  1.00  7.06   -0.370 N
ATOM   6303 1HD2 ASN A 419       2.941  15.162  35.506  1.00  0.00    0.159 HD
ATOM   6304 2HD2 ASN A 419       2.391  16.200  34.174  1.00  0.00    0.159 HD
ATOM   6305  OD1 ASN A 419       4.363  13.726  34.101  1.00 10.74   -0.274 OA
ATOM   6306  N   GLY A 420       4.832  15.662  29.339  1.00  7.79   -0.351 N
ATOM   6307  HN  GLY A 420       5.250  16.410  29.893  1.00  0.00    0.163 HD
ATOM   6308  CA  GLY A 420       4.584  15.870  27.900  1.00  5.43    0.225 C
ATOM   6311  C   GLY A 420       5.545  14.983  27.109  1.00  7.04    0.236 C
ATOM   6312  O   GLY A 420       5.120  14.413  26.083  1.00  7.79   -0.271 OA
ATOM   6313  N   ILE A 421       6.789  14.810  27.555  1.00  6.34   -0.346 N
ATOM   6314  HN  ILE A 421       7.107  15.295  28.394  1.00  0.00    0.163 HD
ATOM   6315  CA  ILE A 421       7.707  13.907  26.820  1.00  6.42    0.180 C
ATOM   6317  C   ILE A 421       7.155  12.474  26.863  1.00  5.44    0.241 C
ATOM   6318  O   ILE A 421       7.170  11.775  25.845  1.00 10.77   -0.271 OA
ATOM   6319  CB  ILE A 421       9.121  13.952  27.465  1.00  8.58    0.013 C
ATOM   6321  CG1 ILE A 421       9.729  15.343  27.253  1.00  8.45    0.002 C
ATOM   6324  CG2 ILE A 421      10.010  12.815  26.964  1.00  9.27    0.012 C
ATOM   6328  CD1 ILE A 421      10.991  15.599  28.074  1.00 10.26    0.005 C
ATOM   6332  N   SER A 422       6.694  12.040  28.030  1.00  7.55   -0.344 N
ATOM   6333  HN  SER A 422       6.741  12.642  28.852  1.00  0.00    0.163 HD
ATOM   6334  CA  SER A 422       6.117  10.696  28.137  1.00  8.61    0.200 C
ATOM   6336  C   SER A 422       4.900  10.523  27.226  1.00 10.79    0.243 C
ATOM   6337  O   SER A 422       4.763   9.503  26.560  1.00  9.12   -0.271 OA
ATOM   6338  CB  SER A 422       5.597  10.524  29.588  1.00  8.40    0.199 C
ATOM   6341  OG ASER A 422       6.724  10.504  30.445  0.50 21.65   -0.398 OA
ATOM   6342  HG ASER A 422       6.405  10.399  31.334  1.00  0.00    0.209 HD
ATOM   6343  N   LEU A 423       3.966  11.483  27.214  1.00  5.42   -0.346 N
ATOM   6344  HN  LEU A 423       4.086  12.301  27.811  1.00  0.00    0.163 HD
ATOM   6345  CA  LEU A 423       2.787  11.387  26.372  1.00  7.82    0.177 C
ATOM   6347  C   LEU A 423       3.102  11.353  24.884  1.00 13.83    0.241 C
ATOM   6348  O   LEU A 423       2.361  10.790  24.083  1.00 10.55   -0.271 OA
ATOM   6349  CB  LEU A 423       1.899  12.634  26.618  1.00  9.01    0.038 C
ATOM   6352  CG  LEU A 423       1.161  12.670  27.983  1.00 13.19   -0.020 C
ATOM   6354  CD1 LEU A 423       0.695  14.095  28.302  1.00 11.04    0.009 C
ATOM   6358  CD2 LEU A 423       0.000  11.687  27.969  1.00 13.54    0.009 C
ATOM   6362  N   HIS A 424       4.185  11.998  24.451  1.00  8.70   -0.346 N
ATOM   6363  HN  HIS A 424       4.823  12.436  25.115  1.00  0.00    0.163 HD
ATOM   6364  CA  HIS A 424       4.449  12.071  23.022  1.00  5.67    0.182 C
ATOM   6366  C   HIS A 424       4.799  10.691  22.480  1.00 12.30    0.241 C
ATOM   6367  O   HIS A 424       4.418  10.384  21.335  1.00 12.72   -0.271 OA
ATOM   6368  CB  HIS A 424       5.686  12.969  22.807  1.00  7.82    0.093 C
ATOM   6371  CG  HIS A 424       6.013  13.157  21.347  1.00 11.33    0.028 A
ATOM   6372  CD2 HIS A 424       5.668  14.119  20.462  1.00 11.63    0.114 A
ATOM   6374  ND1 HIS A 424       6.844  12.247  20.698  1.00 11.76   -0.354 N
ATOM   6375  HD1 HIS A 424       7.265  11.414  21.109  1.00  0.00    0.166 HD
ATOM   6376  CE1 HIS A 424       6.988  12.666  19.436  1.00 14.77    0.180 A
ATOM   6378  NE2 HIS A 424       6.299  13.772  19.244  1.00  9.81   -0.360 N
ATOM   6379  HE2 HIS A 424       6.232  14.290  18.368  1.00  0.00    0.166 HD
ATOM   6380  N   GLY A 425       5.600   9.950  23.227  1.00  9.26   -0.351 N
ATOM   6381  HN  GLY A 425       5.904  10.292  24.139  1.00  0.00    0.163 HD
ATOM   6382  CA  GLY A 425       6.051   8.649  22.756  1.00  8.96    0.225 C
ATOM   6385  C   GLY A 425       7.488   8.757  22.210  1.00 12.50    0.235 C
ATOM   6386  O   GLY A 425       7.963   9.814  21.812  1.00 11.86   -0.272 OA
ATOM   6387  N   GLY A 426       8.261   7.659  22.407  1.00  9.40   -0.351 N
ATOM   6388  HN  GLY A 426       7.867   6.871  22.921  1.00  0.00    0.163 HD
ATOM   6389  CA  GLY A 426       9.623   7.558  21.919  1.00  8.55    0.225 C
ATOM   6392  C   GLY A 426      10.673   7.694  23.013  1.00 13.11    0.236 C
ATOM   6393  O   GLY A 426      11.828   7.400  22.747  1.00 11.46   -0.272 OA
ATOM   6394  N   PHE A 427      10.307   8.124  24.248  1.00  8.56   -0.346 N
ATOM   6395  HN  PHE A 427       9.328   8.296  24.475  1.00  0.00    0.163 HD
ATOM   6396  CA  PHE A 427      11.364   8.334  25.248  1.00  8.10    0.180 C
ATOM   6398  C   PHE A 427      10.941   7.776  26.624  1.00  5.98    0.241 C
ATOM   6399  O   PHE A 427       9.764   7.513  26.819  1.00 11.92   -0.271 OA
ATOM   6400  CB  PHE A 427      11.594   9.873  25.475  1.00 11.66    0.073 C
ATOM   6403  CG  PHE A 427      12.189  10.563  24.258  1.00 12.13   -0.056 A
ATOM   6404  CD1 PHE A 427      13.571  10.463  24.003  1.00 12.02    0.007 A
ATOM   6406  CD2 PHE A 427      11.361  11.253  23.402  1.00 15.32    0.007 A
ATOM   6408  CE1 PHE A 427      14.071  11.069  22.833  1.00  9.15    0.001 A
ATOM   6410  CE2 PHE A 427      11.870  11.856  22.250  1.00 11.15    0.001 A
ATOM   6412  CZ  PHE A 427      13.213  11.751  21.985  1.00  6.93    0.000 A
ATOM   6414  N   LEU A 428      11.917   7.656  27.554  1.00 11.05   -0.346 N
ATOM   6415  HN  LEU A 428      12.889   7.839  27.285  1.00  0.00    0.163 HD
ATOM   6416  CA  LEU A 428      11.562   7.258  28.911  1.00  5.87    0.177 C
ATOM   6418  C   LEU A 428      12.167   8.381  29.746  1.00 10.80    0.243 C
ATOM   6419  O   LEU A 428      13.393   8.416  29.840  1.00  9.31   -0.271 OA
ATOM   6420  CB  LEU A 428      12.366   5.954  29.172  1.00 10.92    0.038 C
ATOM   6423  CG  LEU A 428      11.897   5.148  30.393  1.00 21.66   -0.020 C
ATOM   6425  CD1 LEU A 428      12.561   3.781  30.525  1.00 17.36    0.009 C
ATOM   6429  CD2 LEU A 428      12.119   5.917  31.681  1.00 20.85    0.009 C
ATOM   6433  N   PRO A 429      11.405   9.353  30.221  1.00  8.99   -0.337 N
ATOM   6434  CA  PRO A 429      12.038  10.471  30.911  1.00 10.20    0.179 C
ATOM   6436  C   PRO A 429      12.363  10.192  32.361  1.00  7.62    0.241 C
ATOM   6437  O   PRO A 429      11.627   9.432  33.002  1.00 10.53   -0.271 OA
ATOM   6438  CB  PRO A 429      10.931  11.543  30.795  1.00 12.53    0.037 C
ATOM   6441  CG  PRO A 429       9.630  10.770  30.800  1.00 14.51    0.022 C
ATOM   6444  CD  PRO A 429       9.951   9.472  30.072  1.00  9.31    0.127 C
ATOM   6447  N   TYR A 430      13.461  10.740  32.891  1.00  7.80   -0.346 N
ATOM   6448  HN  TYR A 430      14.138  11.191  32.276  1.00  0.00    0.163 HD
ATOM   6449  CA  TYR A 430      13.718  10.709  34.340  1.00  8.69    0.180 C
ATOM   6451  C   TYR A 430      13.985  12.164  34.735  1.00 10.15    0.241 C
ATOM   6452  O   TYR A 430      14.436  12.959  33.900  1.00  8.47   -0.271 OA
ATOM   6453  CB  TYR A 430      14.834   9.809  34.791  1.00  9.37    0.073 C
ATOM   6456  CG  TYR A 430      16.262  10.046  34.338  1.00  9.71   -0.056 A
ATOM   6457  CD1 TYR A 430      17.101  10.946  34.986  1.00 10.05    0.010 A
ATOM   6459  CD2 TYR A 430      16.816   9.294  33.300  1.00 12.52    0.010 A
ATOM   6461  CE1 TYR A 430      18.418  11.159  34.617  1.00 13.62    0.037 A
ATOM   6463  CE2 TYR A 430      18.146   9.488  32.929  1.00 12.11    0.037 A
ATOM   6465  CZ  TYR A 430      18.939  10.382  33.571  1.00 10.70    0.065 A
ATOM   6466  OH  TYR A 430      20.259  10.609  33.204  1.00 12.98   -0.361 OA
ATOM   6467  HH  TYR A 430      20.612  10.083  32.496  1.00  0.00    0.217 HD
ATOM   6468  N   THR A 431      13.540  12.590  35.922  1.00  6.21   -0.344 N
ATOM   6469  HN  THR A 431      13.071  11.928  36.540  1.00  0.00    0.163 HD
ATOM   6470  CA  THR A 431      13.704  13.966  36.359  1.00  6.58    0.205 C
ATOM   6472  C   THR A 431      14.287  13.881  37.791  1.00  7.86    0.243 C
ATOM   6473  O   THR A 431      14.186  12.834  38.439  1.00  6.93   -0.271 OA
ATOM   6474  CB  THR A 431      12.378  14.763  36.412  1.00  7.69    0.146 C
ATOM   6476  CG2 THR A 431      11.815  14.953  34.992  1.00  5.33    0.042 C
ATOM   6480  OG1 THR A 431      11.457  13.999  37.219  1.00 10.47   -0.393 OA
ATOM   6481  HG1 THR A 431      11.802  13.882  38.096  1.00  0.00    0.210 HD
ATOM   6482  N   SER A 432      14.812  14.984  38.320  1.00  5.08   -0.344 N
ATOM   6483  HN  SER A 432      14.761  15.876  37.829  1.00  0.00    0.163 HD
ATOM   6484  CA  SER A 432      15.463  14.881  39.624  1.00  6.11    0.200 C
ATOM   6486  C   SER A 432      15.617  16.253  40.287  1.00 11.23    0.243 C
ATOM   6487  O   SER A 432      15.804  17.253  39.591  1.00 11.23   -0.271 OA
ATOM   6488  CB  SER A 432      16.938  14.455  39.452  1.00 10.16    0.199 C
ATOM   6491  OG  SER A 432      17.420  14.018  40.728  1.00 16.03   -0.398 OA
ATOM   6492  HG  SER A 432      18.327  13.756  40.622  1.00  0.00    0.209 HD
ATOM   6493  N   THR A 433      15.505  16.200  41.605  1.00  6.68   -0.344 N
ATOM   6494  HN  THR A 433      15.243  15.323  42.055  1.00  0.00    0.163 HD
ATOM   6495  CA  THR A 433      15.756  17.399  42.431  1.00  9.09    0.205 C
ATOM   6497  C   THR A 433      15.837  16.848  43.881  1.00  8.08    0.243 C
ATOM   6498  O   THR A 433      15.693  15.639  44.056  1.00  8.17   -0.271 OA
ATOM   6499  CB  THR A 433      14.630  18.443  42.326  1.00 10.14    0.146 C
ATOM   6501  CG2 THR A 433      13.279  17.908  42.717  1.00 11.04    0.042 C
ATOM   6505  OG1 THR A 433      14.909  19.549  43.224  1.00  7.23   -0.393 OA
ATOM   6506  HG1 THR A 433      14.214  20.193  43.159  1.00  0.00    0.210 HD
ATOM   6507  N   PHE A 434      16.116  17.708  44.840  1.00  6.36   -0.346 N
ATOM   6508  HN  PHE A 434      16.385  18.669  44.629  1.00  0.00    0.163 HD
ATOM   6509  CA  PHE A 434      16.023  17.224  46.236  1.00  8.95    0.180 C
ATOM   6511  C   PHE A 434      14.585  16.861  46.558  1.00  8.53    0.241 C
ATOM   6512  O   PHE A 434      13.637  17.502  46.133  1.00  7.10   -0.271 OA
ATOM   6513  CB  PHE A 434      16.448  18.300  47.233  1.00  8.15    0.073 C
ATOM   6516  CG  PHE A 434      17.901  18.668  47.164  1.00 10.27   -0.056 A
ATOM   6517  CD1 PHE A 434      18.882  17.820  46.680  1.00 13.28    0.007 A
ATOM   6519  CD2 PHE A 434      18.284  19.914  47.661  1.00 16.95    0.007 A
ATOM   6521  CE1 PHE A 434      20.208  18.183  46.633  1.00 19.04    0.001 A
ATOM   6523  CE2 PHE A 434      19.613  20.282  47.618  1.00 20.87    0.001 A
ATOM   6525  CZ  PHE A 434      20.553  19.424  47.111  1.00 16.76    0.000 A
ATOM   6527  N   LEU A 435      14.432  15.862  47.457  1.00  6.53   -0.346 N
ATOM   6528  HN  LEU A 435      15.241  15.418  47.893  1.00  0.00    0.163 HD
ATOM   6529  CA  LEU A 435      13.056  15.433  47.789  1.00  3.99    0.177 C
ATOM   6531  C   LEU A 435      12.153  16.522  48.288  1.00  6.10    0.241 C
ATOM   6532  O   LEU A 435      10.952  16.566  47.990  1.00  7.82   -0.271 OA
ATOM   6533  CB  LEU A 435      13.156  14.302  48.859  1.00  6.31    0.038 C
ATOM   6536  CG  LEU A 435      11.802  13.775  49.379  1.00 15.15   -0.020 C
ATOM   6538  CD1 LEU A 435      10.838  13.311  48.280  1.00 11.62    0.009 C
ATOM   6542  CD2 LEU A 435      12.001  12.649  50.390  1.00 10.81    0.009 C
ATOM   6546  N   MET A 436      12.712  17.460  49.074  1.00  6.80   -0.346 N
ATOM   6547  HN  MET A 436      13.704  17.434  49.308  1.00  0.00    0.163 HD
ATOM   6548  CA  MET A 436      11.827  18.531  49.585  1.00  7.35    0.177 C
ATOM   6550  C   MET A 436      11.129  19.276  48.455  1.00  6.62    0.241 C
ATOM   6551  O   MET A 436       9.974  19.633  48.634  1.00  7.61   -0.271 OA
ATOM   6552  CB  MET A 436      12.703  19.551  50.349  1.00  6.23    0.045 C
ATOM   6555  CG  MET A 436      11.869  20.728  50.922  1.00  7.81    0.076 C
ATOM   6558  SD  MET A 436      10.537  20.188  52.049  1.00 12.23   -0.173 SA
ATOM   6559  CE  MET A 436      11.536  19.601  53.403  1.00  9.74    0.089 C
ATOM   6563  N   PHE A 437      11.800  19.505  47.323  1.00  8.53   -0.346 N
ATOM   6564  HN  PHE A 437      12.741  19.124  47.220  1.00  0.00    0.163 HD
ATOM   6565  CA  PHE A 437      11.227  20.284  46.229  1.00  6.36    0.180 C
ATOM   6567  C   PHE A 437      10.294  19.534  45.324  1.00  7.42    0.241 C
ATOM   6568  O   PHE A 437       9.726  20.105  44.357  1.00 10.66   -0.271 OA
ATOM   6569  CB  PHE A 437      12.361  21.058  45.503  1.00  7.10    0.073 C
ATOM   6572  CG  PHE A 437      13.166  21.799  46.570  1.00 12.06   -0.056 A
ATOM   6573  CD1 PHE A 437      12.516  22.586  47.506  1.00 12.56    0.007 A
ATOM   6575  CD2 PHE A 437      14.536  21.726  46.604  1.00 15.21    0.007 A
ATOM   6577  CE1 PHE A 437      13.206  23.283  48.484  1.00 24.16    0.001 A
ATOM   6579  CE2 PHE A 437      15.225  22.397  47.598  1.00 16.07    0.001 A
ATOM   6581  CZ  PHE A 437      14.589  23.199  48.532  1.00 18.98    0.000 A
ATOM   6583  N   VAL A 438       9.919  18.313  45.741  1.00  6.39   -0.346 N
ATOM   6584  HN  VAL A 438      10.460  17.853  46.473  1.00  0.00    0.163 HD
ATOM   6585  CA  VAL A 438       8.766  17.626  45.181  1.00  8.01    0.180 C
ATOM   6587  C   VAL A 438       7.537  18.474  45.551  1.00 10.75    0.241 C
ATOM   6588  O   VAL A 438       6.553  18.524  44.810  1.00  8.15   -0.271 OA
ATOM   6589  CB  VAL A 438       8.591  16.205  45.689  1.00  9.21    0.009 C
ATOM   6591  CG1 VAL A 438       8.082  16.125  47.153  1.00  9.63    0.012 C
ATOM   6595  CG2 VAL A 438       7.602  15.433  44.808  1.00  8.41    0.012 C
ATOM   6599  N   GLU A 439       7.588  19.269  46.661  1.00  5.67   -0.346 N
ATOM   6600  HN  GLU A 439       8.410  19.263  47.265  1.00  0.00    0.163 HD
ATOM   6601  CA  GLU A 439       6.451  20.124  46.967  1.00  7.63    0.177 C
ATOM   6603  C   GLU A 439       6.285  21.256  45.966  1.00  8.30    0.241 C
ATOM   6604  O   GLU A 439       5.120  21.622  45.705  1.00  9.40   -0.271 OA
ATOM   6605  CB  GLU A 439       6.591  20.697  48.406  1.00  5.32    0.045 C
ATOM   6608  CG  GLU A 439       6.558  19.529  49.427  1.00  7.18    0.116 C
ATOM   6611  CD  GLU A 439       6.169  20.052  50.821  1.00 13.44    0.172 C
ATOM   6612  OE1 GLU A 439       6.274  21.276  51.040  1.00 10.60   -0.648 OA
ATOM   6613  OE2 GLU A 439       5.739  19.247  51.667  1.00 12.10   -0.648 OA
ATOM   6614  N   TYR A 440       7.331  21.724  45.279  1.00  5.88   -0.346 N
ATOM   6615  HN  TYR A 440       8.268  21.370  45.472  1.00  0.00    0.163 HD
ATOM   6616  CA  TYR A 440       7.133  22.733  44.261  1.00  6.84    0.180 C
ATOM   6618  C   TYR A 440       6.425  22.094  43.041  1.00  8.95    0.241 C
ATOM   6619  O   TYR A 440       5.735  22.775  42.299  1.00 11.58   -0.271 OA
ATOM   6620  CB  TYR A 440       8.486  23.299  43.762  1.00  6.50    0.073 C
ATOM   6623  CG  TYR A 440       9.034  24.439  44.637  1.00 10.14   -0.056 A
ATOM   6624  CD1 TYR A 440       9.115  24.268  46.014  1.00  8.29    0.010 A
ATOM   6626  CD2 TYR A 440       9.459  25.619  44.075  1.00  9.31    0.010 A
ATOM   6628  CE1 TYR A 440       9.628  25.272  46.837  1.00  6.36    0.037 A
ATOM   6630  CE2 TYR A 440       9.948  26.657  44.862  1.00  6.08    0.037 A
ATOM   6632  CZ  TYR A 440      10.027  26.456  46.239  1.00  8.04    0.065 A
ATOM   6633  OH  TYR A 440      10.547  27.476  47.019  1.00  9.68   -0.361 OA
ATOM   6634  HH  TYR A 440      10.821  28.288  46.609  1.00  0.00    0.217 HD
ATOM   6635  N   ALA A 441       6.685  20.822  42.791  1.00  8.84   -0.346 N
ATOM   6636  HN  ALA A 441       7.263  20.278  43.432  1.00  0.00    0.163 HD
ATOM   6637  CA  ALA A 441       6.130  20.200  41.575  1.00  9.79    0.172 C
ATOM   6639  C   ALA A 441       4.974  19.267  41.859  1.00  8.41    0.240 C
ATOM   6640  O   ALA A 441       4.648  18.409  41.044  1.00  8.95   -0.271 OA
ATOM   6641  CB  ALA A 441       7.277  19.327  41.016  1.00  9.48    0.042 C
ATOM   6645  N   ARG A 442       4.442  19.311  43.088  1.00  7.98   -0.346 N
ATOM   6646  HN  ARG A 442       4.703  20.067  43.721  1.00  0.00    0.163 HD
ATOM   6647  CA  ARG A 442       3.489  18.289  43.537  1.00  6.62    0.176 C
ATOM   6649  C   ARG A 442       2.334  17.982  42.613  1.00  7.67    0.241 C
ATOM   6650  O   ARG A 442       2.005  16.776  42.492  1.00  8.89   -0.271 OA
ATOM   6651  CB  ARG A 442       2.936  18.747  44.913  1.00  8.40    0.036 C
ATOM   6654  CG  ARG A 442       2.166  17.609  45.620  1.00 13.00    0.023 C
ATOM   6657  CD  ARG A 442       3.269  16.584  45.989  1.00 16.20    0.138 C
ATOM   6660  NE  ARG A 442       2.758  15.399  46.667  1.00 28.06   -0.227 N
ATOM   6661  HE  ARG A 442       3.093  15.194  47.608  1.00  0.00    0.177 HD
ATOM   6662  CZ  ARG A 442       1.869  14.569  46.110  1.00 27.39    0.665 C
ATOM   6663  NH1 ARG A 442       1.413  14.793  44.899  1.00 30.06   -0.235 N
ATOM   6664 1HH1 ARG A 442       1.756  15.619  44.409  1.00  0.00    0.174 HD
ATOM   6665 2HH1 ARG A 442       0.735  14.160  44.474  1.00  0.00    0.174 HD
ATOM   6666  NH2 ARG A 442       1.424  13.496  46.746  1.00 21.84   -0.235 N
ATOM   6667 1HH2 ARG A 442       1.778  13.322  47.687  1.00  0.00    0.174 HD
ATOM   6668 2HH2 ARG A 442       0.746  12.863  46.321  1.00  0.00    0.174 HD
ATOM   6669  N   ASN A 443       1.629  18.981  42.042  1.00  5.83   -0.346 N
ATOM   6670  HN  ASN A 443       1.876  19.960  42.184  1.00  0.00    0.163 HD
ATOM   6671  CA  ASN A 443       0.476  18.582  41.196  1.00  9.24    0.185 C
ATOM   6673  C   ASN A 443       0.936  17.941  39.885  1.00  7.37    0.241 C
ATOM   6674  O   ASN A 443       0.160  17.134  39.355  1.00  6.53   -0.271 OA
ATOM   6675  CB  ASN A 443      -0.469  19.775  40.933  1.00  7.27    0.137 C
ATOM   6678  CG  ASN A 443      -1.851  19.316  40.519  1.00 10.28    0.217 C
ATOM   6679  ND2 ASN A 443      -2.583  18.634  41.409  1.00  8.04   -0.370 N
ATOM   6680 1HD2 ASN A 443      -3.514  18.325  41.130  1.00  0.00    0.159 HD
ATOM   6681 2HD2 ASN A 443      -2.271  18.436  42.360  1.00  0.00    0.159 HD
ATOM   6682  OD1 ASN A 443      -2.227  19.555  39.373  1.00  8.15   -0.274 OA
ATOM   6683  N   ALA A 444       2.117  18.266  39.373  1.00  7.72   -0.346 N
ATOM   6684  HN  ALA A 444       2.682  18.994  39.811  1.00  0.00    0.163 HD
ATOM   6685  CA  ALA A 444       2.607  17.574  38.175  1.00 10.53    0.172 C
ATOM   6687  C   ALA A 444       2.880  16.110  38.462  1.00  8.81    0.240 C
ATOM   6688  O   ALA A 444       2.723  15.214  37.593  1.00  6.70   -0.271 OA
ATOM   6689  CB  ALA A 444       3.885  18.246  37.636  1.00  8.17    0.042 C
ATOM   6693  N   VAL A 445       3.385  15.821  39.653  1.00  5.75   -0.346 N
ATOM   6694  HN  VAL A 445       3.630  16.574  40.296  1.00  0.00    0.163 HD
ATOM   6695  CA  VAL A 445       3.595  14.417  40.053  1.00  4.50    0.180 C
ATOM   6697  C   VAL A 445       2.258  13.716  40.141  1.00  6.61    0.241 C
ATOM   6698  O   VAL A 445       2.112  12.572  39.670  1.00  8.42   -0.271 OA
ATOM   6699  CB  VAL A 445       4.254  14.385  41.461  1.00 10.04    0.009 C
ATOM   6701  CG1 VAL A 445       4.272  12.945  41.997  1.00  9.53    0.012 C
ATOM   6705  CG2 VAL A 445       5.684  14.920  41.366  1.00 12.84    0.012 C
ATOM   6709  N   ARG A 446       1.245  14.384  40.735  1.00  5.04   -0.346 N
ATOM   6710  HN  ARG A 446       1.397  15.296  41.166  1.00  0.00    0.163 HD
ATOM   6711  CA  ARG A 446      -0.091  13.751  40.740  1.00  7.51    0.176 C
ATOM   6713  C   ARG A 446      -0.617  13.525  39.330  1.00  7.74    0.241 C
ATOM   6714  O   ARG A 446      -1.238  12.503  39.051  1.00  7.65   -0.271 OA
ATOM   6715  CB  ARG A 446      -1.129  14.651  41.437  1.00  8.96    0.036 C
ATOM   6718  CG  ARG A 446      -2.489  13.932  41.682  1.00  7.19    0.023 C
ATOM   6721  CD  ARG A 446      -3.453  14.959  42.326  1.00  5.94    0.138 C
ATOM   6724  NE  ARG A 446      -4.489  14.188  43.046  1.00 12.23   -0.227 N
ATOM   6725  HE  ARG A 446      -4.248  13.746  43.933  1.00  0.00    0.177 HD
ATOM   6726  CZ  ARG A 446      -5.733  14.052  42.570  1.00 10.86    0.665 C
ATOM   6727  NH1 ARG A 446      -6.175  14.588  41.442  1.00 10.77   -0.235 N
ATOM   6728 1HH1 ARG A 446      -5.520  15.105  40.856  1.00  0.00    0.174 HD
ATOM   6729 2HH1 ARG A 446      -7.123  14.484  41.079  1.00  0.00    0.174 HD
ATOM   6730  NH2 ARG A 446      -6.590  13.375  43.337  1.00 10.06   -0.235 N
ATOM   6731 1HH2 ARG A 446      -6.250  12.962  44.205  1.00  0.00    0.174 HD
ATOM   6732 2HH2 ARG A 446      -7.538  13.271  42.974  1.00  0.00    0.174 HD
ATOM   6733  N   MET A 447      -0.392  14.461  38.401  1.00  7.06   -0.346 N
ATOM   6734  HN  MET A 447       0.154  15.291  38.631  1.00  0.00    0.163 HD
ATOM   6735  CA  MET A 447      -0.936  14.287  37.047  1.00  9.59    0.177 C
ATOM   6737  C   MET A 447      -0.238  13.150  36.306  1.00 10.75    0.241 C
ATOM   6738  O   MET A 447      -0.918  12.493  35.496  1.00  9.67   -0.271 OA
ATOM   6739  CB  MET A 447      -0.831  15.593  36.243  1.00  6.97    0.045 C
ATOM   6742  CG  MET A 447      -1.807  16.691  36.763  1.00  6.28    0.076 C
ATOM   6745  SD  MET A 447      -3.547  16.300  36.602  1.00 12.34   -0.173 SA
ATOM   6746  CE  MET A 447      -3.662  16.232  34.798  1.00 15.67    0.089 C
ATOM   6750  N   ALA A 448       1.038  12.877  36.574  1.00  7.35   -0.346 N
ATOM   6751  HN  ALA A 448       1.558  13.477  37.214  1.00  0.00    0.163 HD
ATOM   6752  CA  ALA A 448       1.703  11.725  35.961  1.00  9.69    0.172 C
ATOM   6754  C   ALA A 448       0.973  10.441  36.399  1.00  9.45    0.240 C
ATOM   6755  O   ALA A 448       0.679   9.552  35.591  1.00  9.68   -0.271 OA
ATOM   6756  CB  ALA A 448       3.196  11.632  36.383  1.00  7.97    0.042 C
ATOM   6760  N   ALA A 449       0.637  10.368  37.693  1.00  7.11   -0.346 N
ATOM   6761  HN  ALA A 449       0.888  11.122  38.332  1.00  0.00    0.163 HD
ATOM   6762  CA  ALA A 449      -0.104   9.182  38.191  1.00  6.91    0.172 C
ATOM   6764  C   ALA A 449      -1.498   9.024  37.599  1.00  9.82    0.240 C
ATOM   6765  O   ALA A 449      -2.000   7.949  37.175  1.00 10.03   -0.271 OA
ATOM   6766  CB  ALA A 449      -0.159   9.300  39.708  1.00  7.75    0.042 C
ATOM   6770  N   LEU A 450      -2.257  10.135  37.526  1.00  7.26   -0.346 N
ATOM   6771  HN  LEU A 450      -1.852  11.015  37.844  1.00  0.00    0.163 HD
ATOM   6772  CA  LEU A 450      -3.619  10.151  37.020  1.00  8.16    0.177 C
ATOM   6774  C   LEU A 450      -3.654   9.811  35.538  1.00 10.48    0.241 C
ATOM   6775  O   LEU A 450      -4.492   9.019  35.103  1.00  9.38   -0.271 OA
ATOM   6776  CB  LEU A 450      -4.225  11.542  37.286  1.00 12.07    0.038 C
ATOM   6779  CG  LEU A 450      -5.614  11.846  36.661  1.00 16.53   -0.020 C
ATOM   6781  CD1 LEU A 450      -6.656  10.882  37.180  1.00 22.90    0.009 C
ATOM   6785  CD2 LEU A 450      -6.076  13.241  37.086  1.00 25.73    0.009 C
ATOM   6789  N   MET A 451      -2.656  10.289  34.782  1.00  6.98   -0.346 N
ATOM   6790  HN  MET A 451      -1.924  10.857  35.208  1.00  0.00    0.163 HD
ATOM   6791  CA  MET A 451      -2.610   9.996  33.325  1.00  7.51    0.177 C
ATOM   6793  C   MET A 451      -1.975   8.666  33.001  1.00 10.43    0.241 C
ATOM   6794  O   MET A 451      -1.844   8.257  31.825  1.00  9.68   -0.271 OA
ATOM   6795  CB  MET A 451      -1.806  11.158  32.665  1.00  6.07    0.045 C
ATOM   6798  CG  MET A 451      -2.582  12.501  32.684  1.00 11.50    0.076 C
ATOM   6801  SD  MET A 451      -1.830  13.673  31.501  1.00 12.18   -0.173 SA
ATOM   6802  CE  MET A 451      -0.344  14.164  32.340  1.00 12.71    0.089 C
ATOM   6806  N   LYS A 452      -1.483   7.946  34.005  1.00  8.66   -0.346 N
ATOM   6807  HN  LYS A 452      -1.581   8.330  34.945  1.00  0.00    0.163 HD
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ATOM   6808  CA  LYS A 452      -0.816   6.655  33.880  1.00 11.22      0.176 C
ATOM   6810  C   LYS A 452       0.431   6.711  33.013  1.00 10.74      0.241 C
ATOM   6811  O   LYS A 452       0.635   5.827  32.180  1.00 10.94     -0.271 OA
ATOM   6812  CB  LYS A 452      -1.790   5.584  33.342  1.00  9.23      0.035 C
ATOM   6815  CG  LYS A 452      -2.999   5.494  34.324  1.00 12.09      0.004 C
ATOM   6818  CD  LYS A 452      -3.651   4.122  34.136  1.00 35.96      0.027 C
ATOM   6821  CE  LYS A 452      -5.162   4.275  34.129  1.00 45.91      0.229 C
ATOM   6824  NZ  LYS A 452      -5.676   4.151  32.737  1.00 62.39     -0.079 N
ATOM   6825  HZ1 LYS A 452      -6.691   4.254  32.732  1.00  0.00      0.274 HD
ATOM   6826  HZ2 LYS A 452      -5.377   3.282  32.294  1.00  0.00      0.274 HD
ATOM   6827  HZ3 LYS A 452      -5.221   4.806  32.101  1.00  0.00      0.274 HD
ATOM   6828  N   GLN A 453       1.315   7.673  33.240  1.00  7.77     -0.346 N
ATOM   6829  HN  GLN A 453       1.165   8.304  34.027  1.00  0.00      0.163 HD
ATOM   6830  CA  GLN A 453       2.494   7.861  32.404  1.00  9.15      0.177 C
ATOM   6832  C   GLN A 453       3.766   7.439  33.113  1.00 11.08      0.241 C
ATOM   6833  O   GLN A 453       3.924   7.648  34.302  1.00 12.00     -0.271 OA
ATOM   6834  CB  GLN A 453       2.684   9.344  32.004  1.00 10.86      0.044 C
ATOM   6837  CG  GLN A 453       1.400   9.791  31.275  1.00 13.32      0.105 C
ATOM   6840  CD  GLN A 453       1.344   9.095  29.924  1.00 17.55      0.215 C
ATOM   6841  NE2 GLN A 453       0.261   8.445  29.585  1.00 13.85     -0.370 N
ATOM   6842 1HE2 GLN A 453      -0.545   8.406  30.209  1.00  0.00      0.159 HD
ATOM   6843 2HE2 GLN A 453       0.223   7.978  28.679  1.00  0.00      0.159 HD
ATOM   6844  OE1 GLN A 453       2.308   9.142  29.778  1.00 15.69     -0.274 OA
ATOM   6845  N   ARG A 454       4.615   6.735  32.369  1.00  8.20     -0.346 N
ATOM   6846  HN  ARG A 454       4.373   6.498  31.407  1.00  0.00      0.163 HD
ATOM   6847  CA  ARG A 454       5.899   6.298  32.930  1.00  8.27      0.176 C
ATOM   6849  C   ARG A 454       6.877   7.462  33.030  1.00 16.09      0.241 C
ATOM   6850  O   ARG A 454       7.182   8.196  32.071  1.00 13.92     -0.271 OA
ATOM   6851  CB  ARG A 454       6.465   5.235  31.922  1.00 11.59      0.036 C
ATOM   6854  CG  ARG A 454       7.814   4.708  32.438  1.00 16.81      0.023 C
ATOM   6857  CD  ARG A 454       8.263   3.455  31.686  1.00 27.36      0.138 C
ATOM   6860  NE  ARG A 454       8.328   3.790  30.263  1.00 17.17     -0.227 N
ATOM   6861  HE  ARG A 454       7.867   4.644  29.949  1.00  0.00      0.177 HD
ATOM   6862  CZ  ARG A 454       8.958   3.041  29.348  1.00 35.15      0.665 C
ATOM   6863  NH1 ARG A 454       9.567   1.906  29.696  1.00 32.69     -0.235 N
ATOM   6864 1HH1 ARG A 454      10.047   1.336  28.999  1.00  0.00      0.174 HD
ATOM   6865 2HH1 ARG A 454       9.552   1.626  30.677  1.00  0.00      0.174 HD
ATOM   6866  NH2 ARG A 454       8.977   3.404  28.075  1.00 27.58     -0.235 N
ATOM   6867 1HH2 ARG A 454       9.457   2.834  27.378  1.00  0.00      0.174 HD
ATOM   6868 2HH2 ARG A 454       8.511   4.272  27.809  1.00  0.00      0.174 HD
ATOM   6869  N   GLN A 455       7.400   7.724  34.230  1.00  9.93     -0.346 N
ATOM   6870  HN  GLN A 455       7.046   7.234  35.052  1.00  0.00      0.163 HD
ATOM   6871  CA  GLN A 455       8.483   8.713  34.381  1.00 16.36      0.177 C
ATOM   6873  C   GLN A 455       9.225   8.248  35.638  1.00 10.44      0.241 C
ATOM   6874  O   GLN A 455       8.529   7.925  36.606  1.00 11.94     -0.271 OA
ATOM   6875  CB  GLN A 455       7.945  10.128  34.551  1.00 10.69      0.044 C
ATOM   6878  CG  GLN A 455       8.933  11.186  35.013  1.00 12.32      0.105 C
ATOM   6881  CD  GLN A 455       8.329  12.540  35.260  1.00 11.79      0.215 C
ATOM   6882  NE2 GLN A 455       7.114  12.900  34.838  1.00  8.62     -0.370 N
ATOM   6883 1HE2 GLN A 455       6.573  12.212  34.313  1.00  0.00      0.159 HD
ATOM   6884 2HE2 GLN A 455       6.704  13.819  35.006  1.00  0.00      0.159 HD
ATOM   6885  OE1 GLN A 455       8.979  13.367  35.891  1.00 11.20     -0.274 OA
ATOM   6886  N   VAL A 456      10.540   8.286  35.672  1.00 10.36     -0.346 N
ATOM   6887  HN  VAL A 456      11.066   8.574  34.847  1.00  0.00      0.163 HD
ATOM   6888  CA  VAL A 456      11.250   7.910  36.909  1.00 12.32      0.180 C
ATOM   6890  C   VAL A 456      11.611   9.224  37.603  1.00 11.29      0.241 C
ATOM   6891  O   VAL A 456      12.243  10.054  36.977  1.00  7.97     -0.271 OA
ATOM   6892  CB  VAL A 456      12.496   7.046  36.613  1.00  8.68      0.009 C
ATOM   6894  CG1 VAL A 456      13.213   6.803  37.939  1.00  6.87      0.012 C
ATOM   6898  CG2 VAL A 456      12.046   5.717  35.946  1.00 12.08      0.012 C
ATOM   6902  N   MET A 457      11.243   9.440  38.856  1.00  6.21     -0.346 N
ATOM   6903  HN  MET A 457      10.741   8.711  39.363  1.00  0.00      0.163 HD
ATOM   6904  CA  MET A 457      11.544  10.706  39.527  1.00  8.57      0.177 C
ATOM   6906  C   MET A 457      12.614  10.426  40.594  1.00  9.58      0.241 C
ATOM   6907  O   MET A 457      12.405   9.539  41.432  1.00 11.16     -0.271 OA
ATOM   6908  CB  MET A 457      10.238  11.178  40.178  1.00  9.54      0.045 C
ATOM   6911  CG  MET A 457       9.177  11.439  39.075  1.00 13.14      0.076 C
ATOM   6914  SD  MET A 457       7.548  11.360  39.747  1.00 23.30     -0.173 SA
ATOM   6915  CE  MET A 457       6.433  12.017  38.520  1.00 10.86      0.089 C
ATOM   6919  N   VAL A 458      13.781  11.000  40.425  1.00  8.27     -0.346 N
ATOM   6920  HN  VAL A 458      13.906  11.670  39.666  1.00  0.00      0.163 HD
ATOM   6921  CA  VAL A 458      14.915  10.692  41.314  1.00  7.03      0.180 C
ATOM   6923  C   VAL A 458      15.017  11.763  42.407  1.00 11.69      0.241 C
ATOM   6924  O   VAL A 458      15.419  12.891  42.130  1.00 10.83     -0.271 OA
ATOM   6925  CB  VAL A 458      16.167  10.643  40.440  1.00 12.37      0.009 C
ATOM   6927  CG1 VAL A 458      17.417  10.370  41.244  1.00 16.03      0.012 C
ATOM   6931  CG2 VAL A 458      15.994   9.547  39.325  1.00 12.65      0.012 C
ATOM   6935  N   TYR A 459      14.601  11.426  43.628  1.00  9.06     -0.346 N
ATOM   6936  HN  TYR A 459      14.286  10.479  43.837  1.00  0.00      0.163 HD
ATOM   6937  CA  TYR A 459      14.614  12.481  44.670  1.00  5.44      0.180 C
ATOM   6939  C   TYR A 459      15.668  12.128  45.704  1.00  9.75      0.241 C
ATOM   6940  O   TYR A 459      15.562  11.094  46.397  1.00 13.37     -0.271 OA
ATOM   6941  CB  TYR A 459      13.221  12.530  45.304  1.00  7.31      0.073 C
ATOM   6944  CG  TYR A 459      12.111  12.974  44.377  1.00 11.09     -0.056 A
ATOM   6945  CD1 TYR A 459      12.302  14.097  43.565  1.00 13.65      0.010 A
ATOM   6947  CD2 TYR A 459      10.898  12.288  44.302  1.00 10.32      0.010 A
ATOM   6949  CE1 TYR A 459      11.310  14.510  42.665  1.00 14.22      0.037 A
ATOM   6951  CE2 TYR A 459       9.896  12.710  43.424  1.00  7.87      0.037 A
ATOM   6953  CZ  TYR A 459      10.116  13.833  42.621  1.00 10.89      0.065 A
ATOM   6954  OH  TYR A 459       9.157  14.245  41.749  1.00 11.54     -0.361 OA
ATOM   6955  HH  TYR A 459       9.307  15.008  41.203  1.00  0.00      0.217 HD
ATOM   6956  N   THR A 460      16.703  12.969  45.799  1.00  9.45     -0.344 N
ATOM   6957  HN  THR A 460      16.741  13.815  45.230  1.00  0.00      0.163 HD
ATOM   6958  CA  THR A 460      17.786  12.649  46.741  1.00  9.06      0.205 C
ATOM   6960  C   THR A 460      17.654  13.512  47.987  1.00  9.70      0.243 C
ATOM   6961  O   THR A 460      16.808  14.392  48.070  1.00 11.92     -0.271 OA
ATOM   6962  CB  THR A 460      19.149  12.868  46.035  1.00 10.78      0.146 C
ATOM   6964  CG2 THR A 460      19.203  12.140  44.672  1.00  7.28      0.042 C
ATOM   6968  OG1 THR A 460      19.304  14.265  45.813  1.00 12.29     -0.393 OA
ATOM   6969  HG1 THR A 460      20.139  14.399  45.380  1.00  0.00      0.210 HD
ATOM   6970  N   HIS A 461      18.529  13.318  48.953  1.00  9.25     -0.346 N
ATOM   6971  HN  HIS A 461      19.197  12.558  48.827  1.00  0.00      0.163 HD
ATOM   6972  CA  HIS A 461      18.630  14.094  50.191  1.00  6.72      0.182 C
ATOM   6974  C   HIS A 461      17.321  13.891  50.935  1.00  5.96      0.241 C
ATOM   6975  O   HIS A 461      16.518  14.819  51.147  1.00 10.53     -0.271 OA
ATOM   6976  CB  HIS A 461      18.895  15.584  49.860  1.00  9.28      0.093 C
ATOM   6979  CG  HIS A 461      20.284  15.769  49.267  1.00 14.92      0.028 A
ATOM   6980  CD2 HIS A 461      21.352  16.492  49.720  1.00 11.29      0.114 A
ATOM   6982  ND1 HIS A 461      20.671  15.155  48.088  1.00 13.74     -0.354 N
ATOM   6983  HD1 HIS A 461      20.085  14.557  47.505  1.00  0.00      0.166 HD
ATOM   6984  CE1 HIS A 461      21.944  15.480  47.844  1.00 17.26      0.180 A
ATOM   6986  NE2 HIS A 461      22.381  16.286  48.807  1.00 11.96     -0.360 N
ATOM   6987  HE2 HIS A 461      23.319  16.680  48.898  1.00  0.00      0.166 HD
ATOM   6988  N   ASP A 462      17.067  12.640  51.305  1.00  8.26     -0.345 N
ATOM   6989  HN  ASP A 462      17.814  11.945  51.293  1.00  0.00      0.163 HD
ATOM   6990  CA  ASP A 462      15.720  12.254  51.730  1.00  8.68      0.186 C
ATOM   6992  C   ASP A 462      15.364  12.421  53.192  1.00 10.68      0.241 C
ATOM   6993  O   ASP A 462      14.211  12.108  53.514  1.00 11.43     -0.271 OA
ATOM   6994  CB  ASP A 462      15.507  10.754  51.405  1.00  8.11      0.147 C
ATOM   6997  CG  ASP A 462      16.333   9.817  52.285  1.00 12.65      0.175 C
ATOM   6998  OD1 ASP A 462      17.485  10.095  52.680  1.00 13.70     -0.648 OA
ATOM   6999  OD2 ASP A 462      15.813   8.717  52.632  1.00 11.18     -0.648 OA
ATOM   7000  N   SER A 463      16.261  12.917  54.042  1.00  7.05     -0.344 N
ATOM   7001  HN  SER A 463      17.180  13.239  53.740  1.00  0.00      0.163 HD
ATOM   7002  CA  SER A 463      15.832  12.968  55.448  1.00  5.61      0.200 C
ATOM   7004  C   SER A 463      16.762  13.906  56.215  1.00  8.00      0.243 C
ATOM   7005  O   SER A 463      17.643  14.540  55.618  1.00  9.70     -0.271 OA
ATOM   7006  CB  SER A 463      15.956  11.578  56.113  1.00 10.12      0.199 C
ATOM   7009  OG  SER A 463      17.322  11.223  56.343  1.00 13.38     -0.398 OA
ATOM   7010  HG  SER A 463      17.398  10.369  56.752  1.00  0.00      0.209 HD
ATOM   7011  N   ILE A 464      16.671  13.865  57.535  1.00  8.15     -0.346 N
ATOM   7012  HN  ILE A 464      15.946  13.304  57.983  1.00  0.00      0.163 HD
ATOM   7013  CA  ILE A 464      17.622  14.634  58.350  1.00 12.18      0.180 C
ATOM   7015  C   ILE A 464      19.032  14.126  58.139  1.00 13.67      0.241 C
ATOM   7016  O   ILE A 464      20.002  14.829  58.467  1.00 12.17     -0.271 OA
ATOM   7017  CB  ILE A 464      17.269  14.521  59.859  1.00 13.96      0.013 C
ATOM   7019  CG1 ILE A 464      17.033  13.028  60.159  1.00 13.88      0.002 C
ATOM   7022  CG2 ILE A 464      16.089  15.399  60.209  1.00 12.15      0.012 C
ATOM   7026  CD1 ILE A 464      17.000  12.744  61.674  1.00 19.25      0.005 C
ATOM   7030  N   GLY A 465      19.276  12.985  57.494  1.00 14.22     -0.351 N
ATOM   7031  HN  GLY A 465      18.479  12.394  57.260  1.00  0.00      0.163 HD
ATOM   7032  CA  GLY A 465      20.596  12.524  57.101  1.00 14.37      0.225 C
ATOM   7035  C   GLY A 465      21.321  13.466  56.147  1.00 15.73      0.236 C
ATOM   7036  O   GLY A 465      22.556  13.380  56.038  1.00 13.69     -0.272 OA
ATOM   7037  N   LEU A 466      20.675  14.441  55.506  1.00 12.06     -0.346 N
ATOM   7038  HN  LEU A 466      19.660  14.508  55.577  1.00  0.00      0.163 HD
ATOM   7039  CA  LEU A 466      21.397  15.418  54.666  1.00 10.40      0.177 C
ATOM   7041  C   LEU A 466      22.196  16.375  55.533  1.00 11.17      0.240 C
ATOM   7042  O   LEU A 466      23.149  17.054  55.109  1.00 12.80     -0.271 OA
ATOM   7043  CB  LEU A 466      20.441  16.179  53.713  1.00 12.49      0.038 C
ATOM   7046  CG  LEU A 466      19.407  17.150  54.295  1.00 17.03     -0.020 C
ATOM   7048  CD1 LEU A 466      20.087  18.512  54.473  1.00 11.97      0.009 C
ATOM   7052  CD2 LEU A 466      18.192  17.355  53.443  1.00 10.53      0.009 C
ATOM   7056  N   GLY A 467      21.776  16.526  56.793  1.00  9.68     -0.351 N
ATOM   7057  HN  GLY A 467      20.917  16.078  57.112  1.00  0.00      0.163 HD
ATOM   7058  CA  GLY A 467      22.576  17.350  57.710  1.00 10.16      0.225 C
ATOM   7061  C   GLY A 467      22.441  18.837  57.667  1.00 12.90      0.236 C
ATOM   7062  O   GLY A 467      21.355  19.347  57.911  1.00 11.84     -0.272 OA
ATOM   7063  N   GLU A 468      23.534  19.616  57.508  1.00 10.88     -0.346 N
ATOM   7064  HN  GLU A 468      24.377  19.187  57.126  1.00  0.00      0.163 HD
ATOM   7065  CA  GLU A 468      23.580  21.016  57.846  1.00  9.19      0.177 C
ATOM   7067  C   GLU A 468      22.651  21.955  57.113  1.00 12.71      0.241 C
ATOM   7068  O   GLU A 468      22.303  22.968  57.734  1.00 11.44     -0.271 OA
ATOM   7069  CB  GLU A 468      25.040  21.547  57.667  1.00 12.62      0.045 C
ATOM   7072  CG  GLU A 468      25.982  20.872  58.663  1.00 16.03      0.116 C
ATOM   7075  CD  GLU A 468      26.677  19.631  58.152  1.00 19.12      0.117 C
ATOM   7076  OE1 GLU A 468      26.174  18.833  57.338  1.00 14.18     -0.648 OA
ATOM   7077  OE2 GLU A 468      27.825  19.381  58.602  1.00 18.35     -0.648 OA
ATOM   7078  N   ASP A 469      22.198  21.631  55.896  1.00 10.36     -0.346 N
ATOM   7079  HN  ASP A 469      22.478  20.774  55.419  1.00  0.00      0.163 HD
ATOM   7080  CA  ASP A 469      21.254  22.612  55.288  1.00 11.18      0.186 C
ATOM   7082  C   ASP A 469      20.027  22.856  56.139  1.00 11.03      0.241 C
ATOM   7083  O   ASP A 469      19.390  23.939  55.990  1.00 14.20     -0.271 OA
ATOM   7084  CB  ASP A 469      20.874  22.174  53.872  1.00  8.13      0.147 C
ATOM   7087  CG  ASP A 469      21.974  22.450  52.852  1.00 21.25      0.175 C
ATOM   7088  OD1 ASP A 469      22.936  23.221  53.085  1.00 16.83     -0.648 OA
ATOM   7089  OD2 ASP A 469      21.847  21.941  51.722  1.00 16.21     -0.648 OA
ATOM   7090  N   GLY A 470      19.586  21.961  57.036  1.00 14.13     -0.351 N
ATOM   7091  HN  GLY A 470      19.981  21.021  57.078  1.00  0.00      0.163 HD
ATOM   7092  CA  GLY A 470      18.528  22.371  57.946  1.00 13.36      0.225 C
ATOM   7095  C   GLY A 470      17.088  22.112  57.561  1.00 10.36      0.238 C
ATOM   7096  O   GLY A 470      16.779  21.518  56.531  1.00  9.85     -0.272 OA
ATOM   7097  N   PRO A 471      16.172  22.582  58.415  1.00  8.33     -0.337 N
ATOM   7098  CA  PRO A 471      14.778  22.209  58.347  1.00  8.56      0.179 C
ATOM   7100  C   PRO A 471      14.029  22.647  57.099  1.00  9.87      0.241 C
ATOM   7101  O   PRO A 471      13.060  21.935  56.755  1.00  9.28     -0.271 OA
ATOM   7102  CB  PRO A 471      14.178  22.777  59.650  1.00  9.18      0.037 C
ATOM   7105  CG  PRO A 471      15.094  23.907  60.014  1.00 13.75      0.022 C
ATOM   7108  CD  PRO A 471      16.474  23.353  59.665  1.00 10.10      0.127 C
ATOM   7111  N   THR A 472      14.519  23.667  56.396  1.00  5.25     -0.344 N
ATOM   7112  HN  THR A 472      15.349  24.174  56.705  1.00  0.00      0.163 HD
ATOM   7113  CA  THR A 472      13.807  24.039  55.140  1.00 10.57      0.205 C
ATOM   7115  C   THR A 472      14.051  22.974  54.095  1.00 10.69      0.243 C
ATOM   7116  O   THR A 472      13.352  22.931  53.072  1.00 11.40     -0.271 OA
ATOM   7117  CB  THR A 472      14.255  25.415  54.575  1.00 13.49      0.146 C
ATOM   7119  CG2 THR A 472      14.032  26.471  55.645  1.00 10.68      0.042 C
ATOM   7123  OG1 THR A 472      15.655  25.371  54.238  1.00 12.42     -0.393 OA
ATOM   7124  HG1 THR A 472      15.929  26.212  53.892  1.00  0.00      0.210 HD
ATOM   7125  N   HIS A 473      15.139  22.234  54.174  1.00  7.52     -0.346 N
ATOM   7126  HN  HIS A 473      15.758  22.368  54.974  1.00  0.00      0.163 HD
ATOM   7127  CA  HIS A 473      15.502  21.240  53.184  1.00  9.57      0.182 C
ATOM   7129  C   HIS A 473      15.277  19.802  53.648  1.00  8.24      0.241 C
ATOM   7130  O   HIS A 473      15.218  18.913  52.786  1.00 11.28     -0.271 OA
ATOM   7131  CB  HIS A 473      17.018  21.370  52.919  1.00 12.46      0.093 C
ATOM   7134  CG  HIS A 473      17.393  22.458  51.974  1.00  8.68      0.028 A
ATOM   7135  CD2 HIS A 473      18.187  22.432  50.864  1.00 13.87      0.114 A
ATOM   7137  ND1 HIS A 473      16.997  23.769  52.170  1.00 16.29     -0.354 N
ATOM   7138  HD1 HIS A 473      16.430  24.112  52.945  1.00  0.00      0.166 HD
ATOM   7139  CE1 HIS A 473      17.483  24.507  51.173  1.00 19.95      0.180 A
ATOM   7141  NE2 HIS A 473      18.228  23.751  50.393  1.00 17.41     -0.360 N
ATOM   7142  HE2 HIS A 473      18.750  24.073  49.578  1.00  0.00      0.166 HD
ATOM   7143  N   GLN A 474      15.225  19.527  54.945  1.00  8.43     -0.346 N
ATOM   7144  HN  GLN A 474      15.247  20.277  55.636  1.00  0.00      0.163 HD
ATOM   7145  CA  GLN A 474      15.135  18.111  55.371  1.00  6.85      0.177 C
ATOM   7147  C   GLN A 474      13.719  17.602  55.309  1.00  8.21      0.243 C
ATOM   7148  O   GLN A 474      12.813  18.071  56.011  1.00  7.56     -0.271 OA
ATOM   7149  CB  GLN A 474      15.527  18.079  56.896  1.00  7.98      0.044 C
ATOM   7152  CG  GLN A 474      17.059  18.271  56.980  1.00  6.31      0.105 C
ATOM   7155  CD  GLN A 474      17.416  18.711  58.420  1.00 13.90      0.215 C
ATOM   7156  NE2 GLN A 474      18.687  18.747  58.760  1.00 11.05     -0.370 N
ATOM   7157 1HE2 GLN A 474      18.922  19.037  59.709  1.00  0.00      0.159 HD
ATOM   7158 2HE2 GLN A 474      19.415  18.448  58.112  1.00  0.00      0.159 HD
ATOM   7159  OE1 GLN A 474      16.545  19.069  59.195  1.00  9.96     -0.274 OA
ATOM   7160  N   PRO A 475      13.461  16.613  54.468  1.00  8.85     -0.337 N
ATOM   7161  CA  PRO A 475      12.152  16.021  54.366  1.00  7.81      0.179 C
ATOM   7163  C   PRO A 475      11.691  15.350  55.656  1.00  9.99      0.241 C
ATOM   7164  O   PRO A 475      12.535  14.759  56.359  1.00 11.19     -0.271 OA
ATOM   7165  CB  PRO A 475      12.316  14.920  53.309  1.00  5.31      0.037 C
ATOM   7168  CG  PRO A 475      13.488  15.425  52.465  1.00  4.26      0.022 C
ATOM   7171  CD  PRO A 475      14.451  15.986  53.540  1.00  8.35      0.127 C
ATOM   7174  N   VAL A 476      10.393  15.394  55.944  1.00 10.16     -0.346 N
ATOM   7175  HN  VAL A 476       9.779  15.945  55.344  1.00  0.00      0.163 HD
ATOM   7176  CA  VAL A 476       9.810  14.689  57.080  1.00 11.31      0.180 C
ATOM   7178  C   VAL A 476       8.517  13.997  56.628  1.00  8.04      0.241 C
ATOM   7179  O   VAL A 476       8.373  12.782  56.703  1.00 10.40     -0.271 OA
ATOM   7180  CB  VAL A 476       9.549  15.612  58.289  1.00 10.68      0.009 C
ATOM   7182  CG1 VAL A 476       8.745  14.879  59.370  1.00 12.52      0.012 C
ATOM   7186  CG2 VAL A 476      10.878  16.097  58.903  1.00  8.69      0.012 C
ATOM   7190  N   GLU A 477       7.553  14.752  56.083  1.00  8.93     -0.346 N
ATOM   7191  HN  GLU A 477       7.747  15.742  55.936  1.00  0.00      0.163 HD
ATOM   7192  CA  GLU A 477       6.249  14.248  55.689  1.00  5.68      0.177 C
ATOM   7194  C   GLU A 477       6.075  14.051  54.202  1.00  7.76      0.241 C
ATOM   7195  O   GLU A 477       5.016  13.654  53.762  1.00 10.68     -0.271 OA
ATOM   7196  CB  GLU A 477       5.190  15.254  56.273  1.00  8.25      0.045 C
ATOM   7199  CG  GLU A 477       5.185  16.588  55.546  1.00 10.39      0.116 C
ATOM   7202  CD  GLU A 477       6.179  17.650  55.902  1.00 14.36      0.172 C
ATOM   7203  OE1 GLU A 477       7.351  17.439  56.303  1.00  9.92     -0.648 OA
ATOM   7204  OE2 GLU A 477       5.831  18.859  55.835  1.00 10.88     -0.648 OA
ATOM   7205  N   GLN A 478       7.102  14.285  53.385  1.00  5.89     -0.346 N
ATOM   7206  HN  GLN A 478       8.012  14.532  53.775  1.00  0.00      0.163 HD
ATOM   7207  CA  GLN A 478       6.937  14.192  51.944  1.00  7.98      0.177 C
ATOM   7209  C   GLN A 478       6.780  12.763  51.435  1.00 10.78      0.241 C
ATOM   7210  O   GLN A 478       6.016  12.530  50.490  1.00  8.12     -0.271 OA
ATOM   7211  CB  GLN A 478       8.128  14.834  51.225  1.00  9.74      0.044 C
ATOM   7214  CG  GLN A 478       8.102  16.372  51.327  1.00  9.23      0.105 C
ATOM   7217  CD  GLN A 478       8.418  16.880  52.714  1.00 10.44      0.215 C
ATOM   7218  NE2 GLN A 478       7.827  17.988  53.150  1.00  6.39     -0.370 N
ATOM   7219 1HE2 GLN A 478       8.040  18.331  54.087  1.00  0.00      0.159 HD
ATOM   7220 2HE2 GLN A 478       7.207  18.548  52.565  1.00  0.00      0.159 HD
ATOM   7221  OE1 GLN A 478       9.167  16.203  53.421  1.00  7.91     -0.274 OA
ATOM   7222  N   VAL A 479       7.545  11.801  51.965  1.00  9.41     -0.346 N
ATOM   7223  HN  VAL A 479       8.215  12.014  52.704  1.00  0.00      0.163 HD
ATOM   7224  CA  VAL A 479       7.396  10.433  51.457  1.00  7.47      0.180 C
ATOM   7226  C   VAL A 479       5.982   9.939  51.774  1.00  7.60      0.241 C
ATOM   7227  O   VAL A 479       5.369   9.265  50.944  1.00 10.16     -0.271 OA
ATOM   7228  CB  VAL A 479       8.403   9.456  52.115  1.00  6.79      0.009 C
ATOM   7230  CG1 VAL A 479       8.177   8.019  51.615  1.00  8.69      0.012 C
ATOM   7234  CG2 VAL A 479       9.834   9.833  51.727  1.00 11.37      0.012 C
ATOM   7238  N   ALA A 480       5.436  10.208  52.976  1.00  8.56     -0.346 N
ATOM   7239  HN  ALA A 480       5.968  10.724  53.677  1.00  0.00      0.163 HD
ATOM   7240  CA  ALA A 480       4.065   9.753  53.274  1.00 14.55      0.172 C
ATOM   7242  C   ALA A 480       3.054  10.339  52.285  1.00 13.27      0.240 C
ATOM   7243  O   ALA A 480       2.077   9.684  51.896  1.00 10.11     -0.271 OA
ATOM   7244  CB  ALA A 480       3.645  10.085  54.702  1.00 11.49      0.042 C
ATOM   7248  N   SER A 481       3.228  11.586  51.846  1.00 11.57     -0.344 N
ATOM   7249  HN  SER A 481       4.025  12.132  52.173  1.00  0.00      0.163 HD
ATOM   7250  CA  SER A 481       2.278  12.179  50.893  1.00 11.00      0.200 C
ATOM   7252  C   SER A 481       2.339  11.482  49.528  1.00  9.23      0.243 C
ATOM   7253  O   SER A 481       1.314  11.286  48.858  1.00 13.96     -0.271 OA
ATOM   7254  CB  SER A 481       2.662  13.662  50.668  1.00 15.35      0.199 C
ATOM   7257  OG ASER A 481       1.627  14.211  49.842  0.70 18.47     -0.398 OA
ATOM   7258  HG ASER A 481       1.863  15.121  49.704  1.00  0.00      0.209 HD
ATOM   7259  N   LEU A 482       3.498  11.004  49.110  1.00  7.02     -0.346 N
ATOM   7260  HN  LEU A 482       4.331  11.170  49.675  1.00  0.00      0.163 HD
ATOM   7261  CA  LEU A 482       3.627  10.252  47.876  1.00  5.65      0.177 C
ATOM   7263  C   LEU A 482       2.978   8.863  48.005  1.00  7.77      0.241 C
ATOM   7264  O   LEU A 482       2.309   8.347  47.074  1.00  9.79     -0.271 OA
ATOM   7265  CB  LEU A 482       5.121  10.033  47.478  1.00  6.69      0.038 C
ATOM   7268  CG  LEU A 482       5.841  11.324  47.072  1.00 10.85     -0.020 C
ATOM   7270  CD1 LEU A 482       7.325  11.084  46.848  1.00 13.95      0.009 C
ATOM   7274  CD2 LEU A 482       5.252  11.948  45.793  1.00 19.00      0.009 C
ATOM   7278  N   ARG A 483       3.211   8.235  49.166  1.00  6.32     -0.346 N
ATOM   7279  HN  ARG A 483       3.756   8.685  49.901  1.00  0.00      0.163 HD
ATOM   7280  CA  ARG A 483       2.662   6.881  49.357  1.00  8.66      0.176 C
ATOM   7282  C   ARG A 483       1.152   6.846  49.315  1.00 10.72      0.241 C
ATOM   7283  O   ARG A 483       0.631   5.776  49.037  1.00  9.89     -0.271 OA
ATOM   7284  CB  ARG A 483       3.098   6.304  50.726  1.00  7.94      0.036 C
ATOM   7287  CG  ARG A 483       4.572   5.842  50.713  1.00  6.55      0.023 C
ATOM   7290  CD  ARG A 483       4.929   5.298  52.106  1.00  9.28      0.138 C
ATOM   7293  NE  ARG A 483       6.336   4.789  52.163  1.00  7.35     -0.227 N
ATOM   7294  HE  ARG A 483       6.692   4.208  51.403  1.00  0.00      0.177 HD
ATOM   7295  CZ  ARG A 483       7.129   5.083  53.190  1.00 10.20      0.665 C
ATOM   7296  NH1 ARG A 483       6.773   5.877  54.235  1.00  6.77     -0.235 N
ATOM   7297 1HH1 ARG A 483       7.381   6.102  55.022  1.00  0.00      0.174 HD
ATOM   7298 2HH1 ARG A 483       5.822   6.245  54.248  1.00  0.00      0.174 HD
ATOM   7299  NH2 ARG A 483       8.358   4.607  53.173  1.00  8.19     -0.235 N
ATOM   7300 1HH2 ARG A 483       8.966   4.832  53.960  1.00  0.00      0.174 HD
ATOM   7301 2HH2 ARG A 483       8.625   4.011  52.389  1.00  0.00      0.174 HD
ATOM   7302  N   VAL A 484       0.432   7.891  49.709  1.00  7.08     -0.346 N
ATOM   7303  HN  VAL A 484       0.900   8.745  50.013  1.00  0.00      0.163 HD
ATOM   7304  CA  VAL A 484      -1.008   7.822  49.708  1.00 11.32      0.180 C
ATOM   7306  C   VAL A 484      -1.562   8.376  48.381  1.00 10.29      0.241 C
ATOM   7307  O   VAL A 484      -2.766   8.520  48.301  1.00 13.14     -0.271 OA
ATOM   7308  CB  VAL A 484      -1.633   8.519  50.930  1.00 12.66      0.009 C
ATOM   7310  CG1 VAL A 484      -1.214   7.851  52.237  1.00 15.10      0.012 C
ATOM   7314  CG2 VAL A 484      -1.319  10.013  50.978  1.00 10.99      0.012 C
ATOM   7318  N   THR A 485      -0.775   8.634  47.369  1.00 10.44     -0.344 N
ATOM   7319  HN  THR A 485       0.227   8.491  47.493  1.00  0.00      0.163 HD
ATOM   7320  CA  THR A 485      -1.242   9.112  46.079  1.00  6.95      0.205 C
ATOM   7322  C   THR A 485      -1.624   7.887  45.250  1.00 10.36      0.246 C
ATOM   7323  O   THR A 485      -0.735   7.033  45.014  1.00  7.36     -0.271 OA
ATOM   7324  CB  THR A 485      -0.131   9.929  45.389  1.00  7.07      0.146 C
ATOM   7326  CG2 THR A 485      -0.602  10.496  44.055  1.00  7.25      0.042 C
ATOM   7330  OG1 THR A 485       0.191  11.076  46.284  1.00  8.17     -0.393 OA
ATOM   7331  HG1 THR A 485       0.485  10.723  47.116  1.00  0.00      0.210 HD
ATOM   7332  N   PRO A 486      -2.847   7.794  44.761  1.00 10.32     -0.337 N
ATOM   7333  CA  PRO A 486      -3.241   6.644  43.953  1.00 10.47      0.179 C
ATOM   7335  C   PRO A 486      -2.347   6.550  42.716  1.00 10.29      0.241 C
ATOM   7336  O   PRO A 486      -1.978   7.553  42.071  1.00  7.75     -0.271 OA
ATOM   7337  CB  PRO A 486      -4.694   6.893  43.567  1.00 14.97      0.037 C
ATOM   7340  CG  PRO A 486      -5.182   7.933  44.525  1.00 17.08      0.022 C
ATOM   7343  CD  PRO A 486      -3.965   8.746  44.954  1.00 13.72      0.127 C
ATOM   7346  N   ASN A 487      -1.958   5.313  42.394  1.00  7.70     -0.346 N
ATOM   7347  HN  ASN A 487      -2.231   4.552  43.016  1.00  0.00      0.163 HD
ATOM   7348  CA  ASN A 487      -1.169   4.976  41.212  1.00  8.65      0.185 C
ATOM   7350  C   ASN A 487       0.250   5.512  41.180  1.00 11.46      0.241 C
ATOM   7351  O   ASN A 487       0.986   5.407  40.192  1.00 15.07     -0.271 OA
ATOM   7352  CB  ASN A 487      -1.907   5.376  39.912  1.00 10.95      0.137 C
ATOM   7355  CG  ASN A 487      -1.338   4.585  38.736  1.00 17.37      0.217 C
ATOM   7356  ND2 ASN A 487      -1.074   5.213  37.599  1.00 12.77     -0.370 N
ATOM   7357 1HD2 ASN A 487      -0.694   4.685  36.814  1.00  0.00      0.159 HD
ATOM   7358 2HD2 ASN A 487      -1.302   6.197  37.455  1.00  0.00      0.159 HD
ATOM   7359  OD1 ASN A 487      -1.061   3.389  38.911  1.00 12.23     -0.274 OA
ATOM   7360  N   MET A 488       0.749   5.950  42.330  1.00 10.35     -0.346 N
ATOM   7361  HN  MET A 488       0.139   5.997  43.146  1.00  0.00      0.163 HD
ATOM   7362  CA  MET A 488       2.139   6.365  42.465  1.00  9.54      0.177 C
ATOM   7364  C   MET A 488       2.918   5.146  42.998  1.00 15.88      0.241 C
ATOM   7365  O   MET A 488       2.377   4.414  43.844  1.00 13.67     -0.271 OA
ATOM   7366  CB  MET A 488       2.180   7.441  43.552  1.00 10.44      0.045 C
ATOM   7369  CG  MET A 488       3.574   8.015  43.777  1.00 12.65      0.076 C
ATOM   7372  SD  MET A 488       4.090   8.926  42.249  1.00 23.35     -0.173 SA
ATOM   7373  CE  MET A 488       5.736   8.353  42.253  1.00 21.18      0.089 C
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ATOM   7377  N   SER A 489       4.130   4.908  42.541  1.00  8.98    -0.344 N
ATOM   7378  HN  SER A 489       4.465   5.458  41.750  1.00  0.00     0.163 HD
ATOM   7379  CA  SER A 489       5.019   3.898  43.108  1.00  8.42     0.200 C
ATOM   7381  C   SER A 489       6.202   4.640  43.745  1.00  9.10     0.243 C
ATOM   7382  O   SER A 489       6.723   5.612  43.189  1.00 13.56    -0.271 OA
ATOM   7383  CB  SER A 489       5.451   2.854  42.089  1.00  8.24     0.199 C
ATOM   7386  OG  SER A 489       6.277   1.903  42.735  1.00 12.47    -0.398 OA
ATOM   7387  HG  SER A 489       6.547   1.251  42.099  1.00  0.00     0.209 HD
ATOM   7388  N   THR A 490       6.517   4.296  45.002  1.00  7.65    -0.344 N
ATOM   7389  HN  THR A 490       6.018   3.524  45.444  1.00  0.00     0.163 HD
ATOM   7390  CA  THR A 490       7.559   4.999  45.760  1.00  6.18     0.205 C
ATOM   7392  C   THR A 490       8.505   4.007  46.436  1.00  9.83     0.243 C
ATOM   7393  O   THR A 490       7.994   3.050  47.089  1.00  8.43    -0.271 OA
ATOM   7394  CB  THR A 490       6.830   5.762  46.093  1.00 12.98     0.146 C
ATOM   7396  CG2 THR A 490       7.785   6.658  47.693  1.00 15.34     0.042 C
ATOM   7400  OG1 THR A 490       5.853   6.646  46.333  1.00 14.77    -0.393 OA
ATOM   7401  HG1 THR A 490       5.254   6.084  45.855  1.00  0.00     0.210 HD
ATOM   7402  N   TRP A 491      9.784   4.135  46.120  1.00  7.18    -0.346 N
ATOM   7403  HN  TRP A 491      10.075   4.903  45.515  1.00  0.00     0.163 HD
ATOM   7404  CA  TRP A 491      10.796   3.189  46.625  1.00  8.06     0.181 C
ATOM   7406  C   TRP A 491      11.809   3.886  47.499  1.00  6.75     0.241 C
ATOM   7407  O   TRP A 491      12.328   4.939  47.071  1.00  7.74    -0.271 OA
ATOM   7408  CB  TRP A 491      11.571   2.509  45.439  1.00  9.96     0.075 C
ATOM   7411  CG  TRP A 491      10.645   1.550  44.714  1.00  8.62    -0.028 A
ATOM   7412  CD1 TRP A 491       9.596   1.873  43.907  1.00  9.85     0.096 A
ATOM   7414  CD2 TRP A 491      10.649   0.106  44.784  1.00  7.96    -0.002 A
ATOM   7415  CE2 TRP A 491       9.579  -0.356  44.002  1.00  9.02     0.042 A
ATOM   7416  CE3 TRP A 491      11.496  -0.806  45.410  1.00  8.34     0.014 A
ATOM   7418  NE1 TRP A 491       8.927   0.752  43.498  1.00  8.58    -0.365 N
ATOM   7419  HE1 TRP A 491       8.088   0.737  42.918  1.00  0.00     0.165 HD
ATOM   7420  CZ2 TRP A 491       9.273  -0.698  43.848  1.00 13.44     0.030 A
ATOM   7422  CZ3 TRP A 491      11.191  -2.152  45.288  1.00  9.07     0.001 A
ATOM   7424  CH2 TRP A 491      10.081  -2.587  44.553  1.00  7.92     0.002 A
ATOM   7426  N   ARG A 492      12.129   3.371  48.687  1.00  8.25    -0.346 N
ATOM   7427  HN  ARG A 492      11.656   2.528  49.014  1.00  0.00     0.163 HD
ATOM   7428  CA  ARG A 492      13.165   4.009  49.540  1.00  7.04     0.176 C
ATOM   7430  C   ARG A 492      14.156   2.873  49.834  1.00  8.90     0.243 C
ATOM   7431  O   ARG A 492      14.054   2.203  50.847  1.00  9.54    -0.271 OA
ATOM   7432  CB  ARG A 492      12.491   4.497  50.857  1.00  6.46     0.036 C
ATOM   7435  CG  ARG A 492      13.522   5.344  51.637  1.00  4.76     0.023 C
ATOM   7438  CD  ARG A 492      12.858   6.074  52.814  1.00  8.31     0.138 C
ATOM   7441  NE  ARG A 492      13.807   6.935  53.525  1.00 11.10    -0.227 N
ATOM   7442  HE  ARG A 492      14.150   7.757  53.028  1.00  0.00     0.177 HD
ATOM   7443  CZ  ARG A 492      14.267   6.739  54.773  1.00 12.48     0.665 C
ATOM   7444  NH1 ARG A 492      13.877   5.684  55.476  1.00  8.07    -0.235 N
ATOM   7445  1HH1 ARG A 492      14.226   5.535  56.423  1.00  0.00     0.174 HD
ATOM   7446  2HH1 ARG A 492      13.243   4.998  55.066  1.00  0.00     0.174 HD
ATOM   7447  NH2 ARG A 492      15.096   7.637  55.309  1.00  7.31    -0.235 N
ATOM   7448  1HH2 ARG A 492      15.445   7.488  56.256  1.00  0.00     0.174 HD
ATOM   7449  2HH2 ARG A 492      15.396   8.448  54.768  1.00  0.00     0.174 HD
ATOM   7450  N   PRO A 493      15.111   2.609  48.953  1.00  2.42    -0.337 N
ATOM   7451  CA  PRO A 493      16.010   1.472  49.038  1.00  8.45     0.179 C
ATOM   7453  C   PRO A 493      17.012   1.579  50.180  1.00  8.88     0.241 C
ATOM   7454  O   PRO A 493      17.439   2.699  50.506  1.00 10.07    -0.271 OA
ATOM   7455  CB  PRO A 493      16.738   1.475  47.689  1.00  9.35     0.037 C
ATOM   7458  CG  PRO A 493      16.612   2.878  47.150  1.00 12.03     0.022 C
ATOM   7461  CD  PRO A 493      15.302   3.383  47.692  1.00  8.70     0.127 C
ATOM   7464  N   CYS A 494      17.354   0.482  50.840  1.00  9.64    -0.345 N
ATOM   7465  HN  CYS A 494      16.989  -0.419  50.533  1.00  0.00     0.163 HD
ATOM   7466  CA  CYS A 494      18.250   0.536  52.007  1.00 11.16     0.186 C
ATOM   7468  C   CYS A 494      19.731   0.391  51.650  1.00  9.98     0.242 C
ATOM   7469  O   CYS A 494      20.605   0.523  52.509  1.00 10.97    -0.271 OA
ATOM   7470  CB  CYS A 494      17.839  -0.529  53.058  1.00  8.42     0.021 C
ATOM   7473  SG  CYS A 494      18.306  -2.259  52.585  1.00 11.89    -0.095 SA
ATOM   7474  N   ASP A 495      20.075   0.009  50.432  1.00  6.59    -0.345 N
ATOM   7475  HN  ASP A 495      19.330  -0.194  49.765  1.00  0.00     0.163 HD
ATOM   7476  CA  ASP A 495      21.454  -0.139  49.985  1.00  8.25     0.186 C
ATOM   7478  C   ASP A 495      21.553  -0.167  48.467  1.00  8.95     0.241 C
ATOM   7479  O   ASP A 495      20.537   0.043  47.808  1.00  8.25    -0.271 OA
ATOM   7480  CB  ASP A 495      21.996  -1.443  50.620  1.00  5.84     0.147 C
ATOM   7483  CG  ASP A 495      21.368  -2.721  50.155  1.00 10.66     0.175 C
ATOM   7484  OD1 ASP A 495      20.664  -2.824  49.141  1.00 13.92    -0.648 OA
ATOM   7485  OD2 ASP A 495      21.583  -3.766  50.855  1.00 13.00    -0.648 OA
ATOM   7486  N   GLN A 496      22.737  -0.423  47.894  1.00  7.78    -0.346 N
ATOM   7487  HN  GLN A 496      23.519  -0.698  48.488  1.00  0.00     0.163 HD
ATOM   7488  CA  GLN A 496      22.953  -0.323  46.439  1.00 11.67     0.177 C
ATOM   7490  C   GLN A 496      22.207  -1.402  45.669  1.00 11.04     0.241 C
ATOM   7491  O   GLN A 496      21.853  -1.200  44.506  1.00 10.77    -0.271 OA
ATOM   7492  CB  GLN A 496      24.469  -0.360  46.133  1.00  8.21     0.044 C
ATOM   7495  CG  GLN A 496      25.091  -1.747  46.320  1.00 11.18     0.105 C
ATOM   7498  CD  GLN A 496      26.479  -1.836  45.684  1.00 17.30     0.215 C
ATOM   7499  NE2 GLN A 496      27.176  -2.962  45.880  1.00 10.55    -0.370 N
ATOM   7500  1HE2 GLN A 496      28.102  -3.021  45.456  1.00  0.00     0.159 HD
ATOM   7501  2HE2 GLN A 496      26.830  -3.744  46.436  1.00  0.00     0.159 HD
ATOM   7502  OE1 GLN A 496      26.898  -0.889  45.010  1.00 12.81    -0.274 OA
ATOM   7503  N   VAL A 497      21.915  -2.549  46.313  1.00  6.54    -0.346 N
ATOM   7504  HN  VAL A 497      22.215  -2.664  47.281  1.00  0.00     0.163 HD
ATOM   7505  CA  VAL A 497      21.176  -3.639  45.660  1.00  8.54     0.180 C
ATOM   7507  C   VAL A 497      19.694  -3.291  45.547  1.00  9.64     0.241 C
ATOM   7508  O   VAL A 497      19.095  -3.357  44.461  1.00  9.11    -0.271 OA
ATOM   7509  CB  VAL A 497      21.343  -4.945  46.467  1.00  9.74     0.009 C
ATOM   7511  CG1 VAL A 497      20.624  -6.144  45.822  1.00 12.77     0.012 C
ATOM   7515  CG2 VAL A 497      22.846  -5.280  46.612  1.00 12.33     0.012 C
ATOM   7519  N   GLU A 498      19.079  -2.874  46.677  1.00  7.53    -0.346 N
ATOM   7520  HN  GLU A 498      19.564  -2.862  47.574  1.00  0.00     0.163 HD
ATOM   7521  CA  GLU A 498      17.671  -2.436  46.553  1.00  9.42     0.177 C
ATOM   7523  C   GLU A 498      17.605  -1.247  45.581  1.00  6.13     0.241 C
ATOM   7524  O   GLU A 498      16.540  -1.087  44.918  1.00 10.82    -0.271 OA
ATOM   7525  CB  GLU A 498      17.058  -2.000  47.914  1.00  8.80     0.045 C
ATOM   7528  CG  GLU A 498      16.940  -3.195  48.876  1.00  7.91     0.116 C
ATOM   7531  CD  GLU A 498      16.079  -2.900  50.081  1.00 11.69     0.172 C
ATOM   7532  OE1 GLU A 498      15.702  -1.748  50.343  1.00  8.47    -0.648 OA
ATOM   7533  OE2 GLU A 498      15.707  -3.851  50.819  1.00 10.56    -0.648 OA
ATOM   7534  N   SER A 499      19.568  -0.376  45.609  1.00  7.31    -0.344 N
ATOM   7535  HN  SER A 499      19.368  -0.475  46.267  1.00  0.00     0.163 HD
ATOM   7536  CA  SER A 499      18.543   0.759  44.644  1.00  6.72     0.200 C
ATOM   7538  C   SER A 499      18.469   0.302  43.198  1.00 10.98     0.243 C
ATOM   7539  O   SER A 499      17.767   0.951  42.377  1.00 10.45    -0.271 OA
ATOM   7540  CB  SER A 499      19.683   1.756  44.814  1.00  7.95     0.199 C
ATOM   7543  OG  SER A 499      19.781   2.245  46.150  1.00 12.91    -0.398 OA
ATOM   7544  HG  SER A 499      20.492   2.866  46.256  1.00  0.00     0.209 HD
ATOM   7545  N   ALA A 500      19.254  -0.698  42.812  1.00 11.74    -0.346 N
ATOM   7546  HN  ALA A 500      19.890  -1.129  43.483  1.00  0.00     0.163 HD
ATOM   7547  CA  ALA A 500      19.214  -1.187  41.431  1.00 11.69     0.172 C
ATOM   7549  C   ALA A 500      17.894  -1.859  41.134  1.00  9.75     0.240 C
ATOM   7550  O   ALA A 500      17.413  -1.772  39.982  1.00 10.78    -0.271 OA
ATOM   7551  CB  ALA A 500      20.364  -2.183  41.152  1.00  5.21     0.042 C
ATOM   7555  N   VAL A 501      17.308  -2.597  42.087  1.00  8.58    -0.346 N
ATOM   7556  HN  VAL A 501      17.761  -2.691  42.996  1.00  0.00     0.163 HD
ATOM   7557  CA  VAL A 501      16.028  -3.273  41.848  1.00  6.17     0.180 C
ATOM   7559  C   VAL A 501      14.929  -2.191  41.643  1.00  5.26     0.241 C
ATOM   7560  O   VAL A 501      14.021  -2.383  40.821  1.00  9.26    -0.271 OA
ATOM   7561  CB  VAL A 501      15.619  -4.168  43.028  1.00 13.80     0.009 C
ATOM   7563  CG1 VAL A 501      14.189  -4.687  42.902  1.00 10.79     0.012 C
ATOM   7567  CG2 VAL A 501      16.562  -5.374  43.161  1.00 12.49     0.012 C
ATOM   7571  N   ALA A 502      14.977  -1.119  42.426  1.00  7.26    -0.346 N
ATOM   7572  HN  ALA A 502      15.700  -1.054  43.142  1.00  0.00     0.163 HD
ATOM   7573  CA  ALA A 502      14.002  -0.019  42.278  1.00  9.72     0.172 C
ATOM   7575  C   ALA A 502      14.107   0.662  40.914  1.00  8.83     0.240 C
ATOM   7576  O   ALA A 502      13.089   0.977  40.282  1.00 10.07    -0.271 OA
ATOM   7577  CB  ALA A 502      14.223   0.987  43.426  1.00  8.81     0.042 C
ATOM   7581  N   THR A 503      15.333   0.916  40.440  1.00  7.57    -0.346 N
ATOM   7582  HN  THR A 503      16.156   0.697  41.002  1.00  0.00     0.163 HD
ATOM   7583  CA  THR A 503      15.489   1.512  39.103  1.00 10.94     0.181 C
ATOM   7585  C   THR A 503      14.920   0.558  38.064  1.00 11.38     0.241 C
ATOM   7586  O   THR A 503      14.232   0.973  37.134  1.00 10.52    -0.271 OA
ATOM   7587  CB  THR A 503      16.976   1.751  38.814  1.00  9.77     0.075 C
ATOM   7590  CG  THR A 503      17.321   3.209  38.834  1.00  9.33    -0.028 A
ATOM   7591  CD1 THR A 503      18.021   3.859  39.805  1.00 11.59     0.096 A
ATOM   7593  CD2 THR A 503      16.989   4.178  37.837  1.00 11.99    -0.002 A
ATOM   7594  CE2 THR A 503      17.500   5.408  38.250  1.00 11.91     0.042 A
ATOM   7595  CE3 THR A 503      16.303   4.096  36.615  1.00 11.21     0.014 A
ATOM   7597  NE1 THR A 503      18.122   5.205  39.452  1.00 14.20    -0.365 N
ATOM   7598  HE1 THR A 503      18.587   5.926  40.004  1.00  0.00     0.165 HD
ATOM   7599  CZ2 THR A 503      17.358   6.581  37.496  1.00 13.37     0.030 A
ATOM   7601  CZ3 THR A 503      16.173   5.256  35.857  1.00 15.30     0.001 A
ATOM   7603  CH2 THR A 503      16.670   6.476  36.300  1.00 12.07     0.002 A
ATOM   7605  N   LYS A 504      15.186  -0.750  38.168  1.00  9.63    -0.346 N
ATOM   7606  HN  LYS A 504      15.778  -1.076  38.932  1.00  0.00     0.163 HD
ATOM   7607  CA  LYS A 504      14.652  -1.724  37.219  1.00 10.89     0.176 C
ATOM   7609  C   LYS A 504      13.136  -1.734  37.254  1.00 10.59     0.241 C
ATOM   7610  O   LYS A 504      12.437  -1.735  36.204  1.00 11.55    -0.271 OA
ATOM   7611  CB  LYS A 504      15.186  -3.158  37.508  1.00  6.90     0.035 C
ATOM   7614  CG  LYS A 504      14.667  -4.152  36.453  1.00 10.81     0.004 C
ATOM   7617  CD  LYS A 504      15.207  -5.559  36.801  1.00 22.22     0.027 C
ATOM   7620  CE  LYS A 504      14.914  -6.542  35.647  1.00 21.83     0.229 C
ATOM   7623  NZ  LYS A 504      13.567  -7.156  35.823  1.00 20.85    -0.079 N
ATOM   7624  HZ1 LYS A 504      13.373  -7.805  35.061  1.00 16.00     0.274 HD
ATOM   7625  HZ2 LYS A 504      12.836  -6.451  35.918  1.00  0.00     0.274 HD
ATOM   7626  HZ3 LYS A 504      13.467  -7.600  36.736  1.00  0.00     0.274 HD
ATOM   7627  N   TYR A 505      12.534  -1.747  38.443  1.00  8.88    -0.346 N
ATOM   7628  HN  TYR A 505      13.102  -1.813  39.287  1.00  0.00     0.163 HD
ATOM   7629  CA  TYR A 505      11.079  -1.669  38.567  1.00  9.46     0.180 C
ATOM   7631  C   TYR A 505      10.542  -0.400  37.887  1.00 11.57     0.241 C
ATOM   7632  O   TYR A 505       9.528  -0.413  37.163  1.00 10.23    -0.271 OA
ATOM   7633  CB  TYR A 505      10.684  -1.618  40.084  1.00  7.63     0.073 C
ATOM   7636  CG  TYR A 505       9.215  -1.775  40.371  1.00  9.36    -0.056 A
ATOM   7637  CD1 TYR A 505       8.670  -3.064  40.523  1.00 14.54     0.010 A
ATOM   7639  CD2 TYR A 505       8.357  -0.696  40.494  1.00 11.31     0.010 A
ATOM   7641  CE1 TYR A 505       7.341  -3.232  40.814  1.00 17.94     0.037 A
ATOM   7643  CE2 TYR A 505       7.013  -0.844  40.776  1.00 15.68     0.037 A
ATOM   7645  CZ  TYR A 505       6.521  -2.121  40.927  1.00 20.36     0.065 A
ATOM   7646  OH  TYR A 505       5.193  -2.311  41.227  1.00 24.19    -0.361 OA
ATOM   7647  HH  TYR A 505       4.631  -1.549  41.304  1.00  0.00     0.217 HD
ATOM   7648  N   GLY A 506      11.205   0.752  38.100  1.00  9.66    -0.351 N
ATOM   7649  HN  GLY A 506      12.045   0.733  38.678  1.00  0.00     0.163 HD
ATOM   7650  CA  GLY A 506      10.771   2.025  37.539  1.00 10.61     0.225 C
ATOM   7653  C   GLY A 506      10.833   2.065  36.015  1.00 11.77     0.236 C
ATOM   7654  O   GLY A 506       9.860   2.546  35.406  1.00 12.27    -0.272 OA
ATOM   7655  N   VAL A 507      11.891   1.549  35.401  1.00  8.81    -0.346 N
ATOM   7656  HN  VAL A 507      12.665   1.137  35.922  1.00  0.00     0.163 HD
ATOM   7657  CA  VAL A 507      11.891   1.603  33.904  1.00  9.86     0.180 C
ATOM   7659  C   VAL A 507      10.909   0.621  33.308  1.00 11.48     0.241 C
ATOM   7660  O   VAL A 507      10.456   0.811  32.178  1.00 13.85    -0.271 OA
ATOM   7661  CB  VAL A 507      13.305   1.411  33.345  1.00 15.51     0.009 C
ATOM   7663  CG1 VAL A 507      14.222   2.495  33.866  1.00 15.20     0.012 C
ATOM   7667  CG2 VAL A 507      13.895   0.049  33.636  1.00 16.99     0.012 C
ATOM   7671  N   GLU A 508      10.610  -0.488  33.980  1.00 10.23    -0.346 N
ATOM   7672  HN  GLU A 508      11.076  -0.661  34.871  1.00  0.00     0.163 HD
ATOM   7673  CA  GLU A 508       9.644  -1.466  33.495  1.00 10.26     0.177 C
ATOM   7675  C   GLU A 508       8.188  -1.119  33.746  1.00 16.07     0.241 C
ATOM   7676  O   GLU A 508       7.311  -1.811  33.240  1.00 16.43    -0.271 OA
ATOM   7677  CB  GLU A 508       9.937  -2.866  34.102  1.00 13.22     0.045 C
ATOM   7680  CG  GLU A 508      11.285  -3.345  33.539  1.00 13.72     0.116 C
ATOM   7683  CD  GLU A 508      11.734  -4.715  34.004  1.00 24.51     0.172 C
ATOM   7684  OE1 GLU A 508      11.186  -5.229  34.999  1.00 21.75    -0.648 OA
ATOM   7685  OE2 GLU A 508      12.643  -5.272  33.351  1.00 29.99    -0.648 OA
ATOM   7686  N   ARG A 509       7.904  -0.177  34.649  1.00 12.46    -0.346 N
ATOM   7687  HN  ARG A 509       8.670   0.309  35.116  1.00  0.00     0.163 HD
ATOM   7688  CA  ARG A 509       6.528   0.177  34.986  1.00 14.23     0.176 C
ATOM   7690  C   ARG A 509       5.921   0.998  33.874  1.00 17.99     0.241 C
ATOM   7691  O   ARG A 509       6.177   2.214  33.759  1.00 22.90    -0.271 OA
ATOM   7692  CB  ARG A 509       6.586   1.010  36.295  1.00 13.93     0.036 C
ATOM   7695  CG  ARG A 509       5.206   1.170  36.853  1.00 19.12     0.023 C
ATOM   7698  CD  ARG A 509       5.137   1.781  38.246  1.00 13.48     0.138 C
ATOM   7701  NE  ARG A 509       3.730   1.689  38.555  1.00 22.62    -0.227 N
ATOM   7702  HE  ARG A 509       3.346   0.754  38.417  1.00  0.00     0.177 HD
ATOM   7703  CZ  ARG A 509       2.851   2.549  38.972  1.00 19.51     0.665 C
ATOM   7704  NH1 ARG A 509       3.137   3.787  39.313  1.00 11.42    -0.235 N
ATOM   7705  1HH1 ARG A 509       4.080   4.167  39.225  1.00  0.00     0.174 HD
ATOM   7706  2HH1 ARG A 509       2.447   4.463  39.641  1.00  0.00     0.174 HD
ATOM   7707  NH2 ARG A 509       1.635   2.059  39.086  1.00 16.63    -0.235 N
ATOM   7708  1HH2 ARG A 509       1.413   1.099  38.822  1.00  0.00     0.174 HD
ATOM   7709  2HH2 ARG A 509       0.945   2.735  39.414  1.00  0.00     0.174 HD
ATOM   7710  N   GLN A 510       5.010   0.413  33.119  1.00 14.97    -0.346 N
ATOM   7711  HN  GLN A 510       4.688  -0.534  33.319  1.00  0.00     0.163 HD
ATOM   7712  CA  GLN A 510       4.472   1.177  31.973  1.00 20.23     0.177 C
ATOM   7714  C   GLN A 510       3.245   2.024  32.255  1.00 19.19     0.241 C
ATOM   7715  O   GLN A 510       2.857   2.811  31.380  1.00 23.74    -0.271 OA
ATOM   7716  CB  GLN A 510       4.066   0.148  30.910  1.00 23.08     0.044 C
ATOM   7719  CG  GLN A 510       5.176  -0.783  30.449  1.00 43.24     0.105 C
ATOM   7722  CD  GLN A 510       6.095  -0.160  29.404  1.00 53.83     0.215 C
ATOM   7723  NE2 GLN A 510       5.624   0.874  28.702  1.00 49.86    -0.370 N
ATOM   7724  1HE2 GLN A 510       4.688   1.255  28.842  1.00  0.00     0.159 HD
ATOM   7725  2HE2 GLN A 510       6.239   1.291  28.003  1.00  0.00     0.159 HD
ATOM   7726  OE1 GLN A 510       7.235  -0.624  29.234  1.00 58.11    -0.274 OA
ATOM   7727  N   ASP A 511       2.537   1.775  33.329  1.00 14.60    -0.346 N
ATOM   7728  HN  ASP A 511       2.895   1.093  33.998  1.00  0.00     0.163 HD
ATOM   7729  CA  ASP A 511       1.268   2.421  33.616  1.00 14.76     0.186 C
ATOM   7731  C   ASP A 511       1.282   3.426  34.751  1.00 11.64     0.241 C
ATOM   7732  O   ASP A 511       0.204   3.728  35.281  1.00 10.72    -0.271 OA
ATOM   7733  CB  ASP A 511       0.267   1.303  34.021  1.00 27.62     0.147 C
ATOM   7736  CG  ASP A 511       0.727   0.495  35.217  1.00 43.28     0.175 C
ATOM   7737  OD1 ASP A 511       1.918   0.439  35.593  1.00 40.85    -0.648 OA
ATOM   7738  OD2 ASP A 511      -0.156  -0.147  35.852  1.00 59.55    -0.648 OA
ATOM   7739  N   GLY A 512       2.458   3.943  35.088  1.00 12.90    -0.351 N
ATOM   7740  HN  GLY A 512       3.313   3.600  34.651  1.00  0.00     0.163 HD
ATOM   7741  CA  GLY A 512       2.520   5.005  36.088  1.00 11.93     0.225 C
ATOM   7744  C   GLY A 512       3.963   5.319  36.454  1.00  9.37     0.238 C
ATOM   7745  O   GLY A 512       4.895   4.639  36.014  1.00 12.10    -0.272 OA
ATOM   7746  N   PRO A 513       4.121   6.396  37.198  1.00  8.22    -0.337 N
ATOM   7747  CA  PRO A 513       5.433   6.935  37.542  1.00  9.72     0.179 C
ATOM   7749  C   PRO A 513       6.014   6.204  38.749  1.00 10.56     0.241 C
ATOM   7750  O   PRO A 513       5.279   5.561  39.528  1.00 10.42    -0.271 OA
ATOM   7751  CB  PRO A 513       5.157   8.398  37.887  1.00 10.10     0.037 C
ATOM   7754  CG  PRO A 513       3.771   8.353  38.459  1.00 11.96     0.022 C
ATOM   7757  CD  PRO A 513       3.025   7.331  37.590  1.00  8.08     0.127 C
ATOM   7760  N   THR A 514       7.338   6.370  38.870  1.00  6.40    -0.344 N
ATOM   7761  HN  THR A 514       7.863   6.915  38.186  1.00  0.00     0.163 HD
ATOM   7762  CA  THR A 514       8.016   5.741  40.024  1.00  7.17     0.205 C
ATOM   7764  C   THR A 514       8.961   6.739  40.688  1.00  7.96     0.243 C
ATOM   7765  O   THR A 514       9.808   7.321  40.001  1.00 10.07    -0.271 OA
ATOM   7766  CB  THR A 514       8.809   4.495  39.580  1.00 12.13     0.146 C
ATOM   7768  CG2 THR A 514       9.420   3.765  40.786  1.00  8.91     0.042 C
ATOM   7772  OG1 THR A 514       7.960   3.571  38.909  1.00 10.74    -0.393 OA
ATOM   7773  HG1 THR A 514       7.582   4.022  38.163  1.00  0.00     0.210 HD
ATOM   7774  N   ALA A 515       8.782   7.002  42.004  1.00  6.43    -0.346 N
ATOM   7775  HN  ALA A 515       8.021   6.577  42.533  1.00  0.00     0.163 HD
ATOM   7776  CA  ALA A 515       9.734   7.929  42.637  1.00  6.23     0.172 C
ATOM   7778  C   ALA A 515      10.768   7.128  43.431  1.00  9.96     0.240 C
ATOM   7779  O   ALA A 515      10.399   6.236  44.184  1.00 12.18    -0.271 OA
ATOM   7780  CB  ALA A 515       9.048   8.907  43.600  1.00 10.03     0.042 C
ATOM   7784  N   LEU A 516      12.037   7.489  43.331  1.00  6.90    -0.346 N
ATOM   7785  HN  LEU A 516      12.290   8.255  42.707  1.00  0.00     0.163 HD
ATOM   7786  CA  LEU A 516      13.084   6.814  44.096  1.00  7.12     0.177 C
ATOM   7788  C   LEU A 516      13.498   7.786  45.198  1.00 10.54     0.241 C
ATOM   7789  O   LEU A 516      13.734   8.958  44.853  1.00  9.80    -0.271 OA
ATOM   7790  CB  LEU A 516      14.307   6.585  43.184  1.00  6.93     0.038 C
ATOM   7793  CG  LEU A 516      13.997   5.677  41.960  1.00 20.63    -0.020 C
ATOM   7795  CD1 LEU A 516      15.246   5.413  41.131  1.00 28.19     0.009 C
ATOM   7799  CD2 LEU A 516      13.332   4.369  42.358  1.00 13.59     0.009 C
ATOM   7803  N   ILE A 517      13.525   7.355  46.426  1.00  7.52    -0.346 N
ATOM   7804  HN  ILE A 517      13.313   6.374  46.608  1.00  0.00     0.163 HD
ATOM   7805  CA  ILE A 517      13.855   8.245  47.577  1.00  8.34     0.180 C
ATOM   7807  C   ILE A 517      15.240   7.874  48.080  1.00 10.05     0.241 C
ATOM   7808  O   ILE A 517      15.471   6.734  48.579  1.00  8.23    -0.271 OA
ATOM   7809  CB  ILE A 517      12.811   7.937  48.654  1.00  8.85     0.013 C
ATOM   7811  CG1 ILE A 517      11.378   8.106  48.087  1.00  8.60     0.002 C
ATOM   7814  CG2 ILE A 517      13.046   8.820  49.896  1.00  8.03     0.012 C
ATOM   7818  CD1 ILE A 517      11.014   9.474  47.500  1.00  8.00     0.005 C
ATOM   7822  N   LEU A 518      16.220   8.723  47.808  1.00 10.25    -0.346 N
ATOM   7823  HN  LEU A 518      15.976   9.665  47.501  1.00  0.00     0.163 HD
ATOM   7824  CA  LEU A 518      17.629   8.376  47.926  1.00 10.53     0.177 C
ATOM   7826  C   LEU A 518      18.396   9.177  48.944  1.00 10.90     0.241 C
ATOM   7827  O   LEU A 518      18.064  10.356  49.166  1.00 11.52    -0.271 OA
ATOM   7828  CB  LEU A 518      18.255   8.544  46.524  1.00  7.75     0.038 C
ATOM   7831  CG  LEU A 518      17.521   7.770  45.413  1.00 10.10    -0.020 C
ATOM   7833  CD1 LEU A 518      18.111   8.164  44.072  1.00 11.54     0.009 C
ATOM   7837  CD2 LEU A 518      17.648   6.243  45.642  1.00  7.61     0.009 C
ATOM   7841  N   SER A 519      19.438   8.556  49.534  1.00  8.09    -0.344 N
ATOM   7842  HN  SER A 519      19.752   7.637  49.222  1.00  0.00     0.163 HD
ATOM   7843  CA  SER A 519      20.101   9.251  50.640  1.00 11.81     0.200 C
ATOM   7845  C   SER A 519      21.294  10.061  50.178  1.00 13.49     0.243 C
ATOM   7846  O   SER A 519      21.849   9.760  49.136  1.00 14.31    -0.271 OA
ATOM   7847  CB  SER A 519      20.626   8.204  51.650  1.00  8.10     0.199 C
ATOM   7850  OG  SER A 519      21.707   7.474  51.010  1.00 12.17    -0.398 OA
ATOM   7852  HG  SER A 519      22.029   6.831  51.630  1.00  0.00     0.209 HD
ATOM   7853  N   ARG A 520      21.681  11.050  50.987  1.00 13.86    -0.346 N
ATOM   7854  HN  ARG A 520      21.119  11.287  51.804  1.00  0.00     0.163 HD
ATOM   7855  CA  ARG A 520      22.903  11.792  50.707  1.00 13.74     0.176 C
ATOM   7857  C   ARG A 520      24.067  10.996  51.281  1.00 15.06     0.241 C
ATOM   7858  O   ARG A 520      25.151  10.978  50.702  1.00 18.90    -0.271 OA
ATOM   7859  CB  ARG A 520      22.843  13.153  51.451  1.00 11.03     0.036 C
ATOM   7862  CG  ARG A 520      24.167  13.912  51.288  1.00 16.52     0.023 C
ATOM   7865  CD  ARG A 520      24.135  15.217  52.075  1.00 23.92     0.138 C
ATOM   7868  NE  ARG A 520      25.306  16.041  51.688  1.00 26.15    -0.227 N
ATOM   7869  HE  ARG A 520      25.468  16.174  50.690  1.00  0.00     0.177 HD
ATOM   7870  CZ  ARG A 520      26.159  16.619  52.514  1.00 36.03     0.665 C
ATOM   7871  NH1 ARG A 520      26.029  16.504  53.832  1.00 29.44    -0.235 N
ATOM   7872  2HH1 ARG A 520      25.260  15.964  54.229  1.00  0.00     0.174 HD
ATOM   7873  NH2 ARG A 520      27.171  17.330  51.992  1.00 29.73    -0.235 N
ATOM   7874  1HH2 ARG A 520      27.830  17.776  52.630  1.00  0.00     0.174 HD
ATOM   7875  2HH2 ARG A 520      27.271  17.418  50.981  1.00  0.00     0.174 HD
ATOM   7876  N   GLN A 521      23.872  10.381  52.448  1.00 15.47    -0.346 N
ATOM   7877  HN  GLN A 521      22.924  10.407  52.825  1.00  0.00     0.163 HD
ATOM   7878  CA  GLN A 521      24.866   9.678  53.239  1.00 14.31     0.177 C
ATOM   7880  C   GLN A 521      25.013   8.201  52.911  1.00 17.68     0.241 C
ATOM   7881  O   GLN A 521      24.116   7.569  52.333  1.00 12.86    -0.271 OA
ATOM   7882  CB  GLN A 521      24.591   9.868  54.755  1.00 15.88     0.044 C
ATOM   7885  CG  GLN A 521      23.553   8.962  55.409  1.00 14.28     0.105 C
ATOM   7888  CD  GLN A 521      22.113   9.378  55.144  1.00 18.40     0.215 C
ATOM   7889  NE2 GLN A 521      21.147   8.767  55.848  1.00 15.05    -0.370 N
ATOM   7890  1HE2 GLN A 521      21.393   8.057  56.538  1.00  0.00     0.159 HD
ATOM   7891  2HE2 GLN A 521      20.182   9.046  55.670  1.00  0.00     0.159 HD
ATOM   7892  OE1 GLN A 521      21.813  10.243  54.303  1.00 14.85    -0.274 OA
ATOM   7893  N   ASN A 522      26.188   7.611  53.238  1.00 15.84    -0.346 N
ATOM   7894  HN  ASN A 522      26.887   8.135  53.765  1.00  0.00     0.163 HD
ATOM   7895  CA  ASN A 522      26.464   6.229  52.843  1.00 13.36     0.185 C
ATOM   7897  C   ASN A 522      25.598   5.215  53.576  1.00 16.03     0.241 C
ATOM   7898  O   ASN A 522      25.317   5.415  54.772  1.00 17.27    -0.271 OA
ATOM   7899  CB  ASN A 522      27.930   5.839  53.130  1.00 13.86     0.137 C
ATOM   7902  CG  ASN A 522      28.898   6.643  52.300  1.00 22.88     0.217 C
ATOM   7903  ND2 ASN A 522      30.114   6.796  52.827  1.00 27.44    -0.370 N
ATOM   7904  1HD2 ASN A 522      30.769   7.340  52.265  1.00  0.00     0.159 HD
ATOM   7905  2HD2 ASN A 522      30.387   6.383  53.719  1.00  0.00     0.159 HD
ATOM   7906  OD1 ASN A 522      28.570   7.139  51.229  1.00 22.44    -0.274 OA
ATOM   7907  N   LEU A 523      25.236   4.144  52.915  1.00 11.62    -0.346 N
ATOM   7908  HN  LEU A 523      25.582   4.029  51.962  1.00  0.00     0.163 HD
ATOM   7909  CA  LEU A 523      24.371   3.110  53.457  1.00 16.04     0.177 C
ATOM   7911  C   LEU A 523      25.087   1.757  53.433  1.00 15.22     0.241 C
ATOM   7912  O   LEU A 523      25.534   1.394  52.362  1.00 14.09    -0.271 OA
ATOM   7913  CB  LEU A 523      23.078   2.967  52.631  1.00 13.69     0.038 C
ATOM   7916  CG  LEU A 523      22.241   4.233  52.406  1.00 14.89    -0.020 C
ATOM   7918  CD1 LEU A 523      20.958   3.961  51.603  1.00 16.93     0.009 C
ATOM   7922  CD2 LEU A 523      21.863   4.875  53.744  1.00 15.82     0.009 C
ATOM   7926  N   ALA A 524      25.106   1.021  54.537  1.00 13.59    -0.346 N
ATOM   7927  HN  ALA A 524      24.693   1.383  55.396  1.00  0.00     0.163 HD
ATOM   7928  CA  ALA A 524      25.718  -0.309  54.527  1.00 16.96     0.172 C
ATOM   7930  C   ALA A 524      24.883  -1.304  53.723  1.00 15.31     0.240 C
ATOM   7931  O   ALA A 524      23.665  -1.266  53.675  1.00 14.59    -0.271 OA
ATOM   7932  CB  ALA A 524      25.855  -0.830  55.958  1.00 21.88     0.042 C
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ATOM   7936  N   GLN A 525      25.536  -2.270  53.093  1.00 14.50    -0.346 N
ATOM   7937  HN  GLN A 525      26.553  -2.311  53.160  1.00  0.00     0.163 HD
ATOM   7938  CA  GLN A 525      24.834  -3.274  52.307  1.00 13.74     0.177 C
ATOM   7940  C   GLN A 525      24.401  -4.458  53.153  1.00 15.38     0.241 C
ATOM   7941  O   GLN A 525      25.199  -4.958  53.943  1.00 16.59    -0.271 OA
ATOM   7942  CB  GLN A 525      25.744  -3.810  51.190  1.00 13.36     0.044 C
ATOM   7945  CG  GLN A 525      25.066  -4.897  50.344  1.00 12.08     0.105 C
ATOM   7948  CD  GLN A 525      25.753  -5.045  48.998  1.00 13.22     0.215 C
ATOM   7949  NE2 GLN A 525      25.993  -6.297  48.581  1.00 16.06    -0.370 N
ATOM   7950 1HE2 GLN A 525      25.713  -7.136  49.089  1.00  0.00     0.159 HD
ATOM   7951 2HE2 GLN A 525      26.454  -6.396  47.677  1.00  0.00     0.159 HD
ATOM   7952  OE1 GLN A 525      26.091  -4.032  48.385  1.00 14.44    -0.274 OA
ATOM   7953  N   GLN A 526      23.216  -4.998  52.926  1.00 11.55    -0.346 N
ATOM   7954  HN  GLN A 526      22.629  -4.607  52.189  1.00  0.00     0.163 HD
ATOM   7955  CA  GLN A 526      22.724  -6.126  53.688  1.00 14.41     0.177 C
ATOM   7957  C   GLN A 526      22.975  -7.422  52.906  1.00 15.31     0.241 C
ATOM   7958  O   GLN A 526      22.993  -7.404  51.687  1.00 15.42    -0.271 OA
ATOM   7959  CB  GLN A 526      21.226  -6.048  53.986  1.00 12.59     0.044 C
ATOM   7962  CG  GLN A 526      20.792  -4.753  54.682  1.00 11.27     0.105 C
ATOM   7965  CD  GLN A 526      21.357  -4.687  56.080  1.00 18.94     0.215 C
ATOM   7966  NE2 GLN A 526      21.678  -3.510  56.629  1.00 21.06    -0.370 N
ATOM   7967 1HE2 GLN A 526      22.060  -3.465  57.574  1.00  0.00     0.159 HD
ATOM   7968 2HE2 GLN A 526      21.545  -2.630  56.132  1.00  0.00     0.159 HD
ATOM   7969  OE1 GLN A 526      21.518  -5.749  56.680  1.00 19.75    -0.274 OA
ATOM   7970  N   GLU A 527      23.195  -8.490  53.667  1.00 16.52    -0.346 N
ATOM   7971  HN  GLU A 527      23.225  -8.383  54.681  1.00  0.00     0.163 HD
ATOM   7972  CA  GLU A 527      23.396  -9.821  53.078  1.00 14.64     0.177 C
ATOM   7974  C   GLU A 527      22.068 -10.425  52.733  1.00 13.55     0.241 C
ATOM   7975  O   GLU A 527      21.089 -10.257  53.475  1.00 15.07    -0.271 OA
ATOM   7976  CB  GLU A 527      23.960 -10.758  54.192  1.00 25.71     0.045 C
ATOM   7979  CG  GLU A 527      25.430 -10.534  54.469  1.00 41.67     0.116 C
ATOM   7982  CD  GLU A 527      25.966 -11.327  55.651  1.00 61.40     0.172 C
ATOM   7983  OE1 GLU A 527      25.211 -11.750  56.559  1.00 63.65    -0.648 OA
ATOM   7984  OE2 GLU A 527      27.204 -11.540  55.692  1.00 66.54    -0.648 OA
ATOM   7985  N   ARG A 528      21.930 -11.126  51.600  1.00  9.48    -0.346 N
ATOM   7986  HN  ARG A 528      22.757 -11.262  51.019  1.00  0.00     0.163 HD
ATOM   7987  CA  ARG A 528      20.697 -11.696  51.154  1.00 12.35     0.176 C
ATOM   7989  C   ARG A 528      20.948 -13.095  50.519  1.00 16.14     0.241 C
ATOM   7990  O   ARG A 528      21.954 -13.202  49.819  1.00 15.36    -0.271 OA
ATOM   7991  CB  ARG A 528      20.120 -10.816  50.012  1.00 13.64     0.036 C
ATOM   7994  CG  ARG A 528      19.608  -9.469  50.565  1.00 12.39     0.023 C
ATOM   7997  CD  ARG A 528      18.847  -8.680  49.503  1.00 11.90     0.138 C
ATOM   8000  NE  ARG A 528      18.528  -7.375  50.175  1.00  9.68    -0.227 N
ATOM   8001  HE  ARG A 528      17.607  -7.260  50.599  1.00  0.00     0.177 HD
ATOM   8002  CZ  ARG A 528      19.382  -6.367  50.244  1.00 10.34     0.665 C
ATOM   8003  NH1 ARG A 528      20.609  -6.447  49.731  1.00  9.95    -0.235 N
ATOM   8004 1HH1 ARG A 528      21.267  -5.670  49.784  1.00  0.00     0.174 HD
ATOM   8005 2HH1 ARG A 528      20.889  -7.281  49.215  1.00  0.00     0.174 HD
ATOM   8006  NH2 ARG A 528      19.010  -5.259  50.929  1.00 10.23    -0.235 N
ATOM   8007 1HH2 ARG A 528      19.668  -4.482  50.982  1.00  0.00     0.174 HD
ATOM   8008 2HH2 ARG A 528      18.071  -5.198  51.322  1.00  0.00     0.174 HD
ATOM   8009  N   THR A 529      20.012 -14.017  50.716  1.00 15.74    -0.344 N
ATOM   8010  HN  THR A 529      19.241 -13.850  51.362  1.00  0.00     0.163 HD
ATOM   8011  CA  THR A 529      20.117 -15.287  49.977  1.00 20.39     0.205 C
ATOM   8013  C   THR A 529      19.529 -15.007  48.602  1.00 23.35     0.243 C
ATOM   8014  O   THR A 529      18.946 -13.950  48.355  1.00 18.74    -0.271 OA
ATOM   8015  CB  THR A 529      19.253 -16.366  50.636  1.00 19.67     0.146 C
ATOM   8017  CG2 THR A 529      19.686 -16.691  52.056  1.00 16.18     0.042 C
ATOM   8021  OG1 THR A 529      17.897 -15.868  50.691  1.00 16.71    -0.393 OA
ATOM   8022  HG1 THR A 529      17.361 -16.537  51.100  1.00  0.00     0.210 HD
ATOM   8023  N   GLU A 530      19.567 -15.972  47.683  1.00 16.99    -0.346 N
ATOM   8024  HN  GLU A 530      20.021 -16.856  47.912  1.00  0.00     0.163 HD
ATOM   8025  CA  GLU A 530      18.978 -15.801  46.360  1.00 16.98     0.177 C
ATOM   8027  C   GLU A 530      17.474 -15.559  46.442  1.00 14.57     0.241 C
ATOM   8028  O   GLU A 530      16.912 -14.852  45.606  1.00 15.17    -0.271 OA
ATOM   8029  CB  GLU A 530      19.181 -17.115  45.584  1.00 29.71     0.045 C
ATOM   8032  CG  GLU A 530      19.195 -17.061  44.076  1.00 53.99     0.116 C
ATOM   8035  CD  GLU A 530      19.681 -18.416  43.548  1.00 62.01     0.172 C
ATOM   8036  OE1 GLU A 530      20.897 -18.688  43.673  1.00 69.23    -0.648 OA
ATOM   8037  OE2 GLU A 530      18.843 -19.197  43.059  1.00 65.28    -0.648 OA
ATOM   8038  N   GLU A 531      16.785 -16.201  47.372  1.00 15.14    -0.346 N
ATOM   8039  HN  GLU A 531      17.272 -16.858  47.981  1.00  0.00     0.163 HD
ATOM   8040  CA  GLU A 531      15.365 -16.002  47.553  1.00 15.67     0.177 C
ATOM   8042  C   GLU A 531      15.036 -14.577  48.034  1.00 17.35     0.241 C
ATOM   8043  O   GLU A 531      14.020 -14.019  47.604  1.00 14.78    -0.271 OA
ATOM   8044  CB  GLU A 531      14.775 -17.008  48.545  1.00 23.96     0.045 C
ATOM   8047  CG  GLU A 531      13.297 -16.786  48.793  1.00 32.50     0.116 C
ATOM   8050  CD  GLU A 531      12.684 -17.606  49.903  1.00 47.57     0.172 C
ATOM   8051  OE1 GLU A 531      13.281 -17.870  50.964  1.00 34.88    -0.648 OA
ATOM   8052  OE2 GLU A 531      11.511 -18.003  49.725  1.00 50.20    -0.648 OA
ATOM   8053  N   GLN A 532      15.777 -14.057  48.997  1.00 12.88    -0.346 N
ATOM   8054  HN  GLN A 532      16.507 -14.618  49.437  1.00  0.00     0.163 HD
ATOM   8055  CA  GLN A 532      15.551 -12.666  49.438  1.00 14.03     0.177 C
ATOM   8057  C   GLN A 532      15.838 -11.680  48.319  1.00 17.93     0.241 C
ATOM   8058  O   GLN A 532      15.122 -10.674  48.101  1.00 15.53    -0.271 OA
ATOM   8059  CB  GLN A 532      16.487 -12.317  50.621  1.00 11.90     0.044 C
ATOM   8062  CG  GLN A 532      16.091 -13.181  51.824  1.00 12.39     0.105 C
ATOM   8065  CD  GLN A 532      17.099 -13.070  52.968  1.00 15.96     0.215 C
ATOM   8066  NE2 GLN A 532      16.546 -12.897  54.158  1.00 19.74    -0.370 N
ATOM   8067 1HE2 GLN A 532      15.541 -12.873  54.333  1.00  0.00     0.159 HD
ATOM   8068 2HE2 GLN A 532      17.219 -12.823  54.921  1.00  0.00     0.159 HD
ATOM   8069  OE1 GLN A 532      18.292 -13.098  52.760  1.00 17.77    -0.274 OA
ATOM   8070  N   LEU A 533      16.922 -11.931  47.597  1.00 14.69    -0.346 N
ATOM   8071  HN  LEU A 533      17.516 -12.731  47.814  1.00  0.00     0.163 HD
ATOM   8072  CA  LEU A 533      17.255 -11.030  46.470  1.00 13.82     0.177 C
ATOM   8074  C   LEU A 533      16.107 -10.947  45.475  1.00 16.27     0.241 C
ATOM   8075  O   LEU A 533      15.741  -9.865  44.973  1.00 12.45    -0.271 OA
ATOM   8076  CB  LEU A 533      18.536 -11.530  45.853  1.00 15.06     0.038 C
ATOM   8079  CG  LEU A 533      19.211 -10.796  44.706  1.00 25.75    -0.020 C
ATOM   8081  CD1 LEU A 533      19.637  -9.404  45.115  1.00 19.68     0.009 C
ATOM   8085  CD2 LEU A 533      20.437 -11.637  44.296  1.00 23.38     0.009 C
ATOM   8089  N   ALA A 534      15.494 -12.075  45.125  1.00 12.37    -0.346 N
ATOM   8090  HN  ALA A 534      15.836 -12.966  45.484  1.00  0.00     0.163 HD
ATOM   8091  CA  ALA A 534      14.332 -12.052  44.229  1.00 16.87     0.172 C
ATOM   8093  C   ALA A 534      13.122 -11.354  44.855  1.00 20.44     0.240 C
ATOM   8094  O   ALA A 534      12.327 -10.710  44.145  1.00 18.17    -0.271 OA
ATOM   8095  CB  ALA A 534      13.933 -13.485  43.889  1.00 22.40     0.042 C
ATOM   8099  N   ASN A 535      12.910 -11.434  46.172  1.00 11.32    -0.346 N
ATOM   8100  HN  ASN A 535      13.584 -11.937  46.748  1.00  0.00     0.163 HD
ATOM   8101  CA  ASN A 535      11.740 -10.823  46.821  1.00  8.93     0.185 C
ATOM   8103  C   ASN A 535      11.851  -9.308  47.031  1.00 11.42     0.241 C
ATOM   8104  O   ASN A 535      10.869  -8.677  47.495  1.00 11.41    -0.271 OA
ATOM   8105  CB  ASN A 535      11.549 -11.469  48.204  1.00 12.11     0.137 C
ATOM   8108  CG  ASN A 535      10.934 -12.863  48.125  1.00 16.17     0.217 C
ATOM   8109  ND2 ASN A 535      11.044 -13.705  49.143  1.00 17.14    -0.370 N
ATOM   8110 1HD2 ASN A 535      11.562 -13.454  49.985  1.00  0.00     0.159 HD
ATOM   8111 2HD2 ASN A 535      10.633 -14.637  49.090  1.00  0.00     0.159 HD
ATOM   8112  OD1 ASN A 535      10.315 -13.163  47.120  1.00 17.75    -0.274 OA
ATOM   8113  N   ILE A 536      13.010  -8.711  46.730  1.00 11.28    -0.346 N
ATOM   8114  HN  ILE A 536      13.813  -9.252  46.409  1.00  0.00     0.163 HD
ATOM   8115  CA  ILE A 536      13.090  -7.242  46.877  1.00 12.21     0.180 C
ATOM   8117  C   ILE A 536      12.007  -6.599  46.021  1.00 12.33     0.241 C
ATOM   8118  O   ILE A 536      11.284  -5.683  46.405  1.00 10.75    -0.271 OA
ATOM   8119  CB  ILE A 536      14.449  -6.656  46.506  1.00  9.91     0.013 C
ATOM   8121  CG1 ILE A 536      15.552  -7.152  47.469  1.00 13.94     0.002 C
ATOM   8124  CG2 ILE A 536      14.462  -5.110  46.491  1.00  7.74     0.012 C
ATOM   8128  CD1 ILE A 536      16.946  -6.866  46.898  1.00 11.71     0.005 C
ATOM   8132  N   ALA A 537      11.810  -7.115  44.806  1.00 10.86    -0.346 N
ATOM   8133  HN  ALA A 537      12.370  -7.914  44.508  1.00  0.00     0.163 HD
ATOM   8134  CA  ALA A 537      10.810  -6.564  43.890  1.00 15.12     0.172 C
ATOM   8136  C   ALA A 537       9.377  -6.743  44.361  1.00 13.77     0.240 C
ATOM   8137  O   ALA A 537       8.516  -6.109  43.749  1.00 14.74    -0.271 OA
ATOM   8138  CB  ALA A 537      10.938  -7.154  42.483  1.00 19.45     0.042 C
ATOM   8142  N   ARG A 538       9.103  -7.522  45.402  1.00  8.73    -0.346 N
ATOM   8143  HN  ARG A 538       9.859  -8.059  45.828  1.00  0.00     0.163 HD
ATOM   8144  CA  ARG A 538       7.789  -7.633  45.944  1.00  6.72     0.176 C
ATOM   8146  C   ARG A 538       7.540  -6.482  46.933  1.00 10.95     0.240 C
ATOM   8147  O   ARG A 538       6.477  -6.517  47.575  1.00 11.32    -0.271 OA
ATOM   8148  CB  ARG A 538       7.568  -9.000  46.661  1.00  8.96     0.036 C
ATOM   8151  CG  ARG A 538       7.797 -10.083  45.579  1.00 13.51     0.023 C
ATOM   8154  CD  ARG A 538       7.598 -11.504  46.097  1.00 24.62     0.138 C
ATOM   8157  NE  ARG A 538       6.245 -11.916  45.919  1.00 41.64    -0.227 N
ATOM   8158  HE  ARG A 538       5.655 -11.108  45.718  1.00  0.00     0.177 HD
ATOM   8159  CZ  ARG A 538       5.524 -13.009  45.933  1.00 32.48     0.665 C
ATOM   8160  NH1 ARG A 538       5.985 -14.230  46.134  1.00 38.04    -0.235 N
ATOM   8161 1HH1 ARG A 538       6.989 -14.348  46.272  1.00  0.00     0.174 HD
ATOM   8162 2HH1 ARG A 538       5.423 -15.081  46.145  1.00  0.00     0.174 HD
ATOM   8163  NH2 ARG A 538       4.224 -12.856  45.754  1.00 38.94    -0.235 N
ATOM   8164 1HH2 ARG A 538       3.868 -11.913  45.599  1.00  0.00     0.174 HD
ATOM   8165 2HH2 ARG A 538       3.662 -13.707  45.765  1.00  0.00     0.174 HD
ATOM   8166  N   GLY A 539       8.507  -5.577  47.132  1.00 11.12    -0.351 N
ATOM   8167  HN  GLY A 539       9.434  -5.730  46.735  1.00  0.00     0.163 HD
ATOM   8168  CA  GLY A 539       8.242  -4.371  47.914  1.00  8.44     0.225 C
ATOM   8171  C   GLY A 539       8.425  -4.466  49.423  1.00 11.49     0.235 C
ATOM   8172  O   GLY A 539       8.791  -3.491  50.084  1.00  9.65    -0.272 OA
ATOM   8173  N   GLY A 540       8.081  -5.604  49.990  1.00 10.27    -0.351 N
ATOM   8174  HN  GLY A 540       7.631  -6.319  49.419  1.00  0.00     0.163 HD
ATOM   8175  CA  GLY A 540       8.320  -5.886  51.418  1.00  7.92     0.225 C
ATOM   8178  C   GLY A 540       8.808  -7.323  51.527  1.00  9.44     0.236 C
ATOM   8179  O   GLY A 540       8.227  -8.206  50.848  1.00  9.27    -0.272 OA
ATOM   8180  N   TYR A 541       9.831  -7.631  52.342  1.00  9.39    -0.346 N
ATOM   8181  HN  TYR A 541      10.285  -6.903  52.894  1.00  0.00     0.163 HD
ATOM   8182  CA  TYR A 541      10.288  -9.015  52.431  1.00 10.76     0.180 C
ATOM   8184  C   TYR A 541      10.995  -9.221  53.790  1.00 10.53     0.241 C
ATOM   8185  O   TYR A 541      11.413  -8.258  54.438  1.00 10.43    -0.271 OA
ATOM   8186  CB  TYR A 541      11.221  -9.439  51.267  1.00  9.01     0.073 C
ATOM   8189  CG  TYR A 541      12.500  -8.623  51.200  1.00 11.46    -0.056 A
ATOM   8190  CD1 TYR A 541      12.485  -7.299  50.738  1.00  7.53     0.010 A
ATOM   8192  CD2 TYR A 541      13.702  -9.139  51.662  1.00  6.96     0.010 A
ATOM   8194  CE1 TYR A 541      13.621  -6.506  50.723  1.00  7.03     0.037 A
ATOM   8196  CE2 TYR A 541      14.871  -8.384  51.665  1.00  8.90     0.037 A
ATOM   8198  CZ  TYR A 541      14.824  -7.102  51.150  1.00 12.98     0.065 A
ATOM   8199  OH  TYR A 541      15.975  -6.379  51.148  1.00 10.13    -0.361 OA
ATOM   8200  HH  TYR A 541      16.786  -6.781  51.436  1.00  0.00     0.217 HD
ATOM   8201  N   VAL A 542      11.133 -10.502  54.113  1.00  7.95    -0.346 N
ATOM   8202  HN  VAL A 542      10.788 -11.225  53.482  1.00  0.00     0.163 HD
ATOM   8203  CA  VAL A 542      11.779 -10.881  55.373  1.00  6.35     0.180 C
ATOM   8205  C   VAL A 542      13.279 -10.798  55.145  1.00  9.39     0.241 C
ATOM   8206  O   VAL A 542      13.786 -11.572  54.323  1.00 13.29    -0.271 OA
ATOM   8207  CB  VAL A 542      11.358 -12.310  55.803  1.00  9.66     0.009 C
ATOM   8209  CG1 VAL A 542      12.063 -12.690  57.124  1.00 11.90     0.012 C
ATOM   8213  CG2 VAL A 542       9.839 -12.276  56.100  1.00  9.90     0.012 C
ATOM   8217  N   LEU A 543      13.985  -9.963  55.870  1.00  7.03    -0.346 N
ATOM   8218  HN  LEU A 543      13.506  -9.396  56.570  1.00  0.00     0.163 HD
ATOM   8219  CA  LEU A 543      15.439  -9.811  55.715  1.00  9.15     0.177 C
ATOM   8221  C   LEU A 543      16.198 -10.621  56.791  1.00 14.10     0.241 C
ATOM   8222  O   LEU A 543      17.259 -11.162  56.542  1.00 11.51    -0.271 OA
ATOM   8223  CB  LEU A 543      15.800  -8.326  55.864  1.00  9.93     0.038 C
ATOM   8226  CG  LEU A 543      17.285  -7.962  55.750  1.00 10.55    -0.020 C
ATOM   8228  CD1 LEU A 543      17.802  -8.293  54.352  1.00 14.08     0.009 C
ATOM   8232  CD2 LEU A 543      17.490  -6.483  56.097  1.00 14.58     0.009 C
ATOM   8236  N   LYS A 544      15.681 -10.576  58.001  1.00  8.88    -0.346 N
ATOM   8237  HN  LYS A 544      14.859  -9.993  58.159  1.00  0.00     0.163 HD
ATOM   8238  CA  LYS A 544      16.237 -11.331  59.136  1.00 12.00     0.176 C
ATOM   8240  C   LYS A 544      15.077 -12.041  59.823  1.00 12.52     0.241 C
ATOM   8241  O   LYS A 544      13.984 -11.482  59.998  1.00  8.85    -0.271 OA
ATOM   8242  CB  LYS A 544      16.964 -10.443  60.155  1.00 12.54     0.035 C
ATOM   8245  CG  LYS A 544      18.149  -9.645  59.687  1.00 21.48     0.004 C
ATOM   8248  CD  LYS A 544      19.373 -10.499  59.410  1.00 20.33     0.027 C
ATOM   8251  CE  LYS A 544      20.461  -9.649  58.761  1.00 37.72     0.229 C
ATOM   8254  NZ  LYS A 544      21.641 -10.450  58.292  1.00 32.51    -0.079 N
ATOM   8255  HZ1 LYS A 544      22.368  -9.882  57.858  1.00  0.00     0.274 HD
ATOM   8256  HZ2 LYS A 544      21.345 -11.199  57.666  1.00  0.00     0.274 HD
ATOM   8257  HZ3 LYS A 544      22.025 -11.009  59.054  1.00  0.00     0.274 HD
ATOM   8258  N   ASP A 545      15.268 -13.301  60.286  1.00 10.81    -0.346 N
ATOM   8259  HN  ASP A 545      16.176 -13.755  60.185  1.00  0.00     0.163 HD
ATOM   8260  CA  ASP A 545      14.159 -14.003  60.932  1.00 11.70     0.186 C
ATOM   8262  C   ASP A 545      14.618 -14.880  62.095  1.00 16.87     0.241 C
ATOM   8263  O   ASP A 545      15.820 -15.028  62.290  1.00 20.94    -0.271 OA
ATOM   8264  CB  ASP A 545      13.461 -14.845  59.837  1.00 15.23     0.147 C
ATOM   8267  CG  ASP A 545      12.006 -15.118  60.157  1.00 12.56     0.175 C
ATOM   8268  OD1 ASP A 545      11.353 -14.599  61.075  1.00 13.44    -0.648 OA
ATOM   8269  OD2 ASP A 545      11.365 -15.897  59.437  1.00 19.91    -0.648 OA
ATOM   8270  N   CYS A 546      13.700 -15.352  62.903  1.00 14.47    -0.345 N
ATOM   8271  HN  CYS A 546      12.732 -15.070  62.745  1.00  0.00     0.163 HD
ATOM   8272  CA  CYS A 546      13.980 -16.264  64.025  1.00 14.69     0.186 C
ATOM   8274  C   CYS A 546      13.388 -17.633  63.654  1.00 17.51     0.241 C
ATOM   8275  O   CYS A 546      12.610 -17.713  62.692  1.00 13.05    -0.271 OA
ATOM   8276  CB  CYS A 546      13.111 -15.735  65.194  1.00 16.02     0.121 C
ATOM   8279  SG  CYS A 546      11.308 -15.481  64.758  1.00 22.82    -0.095 SA
ATOM   8280  N   ALA A 547      13.565 -18.650  64.476  1.00 16.93    -0.346 N
ATOM   8281  HN  ALA A 547      14.196 -18.540  65.270  1.00  0.00     0.163 HD
ATOM   8282  CA  ALA A 547      12.875 -19.947  64.281  1.00 14.30     0.172 C
ATOM   8284  C   ALA A 547      11.472 -19.886  64.800  1.00 19.69     0.240 C
ATOM   8285  O   ALA A 547      11.207 -19.309  65.881  1.00 18.91    -0.271 OA
ATOM   8286  CB  ALA A 547      13.729 -20.968  65.095  1.00 19.50     0.042 C
ATOM   8290  N   GLY A 548      10.500 -20.414  64.064  1.00 13.90    -0.351 N
ATOM   8291  HN  GLY A 548      10.741 -20.845  63.171  1.00  0.00     0.163 HD
ATOM   8292  CA  GLY A 548       9.117 -20.403  64.476  1.00 15.65     0.225 C
ATOM   8295  C   GLY A 548       8.501 -19.014  64.242  1.00 17.51     0.236 C
ATOM   8296  O   GLY A 548       8.997 -18.194  63.477  1.00 19.04    -0.272 OA
ATOM   8297  N   GLN A 549       7.365 -18.777  64.857  1.00 17.04    -0.346 N
ATOM   8298  HN  GLN A 549       6.967 -19.470  65.491  1.00  0.00     0.163 HD
ATOM   8299  CA  GLN A 549       6.668 -17.493  64.621  1.00 16.57     0.177 C
ATOM   8301  C   GLN A 549       7.319 -16.391  65.422  1.00 15.00     0.243 C
ATOM   8302  O   GLN A 549       7.545 -16.596  66.616  1.00 14.61    -0.271 OA
ATOM   8303  CB  GLN A 549       5.229 -17.655  65.146  1.00 19.52     0.044 C
ATOM   8306  CG  GLN A 549       4.362 -16.502  64.626  1.00 35.66     0.105 C
ATOM   8309  CD  GLN A 549       2.878 -16.664  64.835  1.00 43.42     0.215 C
ATOM   8310  NE2 GLN A 549       2.126 -16.730  63.733  1.00 46.68    -0.370 N
ATOM   8311 1HE2 GLN A 549       1.122 -16.840  63.874  1.00  0.00     0.159 HD
ATOM   8312 2HE2 GLN A 549       2.513 -16.704  62.790  1.00  0.00     0.159 HD
ATOM   8313  OE1 GLN A 549       2.409 -16.695  65.979  1.00 37.39    -0.274 OA
ATOM   8314  N   PRO A 550       7.584 -15.226  64.873  1.00 17.04    -0.337 N
ATOM   8315  CA  PRO A 550       8.211 -14.158  65.633  1.00 11.43     0.179 C
ATOM   8317  C   PRO A 550       7.310 -13.667  66.754  1.00 10.77     0.241 C
ATOM   8318  O   PRO A 550       6.080 -13.718  66.692  1.00 13.41    -0.271 OA
ATOM   8319  CB  PRO A 550       8.322 -12.983  64.657  1.00 14.28     0.037 C
ATOM   8322  CG  PRO A 550       7.608 -13.409  63.423  1.00 17.25     0.022 C
ATOM   8325  CD  PRO A 550       7.350 -14.884  63.445  1.00 16.61     0.127 C
ATOM   8328  N   GLU A 551       7.900 -13.174  67.834  1.00 11.54    -0.346 N
ATOM   8329  HN  GLU A 551       8.912 -13.266  67.923  1.00  0.00     0.163 HD
ATOM   8330  CA  GLU A 551       7.165 -12.507  68.897  1.00 12.34     0.177 C
ATOM   8332  C   GLU A 551       7.129 -10.983  68.616  1.00 11.34     0.241 C
ATOM   8333  O   GLU A 551       6.415 -10.255  69.280  1.00 12.80    -0.271 OA
ATOM   8334  CB  GLU A 551       8.006 -12.575  70.210  1.00 19.35     0.045 C
ATOM   8337  CG  GLU A 551       7.901 -14.005  70.710  1.00 29.27     0.116 C
ATOM   8340  CD  GLU A 551       8.928 -14.392  71.761  1.00 42.92     0.172 C
ATOM   8341  OE1 GLU A 551      10.065 -13.908  71.909  1.00 20.11    -0.648 OA
ATOM   8342  OE2 GLU A 551       8.512 -15.329  72.500  1.00 52.13    -0.648 OA
ATOM   8343  N   LEU A 552       8.099 -10.505  67.835  1.00 12.66    -0.346 N
ATOM   8344  HN  LEU A 552       8.775 -11.140  67.411  1.00  0.00     0.163 HD
ATOM   8345  CA  LEU A 552       8.189  -9.053  67.588  1.00 10.34     0.177 C
ATOM   8347  C   LEU A 552       8.686  -8.836  66.145  1.00 13.46     0.241 C
ATOM   8348  O   LEU A 552       9.589  -9.557  65.722  1.00 11.34    -0.271 OA
ATOM   8349  CB  LEU A 552       9.264  -8.454  68.505  1.00 13.59     0.038 C
ATOM   8352  CG  LEU A 552       9.509  -6.941  68.222  1.00 22.27    -0.020 C
ATOM   8354  CD1 LEU A 552       8.630  -6.136  69.159  1.00 15.48     0.009 C
ATOM   8358  CD2 LEU A 552      10.971  -6.618  68.388  1.00 32.64     0.009 C
ATOM   8362  N   ILE A 553       8.122  -7.854  65.441  1.00  9.57    -0.346 N
ATOM   8363  HN  ILE A 553       7.403  -7.254  65.844  1.00  0.00     0.163 HD
ATOM   8364  CA  ILE A 553       8.587  -7.675  64.048  1.00  6.44     0.180 C
ATOM   8366  C   ILE A 553       8.971  -6.204  63.882  1.00  8.72     0.241 C
ATOM   8367  O   ILE A 553       8.123  -5.327  64.145  1.00 10.52    -0.271 OA
ATOM   8368  CB  ILE A 553       7.432  -7.977  63.039  1.00 14.12     0.013 C
ATOM   8370  CG1 ILE A 553       7.068  -9.469  63.054  1.00 16.69     0.002 C
ATOM   8373  CG2 ILE A 553       7.863  -7.563  61.622  1.00  9.01     0.012 C
ATOM   8377  CD1 ILE A 553       5.795  -9.833  62.280  1.00 18.17     0.005 C
ATOM   8381  N   PHE A 554      10.167  -5.971  63.375  1.00  8.51    -0.346 N
ATOM   8382  HN  PHE A 554      10.825  -6.743  63.266  1.00  0.00     0.163 HD
ATOM   8383  CA  PHE A 554      10.563  -4.630  62.968  1.00 10.99     0.180 C
ATOM   8385  C   PHE A 554      10.269  -4.433  61.468  1.00 12.81     0.241 C
ATOM   8386  O   PHE A 554      10.567  -5.296  60.640  1.00 12.21    -0.271 OA
ATOM   8387  CB  PHE A 554      12.080  -4.456  63.125  1.00 11.57     0.073 C
ATOM   8390  CG  PHE A 554      12.566  -4.449  64.538  1.00 10.84    -0.056 A
ATOM   8391  CD1 PHE A 554      12.411  -3.318  65.311  1.00 12.11     0.007 A
ATOM   8393  CD2 PHE A 554      13.185  -5.581  65.069  1.00 13.79     0.007 A
ATOM   8395  CE1 PHE A 554      12.836  -3.327  66.659  1.00 10.97     0.001 A
ATOM   8397  CE2 PHE A 554      13.650  -5.564  66.399  1.00 15.40     0.001 A
ATOM   8399  CZ  PHE A 554      13.471  -4.437  67.152  1.00 18.62     0.000 A
ATOM   8401  N   ILE A 555       9.762  -3.242  61.116  1.00  8.26    -0.346 N
ATOM   8402  HN  ILE A 555       9.508  -2.571  61.841  1.00  0.00     0.163 HD
ATOM   8403  CA  ILE A 555       9.565  -2.885  59.699  1.00  7.81     0.180 C
ATOM   8405  C   ILE A 555      10.369  -1.603  59.451  1.00  9.05     0.241 C
ATOM   8406  O   ILE A 555      10.259  -0.669  60.269  1.00  9.12    -0.271 OA
ATOM   8407  CB  ILE A 555       8.087  -2.593  59.408  1.00 10.70     0.013 C
ATOM   8409  CG1 ILE A 555       7.222  -3.804  59.851  1.00 12.92     0.002 C
ATOM   8412  CG2 ILE A 555       7.949  -2.229  57.919  1.00 13.10     0.012 C
ATOM   8416  CD1 ILE A 555       5.745  -3.415  59.993  1.00 20.16     0.005 C
ATOM   8420  N   ALA A 556      11.292  -1.657  58.485  1.00  6.28    -0.346 N
ATOM   8421  HN  ALA A 556      11.399  -2.474  57.883  1.00  0.00     0.163 HD
ATOM   8422  CA  ALA A 556      12.142  -0.470  58.343  1.00  8.85     0.172 C
ATOM   8424  C   ALA A 556      12.350  -0.237  56.857  1.00  6.25     0.240 C
ATOM   8425  O   ALA A 556      12.145  -1.129  56.025  1.00  9.70    -0.271 OA
ATOM   8426  CB  ALA A 556      13.490  -0.662  59.044  1.00  8.96     0.042 C
ATOM   8430  N   THR A 557      12.799   0.984  56.522  1.00  8.84    -0.344 N
ATOM   8431  HN  THR A 557      12.982   1.671  57.254  1.00  0.00     0.163 HD
ATOM   8432  CA  THR A 557      13.029   1.341  55.127  1.00  8.61     0.205 C
ATOM   8434  C   THR A 557      14.332   2.155  55.064  1.00  6.19     0.243 C
ATOM   8435  O   THR A 557      14.746   2.682  56.104  1.00  7.23    -0.271 OA
ATOM   8436  CB  THR A 557      11.947   2.279  54.551  1.00  8.18     0.146 C
ATOM   8438  CG2 THR A 557      10.539   1.697  54.754  1.00  9.60     0.042 C
ATOM   8442  OG1 THR A 557      11.996   3.564  55.201  1.00  8.35    -0.393 OA
ATOM   8443  HG1 THR A 557      12.866   3.924  55.076  1.00  0.00     0.210 HD
ATOM   8444  N   GLY A 558      14.859   2.230  53.865  1.00  7.50    -0.350 N
ATOM   8445  HN  GLY A 558      14.447   1.688  53.106  1.00  0.00     0.163 HD
ATOM   8446  CA  GLY A 558      16.025   3.074  53.590  1.00  7.01     0.225 C
ATOM   8449  C   GLY A 558      17.148   3.018  54.587  1.00  9.17     0.236 C
ATOM   8450  O   GLY A 558      17.601   1.931  55.003  1.00  6.90    -0.272 OA
ATOM   8451  N   SER A 559      17.638   4.202  54.940  1.00  8.54    -0.344 N
ATOM   8452  HN  SER A 559      17.227   5.050  54.550  1.00  0.00     0.163 HD
ATOM   8453  CA  SER A 559      18.764   4.313  55.885  1.00 12.28     0.200 C
ATOM   8455  C   SER A 559      18.473   3.732  57.259  1.00 10.55     0.243 C
ATOM   8456  O   SER A 559      19.404   3.556  58.045  1.00 11.79    -0.271 OA
ATOM   8457  CB  SER A 559      19.216   5.781  55.969  1.00  9.13     0.199 C
ATOM   8460  OG  SER A 559      18.122   6.641  56.322  1.00 10.05    -0.398 OA
ATOM   8461  HG  SER A 559      18.401   7.548  56.374  1.00  0.00     0.209 HD
ATOM   8462  N   GLU A 560      17.236   3.465  57.665  1.00  7.26    -0.346 N
ATOM   8463  HN  GLU A 560      16.467   3.659  57.024  1.00  0.00     0.163 HD
ATOM   8464  CA  GLU A 560      16.915   2.909  58.977  1.00  9.23     0.177 C
ATOM   8466  C   GLU A 560      16.929   1.390  59.024  1.00  8.79     0.241 C
ATOM   8467  O   GLU A 560      16.839   0.823  60.125  1.00 10.53    -0.271 OA
ATOM   8468  CB  GLU A 560      15.549   3.433  59.476  1.00  7.42     0.045 C
ATOM   8471  CG  GLU A 560      15.633   4.881  59.973  1.00  7.65     0.116 C
ATOM   8474  CD  GLU A 560      16.048   5.844  58.888  1.00  9.92     0.172 C
ATOM   8475  OE1 GLU A 560      15.210   6.108  57.985  1.00  9.29    -0.648 OA
ATOM   8476  OE2 GLU A 560      17.201   6.324  58.837  1.00 12.30    -0.648 OA
ATOM   8477  N   VAL A 561      17.079   0.687  57.901  1.00  8.41    -0.346 N
ATOM   8478  HN  VAL A 561      17.142   1.162  57.001  1.00  0.00     0.163 HD
ATOM   8479  CA  VAL A 561      17.153  -0.778  57.973  1.00 11.82     0.180 C
ATOM   8481  C   VAL A 561      18.367  -1.195  58.812  1.00 11.54     0.241 C
ATOM   8482  O   VAL A 561      18.278  -2.138  59.612  1.00 10.78    -0.271 OA
ATOM   8483  CB  VAL A 561      17.198  -1.404  56.564  1.00 11.89     0.009 C
ATOM   8485  CG1 VAL A 561      17.548  -2.884  56.663  1.00 10.62     0.012 C
ATOM   8489  CG2 VAL A 561      15.814  -1.230  55.885  1.00  7.46     0.012 C
ATOM   8493  N   GLU A 562      19.508  -0.523  58.663  1.00 10.66    -0.346 N
ATOM   8494  HN  GLU A 562      19.564   0.238  57.986  1.00  0.00     0.163 HD
ATOM   8495  CA  GLU A 562      20.687  -0.873  59.470  1.00 15.24     0.177 C
ATOM   8497  C   GLU A 562      20.458  -0.770  60.964  1.00 11.89     0.241 C
ATOM   8498  O   GLU A 562      20.842  -1.644  61.763  1.00 15.15    -0.271 OA
ATOM   8499  CB  GLU A 562      21.853   0.041  59.037  1.00 22.11     0.045 C
ATOM   8502  CG  GLU A 562      23.116  -0.283  59.792  1.00 42.27     0.116 C
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ATOM   8505  CD  GLU A 562      24.365   0.419  59.285  1.00 55.83     0.172 C
ATOM   8506  OE1 GLU A 562      24.269   1.476  58.622  1.00 48.05    -0.648 OA
ATOM   8507  OE2 GLU A 562      25.459  -0.134  59.574  1.00 64.19    -0.648 OA
ATOM   8508  N   LEU A 563      19.747   0.225  61.456  1.00  9.95    -0.346 N
ATOM   8509  HN  LEU A 563      19.451   0.947  60.799  1.00  0.00     0.163 HD
ATOM   8510  CA  LEU A 563      19.343   0.395  62.844  1.00 10.31     0.177 C
ATOM   8512  C   LEU A 563      18.437  -0.725  63.292  1.00 13.90     0.241 C
ATOM   8513  O   LEU A 563      18.641  -1.321  64.360  1.00 14.78    -0.271 OA
ATOM   8514  CB  LEU A 563      18.546   1.713  62.911  1.00 13.60     0.038 C
ATOM   8517  CG  LEU A 563      18.421   2.513  64.165  1.00 32.79    -0.020 C
ATOM   8519  CD1 LEU A 563      19.802   2.589  64.815  1.00 23.75     0.009 C
ATOM   8523  CD2 LEU A 563      17.908   3.911  63.779  1.00 20.04     0.009 C
ATOM   8527  N   ALA A 564      17.451  -1.094  62.441  1.00  9.59    -0.346 N
ATOM   8528  HN  ALA A 564      17.321  -0.608  61.554  1.00  0.00     0.163 HD
ATOM   8529  CA  ALA A 564      16.578  -2.201  62.817  1.00 11.81     0.172 C
ATOM   8531  C   ALA A 564      17.362  -3.501  62.933  1.00 13.59     0.240 C
ATOM   8532  O   ALA A 564      17.018  -4.334  63.778  1.00 13.33    -0.271 OA
ATOM   8533  CB  ALA A 564      15.436  -2.432  61.788  1.00  9.08     0.042 C
ATOM   8537  N   VAL A 565      18.276  -3.780  61.992  1.00 11.42    -0.346 N
ATOM   8538  HN  VAL A 565      18.425  -3.129  61.221  1.00  0.00     0.163 HD
ATOM   8539  CA  VAL A 565      19.059  -5.011  62.066  1.00  9.14     0.180 C
ATOM   8541  C   VAL A 565      19.910  -4.987  63.352  1.00 13.58     0.241 C
ATOM   8542  O   VAL A 565      20.044  -6.022  64.016  1.00 11.20    -0.271 OA
ATOM   8543  CB  VAL A 565      19.942  -5.183  60.835  1.00  9.69     0.009 C
ATOM   8545  CG1 VAL A 565      20.905  -6.382  61.012  1.00 12.85     0.012 C
ATOM   8549  CG2 VAL A 565      19.062  -5.432  59.568  1.00  8.42     0.012 C
ATOM   8553  N   ALA A 566      20.516  -3.869  63.730  1.00 12.78    -0.346 N
ATOM   8554  HN  ALA A 566      20.443  -3.030  63.154  1.00  0.00     0.163 HD
ATOM   8555  CA  ALA A 566      21.292  -3.837  64.977  1.00 14.73     0.172 C
ATOM   8557  C   ALA A 566      20.406  -4.064  66.178  1.00 17.36     0.240 C
ATOM   8558  O   ALA A 566      20.814  -4.729  67.162  1.00 15.63    -0.271 OA
ATOM   8559  CB  ALA A 566      22.047  -2.493  65.091  1.00 17.56     0.042 C
ATOM   8563  N   ALA A 567      19.178  -3.543  66.205  1.00 11.68    -0.346 N
ATOM   8564  HN  ALA A 567      18.880  -2.948  65.432  1.00  0.00     0.163 HD
ATOM   8565  CA  ALA A 567      18.251  -3.791  67.294  1.00 15.11     0.172 C
ATOM   8567  C   ALA A 567      17.833  -5.263  67.351  1.00 18.09     0.240 C
ATOM   8568  O   ALA A 567      17.658  -5.876  68.436  1.00 13.34    -0.271 OA
ATOM   8569  CB  ALA A 567      17.030  -2.871  67.220  1.00 16.50     0.042 C
ATOM   8573  N   TYR A 568      17.653  -5.910  66.198  1.00 12.23    -0.346 N
ATOM   8574  HN  TYR A 568      17.752  -5.388  65.327  1.00  0.00     0.163 HD
ATOM   8575  CA  TYR A 568      17.322  -7.323  66.124  1.00 11.56     0.180 C
ATOM   8577  C   TYR A 568      18.459  -8.158  66.740  1.00 13.08     0.241 C
ATOM   8578  O   TYR A 568      18.188  -9.123  67.466  1.00 12.35    -0.271 OA
ATOM   8579  CB  TYR A 568      17.113  -7.680  64.630  1.00 10.73     0.073 C
ATOM   8582  CG  TYR A 568      17.295  -9.129  64.268  1.00 11.48    -0.056 A
ATOM   8583  CD1 TYR A 568      18.545  -9.625  63.914  1.00 15.28     0.010 A
ATOM   8585  CD2 TYR A 568      16.190 -10.003  64.283  1.00 11.13     0.010 A
ATOM   8587  CE1 TYR A 568      18.700 -10.962  63.586  1.00 19.33     0.037 A
ATOM   8589  CE2 TYR A 568      16.358 -11.335  63.970  1.00 12.23     0.037 A
ATOM   8591  CZ  TYR A 568      17.603 -11.792  63.618  1.00 17.65     0.065 A
ATOM   8592  OH  TYR A 568      17.764 -13.130  63.313  1.00 19.52    -0.361 OA
ATOM   8593  HH  TYR A 568      18.626 -13.446  63.069  1.00  0.00     0.217 HD
ATOM   8594  N   GLU A 569      19.706  -7.793  66.432  1.00 12.50    -0.346 N
ATOM   8595  HN  GLU A 569      19.872  -6.993  65.822  1.00  0.00     0.163 HD
ATOM   8596  CA  GLU A 569      20.833  -8.551  66.978  1.00 16.81     0.177 C
ATOM   8598  C   GLU A 569      20.847  -8.435  68.505  1.00 17.76     0.241 C
ATOM   8599  O   GLU A 569      21.121  -9.467  69.127  1.00 18.66    -0.271 OA
ATOM   8600  CB  GLU A 569      22.164  -8.026  66.452  1.00 16.21     0.045 C
ATOM   8603  CG  GLU A 569      22.426  -8.320  64.984  1.00 31.34     0.116 C
ATOM   8606  CD  GLU A 569      23.729  -7.703  64.492  1.00 50.17     0.172 C
ATOM   8607  OE1 GLU A 569      24.328  -6.881  65.228  1.00 49.66    -0.648 OA
ATOM   8608  OE2 GLU A 569      24.171  -8.022  63.355  1.00 49.56    -0.648 OA
ATOM   8609  N   LYS A 570      20.551  -7.263  69.068  1.00 13.54    -0.346 N
ATOM   8610  HN  LYS A 570      20.314  -6.452  68.497  1.00  0.00     0.163 HD
ATOM   8611  CA  LYS A 570      20.577  -7.174  70.543  1.00 16.64     0.176 C
ATOM   8613  C   LYS A 570      19.456  -7.948  71.202  1.00 21.25     0.241 C
ATOM   8614  O   LYS A 570      19.608  -8.639  72.222  1.00 19.40    -0.271 OA
ATOM   8615  CB  LYS A 570      20.446  -5.714  71.005  1.00 19.74     0.035 C
ATOM   8618  CG  LYS A 570      21.554  -4.825  70.487  1.00 30.58     0.004 C
ATOM   8621  CD  LYS A 570      22.801  -4.901  71.356  1.00 49.89     0.027 C
ATOM   8624  CE  LYS A 570      23.465  -3.527  71.426  1.00 53.36     0.229 C
ATOM   8627  NZ  LYS A 570      22.599  -2.565  72.165  1.00 65.21    -0.079 N
ATOM   8628  HZ1 LYS A 570      23.042  -1.648  72.212  1.00  0.00     0.274 HD
ATOM   8629  HZ2 LYS A 570      22.350  -2.913  73.091  1.00  0.00     0.274 HD
ATOM   8630  HZ3 LYS A 570      21.662  -2.513  71.765  1.00  0.00     0.274 HD
ATOM   8631  N   LEU A 571      18.252  -7.864  70.607  1.00 13.71    -0.346 N
ATOM   8632  HN  LEU A 571      18.140  -7.323  69.749  1.00  0.00     0.163 HD
ATOM   8633  CA  LEU A 571      17.115  -8.546  71.191  1.00 11.28     0.177 C
ATOM   8635  C   LEU A 571      17.218 -10.062  71.056  1.00 15.45     0.241 C
ATOM   8636  O   LEU A 571      16.795 -10.797  71.943  1.00 17.66    -0.271 OA
ATOM   8637  CB  LEU A 571      15.866  -8.030  70.450  1.00 15.53     0.038 C
ATOM   8640  CG  LEU A 571      15.349  -6.657  70.916  1.00 25.82    -0.020 C
ATOM   8642  CD1 LEU A 571      14.098  -6.329  70.102  1.00 30.32     0.009 C
ATOM   8646  CD2 LEU A 571      15.023  -6.636  72.408  1.00 27.80     0.009 C
ATOM   8650  N   THR A 572      17.725 -10.539  69.909  1.00 13.21    -0.344 N
ATOM   8651  HN  THR A 572      17.983  -9.882  69.173  1.00  0.00     0.163 HD
ATOM   8652  CA  THR A 572      17.920 -11.974  69.678  1.00 13.36     0.205 C
ATOM   8654  C   THR A 572      18.890 -12.507  70.758  1.00 17.64     0.243 C
ATOM   8655  O   THR A 572      18.717 -13.609  71.278  1.00 14.64    -0.271 OA
ATOM   8656  CB  THR A 572      18.560 -12.123  68.266  1.00 15.12     0.146 C
ATOM   8658  CG2 THR A 572      19.111 -13.507  68.070  1.00 27.39     0.042 C
ATOM   8662  OG1 THR A 572      17.473 -11.868  67.304  1.00 21.69    -0.393 OA
ATOM   8663  HG1 THR A 572      17.125 -10.993  67.428  1.00  0.00     0.210 HD
ATOM   8664  N   ALA A 573      19.925 -11.777  71.120  1.00 15.29    -0.346 N
ATOM   8665  HN  ALA A 573      20.075 -10.887  70.645  1.00  0.00     0.163 HD
ATOM   8666  CA  ALA A 573      20.886 -12.175  72.181  1.00 18.96     0.172 C
ATOM   8668  C   ALA A 573      20.250 -12.214  73.555  1.00 20.46     0.240 C
ATOM   8669  O   ALA A 573      20.707 -12.930  74.485  1.00 18.62    -0.271 OA
ATOM   8670  CB  ALA A 573      22.104 -11.266  72.088  1.00 19.35     0.042 C
ATOM   8674  N   GLU A 574      19.119 -11.550  73.817  1.00 15.90    -0.346 N
ATOM   8675  HN  GLU A 574      18.760 -10.934  73.087  1.00  0.00     0.163 HD
ATOM   8676  CA  GLU A 574      18.363 -11.629  75.042  1.00 18.09     0.177 C
ATOM   8678  C   GLU A 574      17.313 -12.735  74.971  1.00 22.37     0.240 C
ATOM   8679  O   GLU A 574      16.440 -12.822  75.846  1.00 24.23    -0.271 OA
ATOM   8680  CB  GLU A 574      17.621 -10.316  75.371  1.00 22.10     0.045 C
ATOM   8683  CG  GLU A 574      18.655  -9.227  75.631  1.00 24.03     0.116 C
ATOM   8686  CD  GLU A 574      18.122  -7.902  76.100  1.00 30.04     0.172 C
ATOM   8687  OE1 GLU A 574      16.912  -7.799  76.373  1.00 34.02    -0.648 OA
ATOM   8688  OE2 GLU A 574      18.950  -6.973  76.209  1.00 29.10    -0.648 OA
ATOM   8689  N   GLY A 575      17.283 -13.489  73.881  1.00 18.84    -0.351 N
ATOM   8690  HN  GLY A 575      17.959 -13.304  73.140  1.00  0.00     0.163 HD
ATOM   8691  CA  GLY A 575      16.326 -14.568  73.698  1.00 20.55     0.225 C
ATOM   8694  C   GLY A 575      14.980 -14.226  73.097  1.00 23.90     0.236 C
ATOM   8695  O   GLY A 575      14.025 -15.018  73.178  1.00 23.38    -0.272 OA
ATOM   8696  N   VAL A 576      14.766 -13.041  72.536  1.00 16.53    -0.346 N
ATOM   8697  HN  VAL A 576      15.518 -12.352  72.504  1.00  0.00     0.163 HD
ATOM   8698  CA  VAL A 576      13.440 -12.713  71.955  1.00 13.25     0.180 C
ATOM   8700  C   VAL A 576      13.404 -13.303  70.540  1.00 13.98     0.241 C
ATOM   8701  O   VAL A 576      14.453 -13.162  69.895  1.00 11.46    -0.271 OA
ATOM   8702  CB  VAL A 576      13.283 -11.180  71.872  1.00 22.04     0.009 C
ATOM   8704  CG1 VAL A 576      11.937 -10.726  71.277  1.00 18.29     0.012 C
ATOM   8708  CG2 VAL A 576      13.420 -10.634  73.305  1.00 21.58     0.012 C
ATOM   8712  N   LYS A 577      12.266 -13.792  70.083  1.00 10.69    -0.346 N
ATOM   8713  HN  LYS A 577      11.445 -13.841  70.686  1.00  0.00     0.163 HD
ATOM   8714  CA  LYS A 577      12.199 -14.261  68.703  1.00  8.36     0.176 C
ATOM   8716  C   LYS A 577      11.811 -13.059  67.819  1.00 14.03     0.241 C
ATOM   8717  O   LYS A 577      10.657 -12.659  67.910  1.00 13.93    -0.271 OA
ATOM   8718  CB  LYS A 577      11.050 -15.267  68.587  1.00 11.94     0.035 C
ATOM   8721  CG  LYS A 577      11.497 -16.653  69.154  1.00 21.70     0.004 C
ATOM   8724  CD  LYS A 577      10.394 -17.609  68.684  1.00 31.51     0.027 C
ATOM   8727  CE  LYS A 577      10.538 -19.046  69.151  1.00 41.08     0.229 C
ATOM   8730  NZ  LYS A 577      11.738 -19.720  68.587  1.00 38.30    -0.079 N
ATOM   8731  HZ1 LYS A 577      11.835 -20.686  68.901  1.00  0.00     0.274 HD
ATOM   8732  HZ2 LYS A 577      12.584 -19.185  68.786  1.00  0.00     0.274 HD
ATOM   8733  HZ3 LYS A 577      11.742 -19.665  67.568  1.00  0.00     0.274 HD
ATOM   8734  N   ALA A 578      12.742 -12.455  67.138  1.00 12.68    -0.346 N
ATOM   8735  HN  ALA A 578      13.695 -12.819  67.126  1.00  0.00     0.163 HD
ATOM   8736  CA  ALA A 578      12.395 -11.231  66.381  1.00  9.11     0.172 C
ATOM   8738  C   ALA A 578      12.585 -11.460  64.885  1.00  9.26     0.240 C
ATOM   8739  O   ALA A 578      13.340 -12.347  64.478  1.00 13.18    -0.271 OA
ATOM   8740  CB  ALA A 578      13.375 -10.127  66.817  1.00  9.53     0.042 C
ATOM   8744  N   ARG A 579      12.021 -10.539  64.085  1.00  9.61    -0.346 N
ATOM   8745  HN  ARG A 579      11.504  -9.766  64.503  1.00  0.00     0.163 HD
ATOM   8746  CA  ARG A 579      12.131 -10.619  62.639  1.00  7.97     0.176 C
ATOM   8748  C   ARG A 579      12.361  -9.173  62.142  1.00 11.35     0.241 C
ATOM   8749  O   ARG A 579      11.844  -8.226  62.743  1.00 11.34    -0.271 OA
ATOM   8750  CB  ARG A 579      10.765 -11.123  62.109  1.00  7.45     0.036 C
ATOM   8753  CG  ARG A 579      10.645 -10.926  60.560  1.00 12.32     0.023 C
ATOM   8756  CD  ARG A 579       9.268 -11.447  60.091  1.00  9.62     0.138 C
ATOM   8759  NE  ARG A 579       9.332 -12.951  60.052  1.00  8.45    -0.227 N
ATOM   8760  HE  ARG A 579      10.140 -13.427  60.454  1.00  0.00     0.177 HD
ATOM   8761  CZ  ARG A 579       8.364 -13.668  59.508  1.00 15.61     0.665 C
ATOM   8762  NH1 ARG A 579       7.285 -13.069  59.013  1.00 10.33    -0.235 N
ATOM   8763 1HH1 ARG A 579       7.305 -12.051  59.081  1.00  0.00     0.174 HD
ATOM   8764 2HH1 ARG A 579       6.538 -13.622  58.593  1.00  0.00     0.174 HD
ATOM   8765  NH2 ARG A 579       8.338 -14.996  59.419  1.00 13.19    -0.235 N
ATOM   8766 1HH2 ARG A 579       9.166 -15.455  59.799  1.00  0.00     0.174 HD
ATOM   8767 2HH2 ARG A 579       7.591 -15.549  58.999  1.00  0.00     0.174 HD
ATOM   8768  N   VAL A 580      13.071  -8.974  61.053  1.00  8.97    -0.346 N
ATOM   8769  HN  VAL A 580      13.544  -9.767  60.619  1.00  0.00     0.163 HD
ATOM   8770  CA  VAL A 580      13.202  -7.653  60.448  1.00  5.63     0.180 C
ATOM   8772  C   VAL A 580      12.621  -7.759  59.004  1.00  8.76     0.241 C
ATOM   8773  O   VAL A 580      13.038  -8.630  58.252  1.00  9.25    -0.271 OA
ATOM   8774  CB  VAL A 580      14.670  -7.203  60.307  1.00 10.56     0.009 C
ATOM   8776  CG1 VAL A 580      14.755  -5.890  59.488  1.00 12.26     0.012 C
ATOM   8780  CG2 VAL A 580      15.333  -7.066  61.694  1.00  9.82     0.012 C
ATOM   8784  N   VAL A 581      11.726  -6.853  58.684  1.00  7.30    -0.346 N
ATOM   8785  HN  VAL A 581      11.433  -6.176  59.388  1.00  0.00     0.163 HD
ATOM   8786  CA  VAL A 581      11.138  -6.788  57.347  1.00  8.55     0.180 C
ATOM   8788  C   VAL A 581      11.687  -5.526  56.694  1.00 10.14     0.241 C
ATOM   8789  O   VAL A 581      11.583  -4.476  57.319  1.00 10.22    -0.271 OA
ATOM   8790  CB  VAL A 581       9.598  -6.761  57.454  1.00  8.06     0.009 C
ATOM   8792  CG1 VAL A 581       8.907  -6.370  56.152  1.00  6.99     0.012 C
ATOM   8796  CG2 VAL A 581       9.032  -8.146  57.835  1.00  9.41     0.012 C
ATOM   8800  N   SER A 582      12.306  -5.637  55.531  1.00  5.67    -0.344 N
ATOM   8801  HN  SER A 582      12.485  -6.557  55.129  1.00  0.00     0.163 HD
ATOM   8802  CA  SER A 582      12.732  -4.426  54.826  1.00  8.19     0.200 C
ATOM   8804  C   SER A 582      11.537  -4.078  53.942  1.00  7.48     0.243 C
ATOM   8805  O   SER A 582      11.019  -4.998  53.268  1.00  8.75    -0.271 OA
ATOM   8806  CB  SER A 582      13.963  -4.692  53.978  1.00  8.70     0.199 C
ATOM   8809  OG  SER A 582      14.321  -3.548  53.202  1.00 10.90    -0.398 OA
ATOM   8810  HG  SER A 582      15.091  -3.714  52.671  1.00  0.00     0.209 HD
ATOM   8811  N   MET A 583      11.120  -2.804  53.862  1.00  4.82    -0.346 N
ATOM   8812  HN  MET A 583      11.617  -2.069  54.364  1.00  0.00     0.163 HD
ATOM   8813  CA  MET A 583       9.951  -2.478  53.052  1.00  7.55     0.177 C
ATOM   8815  C   MET A 583      10.319  -1.321  52.112  1.00  5.90     0.243 C
ATOM   8816  O   MET A 583       9.799  -0.200  52.270  1.00  9.42    -0.271 OA
ATOM   8817  CB  MET A 583       8.780  -2.116  53.986  1.00  8.69     0.045 C
ATOM   8820  CG AMET A 583       7.454  -1.669  53.364  0.50  2.23     0.076 C
ATOM   8823  SD AMET A 583       6.422  -3.073  52.949  0.50  9.70    -0.173 SA
ATOM   8824  CE AMET A 583       6.167  -3.840  54.561  0.50  7.48     0.089 C
ATOM   8828  N   PRO A 584      11.097  -1.585  51.076  1.00  8.28    -0.337 N
ATOM   8829  CA  PRO A 584      11.477  -0.526  50.147  1.00  9.43     0.179 C
ATOM   8831  C   PRO A 584      10.261   0.083  49.460  1.00 10.29     0.241 C
ATOM   8832  O   PRO A 584      10.327   1.272  49.103  1.00 11.65    -0.271 OA
ATOM   8833  CB  PRO A 584      12.507  -1.169  49.217  1.00  8.94     0.037 C
ATOM   8836  CG  PRO A 584      12.232  -2.651  49.275  1.00  8.03     0.022 C
ATOM   8839  CD  PRO A 584      11.785  -2.851  50.728  1.00  8.08     0.127 C
ATOM   8842  N   SER A 585       9.215  -0.698  49.151  1.00  6.48    -0.344 N
ATOM   8843  HN  SER A 585       9.230  -1.699  49.346  1.00  0.00     0.163 HD
ATOM   8844  CA  SER A 585       8.039  -0.060  48.518  1.00 11.22     0.200 C
ATOM   8846  C   SER A 585       6.743  -0.547  49.168  1.00  9.30     0.243 C
ATOM   8847  O   SER A 585       6.382  -1.725  48.985  1.00  7.95    -0.271 OA
ATOM   8848  CB  SER A 585       7.984  -0.421  47.010  1.00  7.84     0.199 C
ATOM   8851  OG  SER A 585       6.757   0.098  46.455  1.00  9.32    -0.398 OA
ATOM   8852  HG  SER A 585       6.723  -0.123  45.532  1.00  0.00     0.209 HD
ATOM   8853  N   THR A 586       6.012   0.297  49.864  1.00  7.65    -0.344 N
ATOM   8854  HN  THR A 586       6.347   1.248  50.017  1.00  0.00     0.163 HD
ATOM   8855  CA  THR A 586       4.717  -0.116  50.424  1.00  9.12     0.205 C
ATOM   8857  C   THR A 586       3.721  -0.416  49.316  1.00 12.61     0.243 C
ATOM   8858  O   THR A 586       2.896  -1.307  49.493  1.00  8.57    -0.271 OA
ATOM   8859  CB  THR A 586       4.122   1.009  51.325  1.00 11.45     0.146 C
ATOM   8861  CG2 THR A 586       5.021   1.243  52.526  1.00  8.64     0.042 C
ATOM   8865  OG1 THR A 586       4.042   2.234  50.527  1.00  8.60    -0.393 OA
ATOM   8866  HG1 THR A 586       3.480   2.088  49.776  1.00  0.00     0.210 HD
ATOM   8867  N   ASP A 587       3.755   0.371  48.208  1.00  8.37    -0.345 N
ATOM   8868  HN  ASP A 587       4.427   1.133  48.117  1.00  0.00     0.163 HD
ATOM   8869  CA  ASP A 587       2.789   0.080  47.154  1.00  9.57     0.186 C
ATOM   8871  C   ASP A 587       3.031  -1.234  46.434  1.00  9.13     0.241 C
ATOM   8872  O   ASP A 587       2.049  -1.967  46.133  1.00  7.20    -0.271 OA
ATOM   8873  CB  ASP A 587       2.699   1.231  46.129  1.00 11.78     0.147 C
ATOM   8876  CG  ASP A 587       4.061   1.532  45.544  1.00  9.54     0.175 C
ATOM   8877  OD1 ASP A 587       4.829   2.260  46.230  1.00  8.23    -0.648 OA
ATOM   8878  OD2 ASP A 587       4.352   0.981  44.464  1.00 12.01    -0.648 OA
ATOM   8879  N   ALA A 588       4.283  -1.612  46.183  1.00  8.58    -0.346 N
ATOM   8880  HN  ALA A 588       5.071  -1.002  46.402  1.00  0.00     0.163 HD
ATOM   8881  CA  ALA A 588       4.495  -2.944  45.576  1.00 10.51     0.172 C
ATOM   8883  C   ALA A 588       4.128  -4.032  46.592  1.00 11.05     0.240 C
ATOM   8884  O   ALA A 588       3.554  -5.039  46.203  1.00  9.68    -0.271 OA
ATOM   8885  CB  ALA A 588       5.962  -3.095  45.158  1.00  5.31     0.042 C
ATOM   8889  N   PHE A 589       4.335  -3.830  47.894  1.00  9.80    -0.346 N
ATOM   8890  HN  PHE A 589       4.767  -2.959  48.203  1.00  0.00     0.163 HD
ATOM   8891  CA  PHE A 589       3.953  -4.838  48.890  1.00 10.97     0.180 C
ATOM   8893  C   PHE A 589       2.447  -5.009  48.965  1.00 11.54     0.241 C
ATOM   8894  O   PHE A 589       1.904  -6.124  49.006  1.00  9.28    -0.271 OA
ATOM   8895  CB  PHE A 589       4.517  -4.446  50.282  1.00  8.64     0.073 C
ATOM   8898  CG  PHE A 589       4.121  -5.435  51.354  1.00 10.67    -0.056 A
ATOM   8899  CD1 PHE A 589       4.773  -6.645  51.437  1.00  7.58     0.007 A
ATOM   8901  CD2 PHE A 589       3.152  -5.109  52.288  1.00 11.56     0.007 A
ATOM   8903  CE1 PHE A 589       4.431  -7.566  52.442  1.00 10.92     0.001 A
ATOM   8905  CE2 PHE A 589       2.792  -6.016  53.292  1.00 12.64     0.001 A
ATOM   8907  CZ  PHE A 589       3.437  -7.269  53.378  1.00  7.79     0.000 A
ATOM   8909  N   ASP A 590       1.699  -3.896  48.976  1.00  6.93    -0.345 N
ATOM   8910  HN  ASP A 590       2.146  -2.980  48.941  1.00  0.00     0.163 HD
ATOM   8911  CA  ASP A 590       0.249  -3.997  49.038  1.00  7.80     0.186 C
ATOM   8913  C   ASP A 590      -0.368  -4.716  47.837  1.00 15.69     0.241 C
ATOM   8914  O   ASP A 590      -1.441  -5.306  47.994  1.00 10.96    -0.271 OA
ATOM   8915  CB  ASP A 590      -0.400  -2.591  49.058  1.00  8.15     0.147 C
ATOM   8918  CG  ASP A 590      -0.193  -1.897  50.391  1.00 16.81     0.175 C
ATOM   8919  OD1 ASP A 590       0.310  -2.480  51.361  1.00 13.04    -0.648 OA
ATOM   8920  OD2 ASP A 590      -0.484  -0.690  50.445  1.00 15.48    -0.648 OA
ATOM   8921  N   LYS A 591       0.265  -4.688  46.693  1.00 10.49    -0.346 N
ATOM   8922  HN  LYS A 591       1.145  -4.176  46.638  1.00  0.00     0.163 HD
ATOM   8923  CA  LYS A 591      -0.227  -5.355  45.488  1.00 14.53     0.176 C
ATOM   8925  C   LYS A 591       0.083  -6.836  45.507  1.00 15.62     0.241 C
ATOM   8926  O   LYS A 591      -0.428  -7.541  44.628  1.00 14.03    -0.271 OA
ATOM   8927  CB  LYS A 591       0.485  -4.711  44.244  1.00 10.31     0.035 C
ATOM   8930  CG  LYS A 591      -0.215  -3.401  43.927  1.00 20.40     0.004 C
ATOM   8933  CD  LYS A 591       0.579  -2.556  42.911  1.00 25.16     0.027 C
ATOM   8936  CE  LYS A 591      -0.016  -1.130  42.934  1.00 31.35     0.229 C
ATOM   8939  NZ  LYS A 591       0.705  -0.262  41.949  1.00 43.42    -0.079 N
ATOM   8940  HZ1 LYS A 591       0.312   0.679  41.964  1.00  0.00     0.274 HD
ATOM   8941  HZ2 LYS A 591       0.703  -0.663  41.011  1.00  0.00     0.274 HD
ATOM   8942  HZ3 LYS A 591       1.713  -0.259  42.106  1.00  0.00     0.274 HD
ATOM   8943  N   GLN A 592       0.918  -7.330  46.429  1.00  7.38    -0.346 N
ATOM   8944  HN  GLN A 592       1.397  -6.707  47.080  1.00  0.00     0.163 HD
ATOM   8945  CA  GLN A 592       1.134  -8.774  46.490  1.00 10.03     0.177 C
ATOM   8947  C   GLN A 592      -0.125  -9.531  46.890  1.00 13.63     0.241 C
ATOM   8948  O   GLN A 592      -1.032  -9.020  47.565  1.00  9.92    -0.271 OA
ATOM   8949  CB  GLN A 592       2.317  -9.121  47.424  1.00 10.51     0.044 C
ATOM   8952  CG  GLN A 592       3.598  -8.396  47.020  1.00 12.62     0.105 C
ATOM   8955  CD  GLN A 592       4.020  -8.677  45.599  1.00 17.17     0.215 C
ATOM   8956  NE2 GLN A 592       4.214  -7.646  44.819  1.00 11.33    -0.370 N
ATOM   8957 1HE2 GLN A 592       4.081  -6.687  45.140  1.00  0.00     0.159 HD
ATOM   8958 2HE2 GLN A 592       4.499  -7.836  43.858  1.00  0.00     0.159 HD
ATOM   8959  OE1 GLN A 592       4.182  -9.841  45.209  1.00 17.15    -0.274 OA
ATOM   8960  N   ASP A 593      -0.139 -10.833  46.598  1.00 11.63    -0.346 N
ATOM   8961  HN  ASP A 593       0.643 -11.283  46.122  1.00  0.00     0.163 HD
ATOM   8962  CA  ASP A 593      -1.338 -11.587  46.997  1.00 12.87     0.186 C
ATOM   8964  C   ASP A 593      -1.418 -11.738  48.521  1.00 15.85     0.241 C
ATOM   8965  O   ASP A 593      -0.434 -11.593  49.218  1.00 12.01    -0.271 OA
ATOM   8966  CB  ASP A 593      -1.444 -12.929  46.325  1.00 21.80     0.147 C
ATOM   8969  CG  ASP A 593      -0.459 -14.016  46.635  1.00 34.64     0.175 C
ATOM   8970  OD1 ASP A 593      -0.005 -14.250  47.769  1.00 28.67    -0.648 OA
ATOM   8971  OD2 ASP A 593      -0.143 -14.748  45.660  1.00 54.95    -0.648 OA
ATOM   8972  N   ALA A 594      -2.598 -12.093  49.010  1.00 15.56    -0.346 N
ATOM   8973  HN  ALA A 594      -3.355 -12.309  48.361  1.00  0.00     0.163 HD
ATOM   8974  CA  ALA A 594      -2.855 -12.186  50.456  1.00 17.79     0.172 C
ATOM   8976  C   ALA A 594      -1.965 -13.181  51.184  1.00 18.03     0.240 C
ATOM   8977  O   ALA A 594      -1.535 -12.900  52.324  1.00 14.13    -0.271 OA
ATOM   8978  CB  ALA A 594      -4.321 -12.500  50.693  1.00 23.17     0.042 C
ATOM   8982  N   ALA A 595      -1.661 -14.308  50.594  1.00 13.66    -0.346 N
ATOM   8983  HN  ALA A 595      -2.058 -14.483  49.671  1.00  0.00     0.163 HD
ATOM   8984  CA  ALA A 595      -0.796 -15.329  51.163  1.00 16.69     0.172 C
ATOM   8986  C   ALA A 595       0.623 -14.797  51.360  1.00 14.18     0.240 C
ATOM   8987  O   ALA A 595       1.158 -15.040  52.435  1.00  9.84    -0.271 OA
ATOM   8988  CB  ALA A 595      -0.707 -16.524  50.218  1.00 14.81     0.042 C
ATOM   8992  N   TYR A 596       1.153 -14.055  50.380  1.00  9.49    -0.346 N
ATOM   8993  HN  TYR A 596       0.629 -13.865  49.525  1.00  0.00     0.163 HD
ATOM   8994  CA  TYR A 596       2.515 -13.519  50.569  1.00 11.15     0.180 C
ATOM   8996  C   TYR A 596       2.516 -12.487  51.705  1.00  8.79     0.241 C
ATOM   8997  O   TYR A 596       3.428 -12.522  52.560  1.00 10.39    -0.271 OA
ATOM   8998  CB  TYR A 596       3.053 -12.879  49.272  1.00 12.77     0.073 C
ATOM   9001  CG  TYR A 596       4.446 -12.301  49.479  1.00 13.27    -0.056 A
ATOM   9002  CD1 TYR A 596       5.537 -13.159  49.475  1.00 14.40     0.010 A
ATOM   9004  CD2 TYR A 596       4.632 -10.932  49.711  1.00 10.64     0.010 A
ATOM   9006  CE1 TYR A 596       6.840 -12.669  49.688  1.00 14.49     0.037 A
ATOM   9008  CE2 TYR A 596       5.924 -10.436  49.901  1.00 10.02     0.037 A
ATOM   9010  CZ  TYR A 596       7.007 -11.322  49.896  1.00 11.49     0.065 A
ATOM   9011  OH  TYR A 596       8.269 -10.837  50.130  1.00  8.89    -0.361 OA
ATOM   9012  HH  TYR A 596       8.385  -9.905  50.274  1.00  0.00     0.217 HD
ATOM   9013  N   ARG A 597       1.549 -11.552  51.735  1.00  8.71    -0.346 N
ATOM   9014  HN  ARG A 597       0.825 -11.563  51.016  1.00  0.00     0.163 HD
ATOM   9015  CA  ARG A 597       1.508 -10.536  52.754  1.00 12.31     0.176 C
ATOM   9017  C   ARG A 597       1.383 -11.157  54.150  1.00  9.30     0.241 C
ATOM   9018  O   ARG A 597       2.073 -10.672  55.048  1.00 11.16    -0.271 OA
ATOM   9019  CB  ARG A 597       0.407  -9.496  52.552  1.00 10.57     0.036 C
ATOM   9022  CG  ARG A 597       0.704  -8.734  51.200  1.00  9.91     0.023 C
ATOM   9025  CD  ARG A 597      -0.294  -7.553  51.180  1.00 16.53     0.138 C
ATOM   9028  NE  ARG A 597      -1.363  -8.005  50.316  1.00 24.05    -0.227 N
ATOM   9029  HE  ARG A 597      -1.115  -8.144  49.337  1.00  0.00     0.177 HD
ATOM   9030  CZ  ARG A 597      -2.617  -8.260  50.633  1.00 28.67     0.665 C
ATOM   9031  NH1 ARG A 597      -3.013  -8.083  51.870  1.00 21.73    -0.235 N
ATOM   9032 1HH1 ARG A 597      -2.377  -7.751  52.595  1.00  0.00     0.174 HD
ATOM   9033 2HH1 ARG A 597      -3.983  -8.280  52.115  1.00  0.00     0.174 HD
ATOM   9034  NH2 ARG A 597      -3.438  -8.689  49.696  1.00 37.10    -0.235 N
ATOM   9035 1HH2 ARG A 597      -3.130  -8.827  48.733  1.00  0.00     0.174 HD
ATOM   9036 2HH2 ARG A 597      -4.408  -8.886  49.941  1.00  0.00     0.174 HD
ATOM   9037  N   GLU A 598       0.540 -12.159  54.311  1.00  9.87    -0.346 N
ATOM   9038  HN  GLU A 598      -0.030 -12.479  53.528  1.00  0.00     0.163 HD
ATOM   9039  CA  GLU A 598       0.423 -12.821  55.640  1.00 10.79     0.177 C
ATOM   9041  C   GLU A 598       1.713 -13.513  56.029  1.00  9.12     0.241 C
ATOM   9042  O   GLU A 598       2.037 -13.605  57.246  1.00 11.78    -0.271 OA
ATOM   9043  CB  GLU A 598      -0.735 -13.834  55.518  1.00 13.93     0.045 C
ATOM   9046  CG  GLU A 598      -0.886 -14.862  56.643  1.00 13.94     0.116 C
ATOM   9049  CD  GLU A 598      -1.195 -14.291  57.995  1.00 19.05     0.172 C
ATOM   9050  OE1 GLU A 598      -1.626 -13.128  58.158  1.00 11.83    -0.648 OA
ATOM   9051  OE2 GLU A 598      -0.979 -14.997  59.021  1.00 14.98    -0.648 OA
ATOM   9052  N   SER A 599       2.480 -14.076  55.087  1.00  9.48    -0.344 N
ATOM   9053  HN  SER A 599       2.199 -14.027  54.108  1.00  0.00     0.163 HD
ATOM   9054  CA  SER A 599       3.714 -14.759  55.453  1.00 10.96     0.200 C
ATOM   9056  C   SER A 599       4.738 -13.742  55.994  1.00 15.56     0.243 C
ATOM   9057  O   SER A 599       5.637 -14.103  56.765  1.00 13.42    -0.271 OA
ATOM   9058  CB  SER A 599       4.374 -15.559  54.355  1.00  9.37     0.199 C
ATOM   9061  OG ASER A 599       4.998 -14.887  53.305  0.50 13.46    -0.398 OA
ATOM   9062  HG ASER A 599       5.413 -15.390  52.614  1.00  0.00     0.209 HD
ATOM   9063  N   VAL A 600       4.773 -12.556  55.410  1.00  7.81    -0.346 N
ATOM   9064  HN  VAL A 600       4.146 -12.359  54.630  1.00  0.00     0.163 HD
ATOM   9065  CA  VAL A 600       5.711 -11.513  55.875  1.00  5.83     0.180 C
ATOM   9067  C   VAL A 600       5.288 -10.807  57.140  1.00  6.54     0.241 C
ATOM   9068  O   VAL A 600       6.114 -10.555  58.062  1.00 10.58    -0.271 OA
ATOM   9069  CB  VAL A 600       5.892 -10.488  54.735  1.00 11.16     0.009 C
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ATOM   9071  CG1 VAL A 600       6.815  -9.341  55.134  1.00 14.04      0.012 C
ATOM   9075  CG2 VAL A 600       6.452 -11.244  53.516  1.00  8.34      0.012 C
ATOM   9079  N   LEU A 601       4.034 -10.447  57.267  1.00  7.75     -0.346 N
ATOM   9080  HN  LEU A 601       3.410 -10.701  56.501  1.00  0.00      0.163 HD
ATOM   9081  CA  LEU A 601       3.435  -9.728  58.375  1.00  8.43      0.177 C
ATOM   9083  C   LEU A 601       2.209 -10.495  58.891  1.00  8.51      0.243 C
ATOM   9084  O   LEU A 601       1.057 -10.166  58.647  1.00  9.65     -0.271 OA
ATOM   9085  CB  LEU A 601       2.958  -8.296  57.977  1.00  9.84      0.038 C
ATOM   9088  CG  LEU A 601       4.097  -7.337  57.618  1.00 17.98     -0.020 C
ATOM   9090  CD1 LEU A 601       3.582  -5.963  57.149  1.00 14.72      0.009 C
ATOM   9094  CD2 LEU A 601       5.010  -7.091  58.827  1.00 14.72      0.009 C
ATOM   9098  N   PRO A 602       2.423 -11.591  59.615  1.00  9.14     -0.337 N
ATOM   9099  CA  PRO A 602       1.345 -12.421  60.092  1.00 12.08      0.179 C
ATOM   9101  C   PRO A 602       0.372 -11.606  60.891  1.00 10.76      0.241 C
ATOM   9102  O   PRO A 602       0.756 -10.939  61.891  1.00 11.49     -0.271 OA
ATOM   9103  CB  PRO A 602       2.029 -13.532  60.902  1.00 12.32      0.037 C
ATOM   9106  CG  PRO A 602       3.470 -13.200  60.958  1.00 18.23      0.022 C
ATOM   9109  CD  PRO A 602       3.764 -12.165  59.929  1.00 13.02      0.127 C
ATOM   9112  N   LYS A 603      -0.927 -11.826  60.686  1.00 12.41     -0.346 N
ATOM   9113  HN  LYS A 603      -1.222 -12.541  60.021  1.00  0.00      0.163 HD
ATOM   9114  CA  LYS A 603      -1.926 -11.024  61.410  1.00 16.35      0.176 C
ATOM   9116  C   LYS A 603      -1.916 -11.336  62.896  1.00 14.74      0.241 C
ATOM   9117  O   LYS A 603      -2.239 -10.490  63.710  1.00 16.51     -0.271 OA
ATOM   9118  CB  LYS A 603      -3.284 -11.222  60.761  1.00 23.85      0.035 C
ATOM   9121  CG  LYS A 603      -4.254 -12.143  61.478  1.00 36.12      0.004 C
ATOM   9124  CD  LYS A 603      -5.563 -12.207  60.676  1.00 52.03      0.027 C
ATOM   9127  CE  LYS A 603      -6.484 -11.052  61.048  1.00 58.66      0.229 C
ATOM   9130  NZ  LYS A 603      -6.632 -10.069  59.937  1.00 66.03     -0.079 N
ATOM   9131  HZ1 LYS A 603      -7.249  -9.296  60.186  1.00  0.00      0.274 HD
ATOM   9132  HZ2 LYS A 603      -6.941 -10.526  59.079  1.00  0.00      0.274 HD
ATOM   9133  HZ3 LYS A 603      -5.723  -9.729  59.621  1.00  0.00      0.274 HD
ATOM   9134  N   ALA A 604      -1.531 -12.556  63.268  1.00 13.72     -0.346 N
ATOM   9135  HN  ALA A 604      -1.262 -13.254  62.574  1.00  0.00      0.163 HD
ATOM   9136  CA  ALA A 604      -1.503 -12.871  64.703  1.00 19.11      0.172 C
ATOM   9138  C   ALA A 604      -0.407 -12.127  65.471  1.00 20.98      0.240 C
ATOM   9139  O   ALA A 604      -0.485 -12.094  66.723  1.00 17.28     -0.271 OA
ATOM   9140  CB  ALA A 604      -1.276 -14.377  64.874  1.00 21.88      0.042 C
ATOM   9144  N   VAL A 605       0.626 -11.620  64.800  1.00 10.94     -0.346 N
ATOM   9145  HN  VAL A 605       0.668 -11.688  63.783  1.00  0.00      0.163 HD
ATOM   9146  CA  VAL A 605       1.710 -10.958  65.554  1.00 14.07      0.180 C
ATOM   9148  C   VAL A 605       1.391  -9.486  65.620  1.00 16.61      0.241 C
ATOM   9149  O   VAL A 605       1.491  -8.794  64.589  1.00 16.70     -0.271 OA
ATOM   9150  CB  VAL A 605       3.062 -11.198  64.865  1.00 18.47      0.009 C
ATOM   9152  CG1 VAL A 605       4.212 -10.525  65.614  1.00 16.89      0.012 C
ATOM   9156  CG2 VAL A 605       3.338 -12.698  64.741  1.00 20.23      0.012 C
ATOM   9160  N   THR A 606       1.065  -8.966  66.814  1.00 10.40     -0.344 N
ATOM   9161  HN  THR A 606       1.050  -9.536  67.660  1.00  0.00      0.163 HD
ATOM   9162  CA  THR A 606       0.732  -7.538  66.842  1.00 16.41      0.205 C
ATOM   9164  C   THR A 606       1.837  -6.683  67.414  1.00 13.89      0.243 C
ATOM   9165  O   THR A 606       1.692  -5.452  67.426  1.00 14.06     -0.271 OA
ATOM   9166  CB  THR A 606      -0.545  -7.330  67.694  1.00 17.52      0.146 C
ATOM   9168  CG2 THR A 606      -1.722  -8.029  67.048  1.00 22.63      0.042 C
ATOM   9172  OG1 THR A 606      -0.248  -7.891  68.972  1.00 18.91     -0.393 OA
ATOM   9173  HG1 THR A 606      -1.031  -7.763  69.494  1.00  0.00      0.210 HD
ATOM   9174  N   ALA A 607       2.926  -7.283  67.904  1.00 11.85     -0.346 N
ATOM   9175  HN  ALA A 607       3.007  -8.300  67.884  1.00  0.00      0.163 HD
ATOM   9176  CA  ALA A 607       4.012  -6.458  68.475  1.00 13.72      0.172 C
ATOM   9178  C   ALA A 607       4.879  -6.049  67.284  1.00 13.87      0.240 C
ATOM   9179  O   ALA A 607       5.739  -6.807  66.860  1.00 12.08     -0.271 OA
ATOM   9180  CB  ALA A 607       4.840  -7.220  69.502  1.00 14.27      0.042 C
ATOM   9184  N   ARG A 608       4.566  -4.891  66.686  1.00 10.56     -0.346 N
ATOM   9185  HN  ARG A 608       3.828  -4.306  67.079  1.00  0.00      0.163 HD
ATOM   9186  CA  ARG A 608       5.263  -4.455  65.484  1.00  8.65      0.176 C
ATOM   9188  C   ARG A 608       5.892  -3.069  65.702  1.00  9.54      0.241 C
ATOM   9189  O   ARG A 608       5.225  -2.257  66.323  1.00 12.83     -0.271 OA
ATOM   9190  CB  ARG A 608       4.272  -4.314  64.308  1.00 11.81      0.036 C
ATOM   9193  CG  ARG A 608       3.672  -5.683  63.885  1.00  9.21      0.023 C
ATOM   9196  CD  ARG A 608       2.616  -5.492  62.801  1.00 14.32      0.138 C
ATOM   9199  NE  ARG A 608       1.909  -6.783  62.553  1.00 12.30     -0.227 N
ATOM   9200  HE  ARG A 608       2.024  -7.554  63.211  1.00  0.00      0.177 HD
ATOM   9201  CZ  ARG A 608       1.135  -6.941  61.492  1.00 22.08      0.665 C
ATOM   9202  NH1 ARG A 608       0.986  -5.931  60.636  1.00  8.44     -0.235 N
ATOM   9203 1HH1 ARG A 608       1.417  -5.012  60.735  1.00  0.00      0.174 HD
ATOM   9204 2HH1 ARG A 608       0.389  -6.053  59.818  1.00  0.00      0.174 HD
ATOM   9205  NH2 ARG A 608       0.578  -8.129  61.364  1.00 11.66     -0.235 N
ATOM   9206 1HH2 ARG A 608       0.692  -8.902  62.019  1.00  0.00      0.174 HD
ATOM   9207 2HH2 ARG A 608      -0.019  -8.251  60.546  1.00  0.00      0.174 HD
ATOM   9208  N   VAL A 609       7.143  -2.895  65.244  1.00 10.12     -0.346 N
ATOM   9209  HN  VAL A 609       7.622  -3.652  64.756  1.00  0.00      0.163 HD
ATOM   9210  CA  VAL A 609       7.817  -1.602  65.453  1.00  8.93      0.180 C
ATOM   9212  C   VAL A 609       8.232  -1.114  64.053  1.00  9.93      0.241 C
ATOM   9213  O   VAL A 609       9.053  -1.737  63.386  1.00 10.04     -0.271 OA
ATOM   9214  CB  VAL A 609       9.082  -1.765  66.316  1.00 11.13      0.009 C
ATOM   9216  CG1 VAL A 609       9.753 -10.417  66.591  1.00  8.14      0.012 C
ATOM   9220  CG2 VAL A 609       8.776  -2.394  67.699  1.00 10.86      0.012 C
ATOM   9224  N   ALA A 610       7.797   0.101  63.690  1.00  9.86     -0.346 N
ATOM   9225  HN  ALA A 610       7.153   0.612  64.294  1.00  0.00      0.163 HD
ATOM   9226  CA  ALA A 610       8.243   0.697  62.429  1.00  9.88      0.172 C
ATOM   9228  C   ALA A 610       9.370   1.709  62.692  1.00  8.84      0.240 C
ATOM   9229  O   ALA A 610       9.306   2.426  63.711  1.00 11.19     -0.271 OA
ATOM   9230  CB  ALA A 610       7.046   1.507  61.861  1.00 10.52      0.042 C
ATOM   9234  N   VAL A 611      10.412  -1.695  61.888  1.00 14.48     -0.346 N
ATOM   9235  HN  VAL A 611      10.416   1.036  61.109  1.00  0.00      0.163 HD
ATOM   9236  CA  VAL A 611      11.545   2.564  62.055  1.00  6.87      0.180 C
ATOM   9238  C   VAL A 611      11.800   3.316  60.738  1.00  7.50      0.241 C
ATOM   9239  O   VAL A 611      12.175   2.691  59.752  1.00  8.23     -0.271 OA
ATOM   9240  CB  VAL A 611      12.825   1.827  62.451  1.00  9.84      0.009 C
ATOM   9242  CG1 VAL A 611      13.819   2.911  62.950  1.00 12.04      0.012 C
ATOM   9246  CG2 VAL A 611      12.629   0.825  63.591  1.00  7.65      0.012 C
ATOM   9250  N   GLU A 612      11.660   4.614  60.734  1.00  7.26     -0.346 N
ATOM   9251  HN  GLU A 612      11.395   5.104  61.588  1.00  0.00      0.163 HD
ATOM   9252  CA  GLU A 612      11.888   5.369  59.484  1.00  5.83      0.177 C
ATOM   9254  C   GLU A 612      12.110   6.838  59.866  1.00  7.69      0.241 C
ATOM   9255  O   GLU A 612      11.295   7.394  60.603  1.00  8.75     -0.271 OA
ATOM   9256  CB  GLU A 612      10.649   5.311  58.557  1.00  6.92      0.045 C
ATOM   9259  CG  GLU A 612      10.829   6.221  57.295  1.00  4.90      0.116 C
ATOM   9262  CD  GLU A 612       9.710   5.969  56.286  1.00  9.29      0.172 C
ATOM   9263  OE1 GLU A 612       8.581   6.493  56.344  1.00  8.26     -0.648 OA
ATOM   9264  OE2 GLU A 612       9.964   5.162  55.369  1.00 11.13     -0.648 OA
ATOM   9265  N   ALA A 613      13.080   7.518  59.231  1.00  5.56     -0.346 N
ATOM   9266  HN  ALA A 613      13.685   7.047  58.558  1.00  0.00      0.163 HD
ATOM   9267  CA  ALA A 613      13.256   8.935  59.516  1.00  8.35      0.172 C
ATOM   9269  C   ALA A 613      12.258   9.793  58.671  1.00 10.34      0.240 C
ATOM   9270  O   ALA A 613      12.651  10.494  57.727  1.00  9.97     -0.271 OA
ATOM   9271  CB  ALA A 613      14.680   9.361  59.248  1.00  8.08      0.042 C
ATOM   9275  N   GLY A 614      11.011   9.670  59.013  1.00  9.83     -0.351 N
ATOM   9276  HN  GLY A 614      10.776   9.040  59.780  1.00  0.00      0.163 HD
ATOM   9277  CA  GLY A 614       9.909  10.407  58.337  1.00 11.11      0.225 C
ATOM   9280  C   GLY A 614       8.747  10.460  59.322  1.00  9.91      0.236 C
ATOM   9281  O   GLY A 614       8.830   9.840  60.398  1.00 10.33     -0.272 OA
ATOM   9282  N   ILE A 615       7.690  11.172  58.934  1.00  7.06     -0.346 N
ATOM   9283  HN  ILE A 615       7.672  11.559  57.990  1.00  0.00      0.163 HD
ATOM   9284  CA  ILE A 615       6.559  11.413  59.821  1.00  7.45      0.180 C
ATOM   9286  C   ILE A 615       5.975  10.103  60.337  1.00  7.53      0.241 C
ATOM   9287  O   ILE A 615       5.750   9.122  59.619  1.00  6.68     -0.271 OA
ATOM   9288  CB  ILE A 615       5.475  12.286  59.146  1.00  7.74      0.013 C
ATOM   9290  CG1 ILE A 615       4.502  12.817  60.231  1.00  9.74      0.002 C
ATOM   9293  CG2 ILE A 615       4.713  11.497  58.090  1.00  9.10      0.012 C
ATOM   9297  CD1 ILE A 615       5.207  13.997  60.966  1.00 12.80      0.005 C
ATOM   9301  N   ALA A 616       5.812  10.002  61.657  1.00  9.06     -0.346 N
ATOM   9302  HN  ALA A 616       5.987  10.817  62.245  1.00  0.00      0.163 HD
ATOM   9303  CA  ALA A 616       5.389   8.751  62.278  1.00  9.39      0.172 C
ATOM   9305  C   ALA A 616       4.001   8.304  61.952  1.00  9.16      0.240 C
ATOM   9306  O   ALA A 616       3.753   7.100  61.808  1.00  8.64     -0.271 OA
ATOM   9307  CB  ALA A 616       5.424   8.935  63.843  1.00 10.13      0.042 C
ATOM   9311  N   ASP A 617       3.022   9.217  61.772  1.00  9.19     -0.346 N
ATOM   9312  HN  ASP A 617       3.269  10.206  61.729  1.00  0.00      0.163 HD
ATOM   9313  CA  ASP A 617       1.626   8.831  61.638  1.00  8.93      0.186 C
ATOM   9315  C   ASP A 617       1.327   7.949  60.416  1.00  9.43      0.241 C
ATOM   9316  O   ASP A 617       0.330   7.225  60.422  1.00 10.60     -0.271 OA
ATOM   9317  CB  ASP A 617       0.745  10.105  61.430  1.00 10.36      0.147 C
ATOM   9320  CG  ASP A 617       0.494  10.837  62.741  1.00 26.01      0.175 C
ATOM   9321  OD1 ASP A 617       0.878  10.311  63.805  1.00 35.33     -0.648 OA
ATOM   9322  OD2 ASP A 617      -0.118  11.916  62.709  1.00 26.98     -0.648 OA
ATOM   9323  N   TYR A 618      -1.186   7.972  59.402  1.00 12.88     -0.346 N
ATOM   9324  HN  TYR A 618       3.000   8.586  59.425  1.00  0.00      0.163 HD
ATOM   9325  CA  TYR A 618       1.938   7.089  58.238  1.00  9.75      0.180 C
ATOM   9327  C   TYR A 618       1.854   5.617  58.659  1.00 10.93      0.241 C
ATOM   9328  O   TYR A 618       1.050   4.799  58.150  1.00 11.64     -0.271 OA
ATOM   9329  CB  TYR A 618       3.133   7.239  57.219  1.00  6.88      0.073 C
ATOM   9332  CG  TYR A 618       2.901   6.231  56.098  1.00  9.27     -0.056 A
ATOM   9333  CD1 TYR A 618       1.930   6.440  55.129  1.00 12.44      0.010 A
ATOM   9335  CD2 TYR A 618       3.610   5.034  56.018  1.00  9.53      0.010 A
ATOM   9337  CE1 TYR A 618       1.651   5.472  54.170  1.00 10.00      0.037 A
ATOM   9339  CE2 TYR A 618       3.299   4.049  55.156  1.00 13.13      0.037 A
ATOM   9341  CZ  TYR A 618       2.349   4.275  54.204  1.00 12.16      0.065 A
ATOM   9342  OH  TYR A 618       2.057   3.288  53.252  1.00 11.69     -0.361 OA
ATOM   9343  HH  TYR A 618       2.535   2.468  53.275  1.00  0.00      0.217 HD
ATOM   9344  N   TRP A 619       2.734   5.219  59.596  1.00 10.12     -0.346 N
ATOM   9345  HN  TRP A 619       3.235   5.929  60.130  1.00  0.00      0.163 HD
ATOM   9346  CA  TRP A 619       3.001   3.816  59.879  1.00 11.03      0.181 C
ATOM   9348  C   TRP A 619       1.946   3.070  60.643  1.00 11.98      0.241 C
ATOM   9349  O   TRP A 619       2.026   1.835  60.763  1.00  9.75     -0.271 OA
ATOM   9350  CB  TRP A 619       4.409   3.645  60.553  1.00  8.20      0.075 C
ATOM   9353  CG  TRP A 619       5.443   3.856  59.474  1.00  8.15     -0.028 A
ATOM   9354  CD1 TRP A 619       6.156   5.013  59.261  1.00  5.43      0.096 A
ATOM   9356  CD2 TRP A 619       5.822   2.937  58.449  1.00 10.12     -0.002 A
ATOM   9357  CE2 TRP A 619       6.759   3.578  57.630  1.00 11.75      0.042 A
ATOM   9358  CE3 TRP A 619       5.409   1.636  58.128  1.00 10.12      0.014 A
ATOM   9360  NE1 TRP A 619       6.982   4.834  58.135  1.00  7.55     -0.365 N
ATOM   9361  HE1 TRP A 619       7.635   5.521  57.759  1.00  0.00      0.165 HD
ATOM   9362  CZ2 TRP A 619       7.363   2.955  56.527  1.00 11.00      0.030 A
ATOM   9364  CZ3 TRP A 619       5.991   1.027  57.023  1.00 13.96      0.001 A
ATOM   9366  CH2 TRP A 619       6.933   1.696  56.224  1.00 14.53      0.002 A
ATOM   9368  N   TYR A 620       0.880   3.722  61.150  1.00  7.86     -0.346 N
ATOM   9369  HN  TYR A 620       0.831   4.738  61.078  1.00  0.00      0.163 HD
ATOM   9370  CA  TYR A 620      -0.214   2.986  61.804  1.00  9.30      0.180 C
ATOM   9372  C   TYR A 620      -0.855   1.995  60.846  1.00  9.37      0.241 C
ATOM   9373  O   TYR A 620      -1.434   0.962  61.226  1.00  9.05     -0.271 OA
ATOM   9374  CB  TYR A 620      -1.321   3.951  62.297  1.00  9.50      0.073 C
ATOM   9377  CG  TYR A 620      -0.822   4.652  63.549  1.00  7.81     -0.056 A
ATOM   9378  CD1 TYR A 620      -0.846   3.991  64.769  1.00 15.69      0.010 A
ATOM   9380  CD2 TYR A 620      -0.384   5.964  63.498  1.00 10.63      0.010 A
ATOM   9382  CE1 TYR A 620      -0.393   4.627  65.933  1.00 17.22      0.037 A
ATOM   9384  CE2 TYR A 620       0.087   6.615  64.630  1.00 13.99      0.037 A
ATOM   9386  CZ  TYR A 620       0.079   5.926  65.827  1.00 24.13      0.065 A
ATOM   9387  OH  TYR A 620       0.522   6.565  66.965  1.00 22.12     -0.361 OA
ATOM   9388  HH  TYR A 620       0.845   7.455  66.892  1.00  0.00      0.217 HD
ATOM   9389  N   LYS A 621      -0.771   2.282  59.540  1.00  7.00     -0.346 N
ATOM   9390  HN  LYS A 621      -0.358   3.160  59.227  1.00  0.00      0.163 HD
ATOM   9391  CA  LYS A 621      -1.282   1.313  58.573  1.00  5.94      0.176 C
ATOM   9393  C   LYS A 621      -0.676  -0.063  58.721  1.00  9.22      0.241 C
ATOM   9394  O   LYS A 621      -1.386  -1.031  58.363  1.00 10.73     -0.271 OA
ATOM   9395  CB  LYS A 621      -0.986   1.879  57.157  1.00  9.23      0.035 C
ATOM   9398  CG  LYS A 621      -1.360   0.904  56.058  1.00 13.27      0.004 C
ATOM   9401  CD  LYS A 621      -1.098   1.543  54.674  1.00 13.68      0.027 C
ATOM   9404  CE  LYS A 621      -1.526   0.494  53.611  1.00 19.60      0.229 C
ATOM   9407  NZ  LYS A 621      -0.948   0.934  52.313  1.00 27.94     -0.079 N
ATOM   9408  HZ1 LYS A 621      -1.229   0.245  51.615  1.00  0.00      0.274 HD
ATOM   9409  HZ2 LYS A 621       0.061   1.078  52.351  1.00  0.00      0.274 HD
ATOM   9410  HZ3 LYS A 621      -1.206   1.888  52.062  1.00  0.00      0.274 HD
ATOM   9411  N   TYR A 622       0.594  -0.222  59.113  1.00  6.32     -0.346 N
ATOM   9412  HN  TYR A 622       1.151   0.601  59.343  1.00  0.00      0.163 HD
ATOM   9413  CA  TYR A 622       1.196  -1.534  59.218  1.00  4.95      0.180 C
ATOM   9415  C   TYR A 622       1.411  -1.932  60.685  1.00 12.09      0.241 C
ATOM   9416  O   TYR A 622       1.554  -3.151  60.867  1.00 13.02     -0.271 OA
ATOM   9417  CB  TYR A 622       2.551  -1.604  58.492  1.00  6.13      0.073 C
ATOM   9420  CG  TYR A 622       2.335  -1.386  56.975  1.00 13.56     -0.056 A
ATOM   9421  CD1 TYR A 622       1.834  -2.425  56.194  1.00 14.59      0.010 A
ATOM   9423  CD2 TYR A 622       2.606  -0.154  56.401  1.00 13.52      0.010 A
ATOM   9425  CE1 TYR A 622       1.629  -2.241  54.830  1.00 13.94      0.037 A
ATOM   9427  CE2 TYR A 622       2.442   0.045  55.020  1.00 11.19      0.037 A
ATOM   9429  CZ  TYR A 622       1.955  -1.004  54.269  1.00 16.54      0.065 A
ATOM   9430  OH  TYR A 622       1.743  -0.793  52.939  1.00 20.37     -0.361 OA
ATOM   9431  HH  TYR A 622       1.965   0.048  52.557  1.00  0.00      0.217 HD
ATOM   9432  N   VAL A 623       1.459  -0.988  61.614  1.00 10.21     -0.346 N
ATOM   9433  HN  VAL A 623       1.298  -0.007  61.385  1.00  0.00      0.163 HD
ATOM   9434  CA  VAL A 623       1.756  -1.418  62.994  1.00 11.43      0.180 C
ATOM   9436  C   VAL A 623       0.497  -1.475  63.846  1.00 16.41      0.241 C
ATOM   9437  O   VAL A 623       0.593  -2.025  64.941  1.00 15.90     -0.271 OA
ATOM   9438  CB  VAL A 623       2.809  -0.586  63.731  1.00 13.76      0.009 C
ATOM   9440  CG1 VAL A 623       4.124  -0.511  62.918  1.00 13.56      0.012 C
ATOM   9444  CG2 VAL A 623       2.367   0.812  64.119  1.00 14.18      0.012 C
ATOM   9448  N   GLY A 624      -0.549  -0.786  63.445  1.00  9.57     -0.351 N
ATOM   9449  HN  GLY A 624      -0.477  -0.220  62.600  1.00  0.00      0.163 HD
ATOM   9450  CA  GLY A 624      -1.821  -0.811  64.185  1.00 13.61      0.225 C
ATOM   9453  C   GLY A 624      -1.755   0.001  65.486  1.00 15.86      0.236 C
ATOM   9454  O   GLY A 624      -0.837   0.774  65.747  1.00 15.98     -0.272 OA
ATOM   9455  N   LEU A 625      -2.709  -0.246  66.364  1.00 14.26     -0.346 N
ATOM   9456  HN  LEU A 625      -3.403  -0.967  66.166  1.00  0.00      0.163 HD
ATOM   9457  CA  LEU A 625      -2.783   0.507  67.625  1.00 14.42      0.177 C
ATOM   9459  C   LEU A 625      -1.980  -0.137  68.734  1.00 19.22      0.241 C
ATOM   9460  O   LEU A 625      -1.828   0.478  69.789  1.00 23.34     -0.271 OA
ATOM   9461  CB  LEU A 625      -4.255   0.588  68.044  1.00 15.03      0.038 C
ATOM   9464  CG  LEU A 625      -5.185   1.283  67.031  1.00 18.05     -0.020 C
ATOM   9466  CD1 LEU A 625      -6.656   1.159  67.485  1.00 22.90      0.009 C
ATOM   9470  CD2 LEU A 625      -4.792   2.744  66.911  1.00 34.24      0.009 C
ATOM   9474  N   ASN A 626      -1.447  -1.340  68.596  1.00 15.73     -0.346 N
ATOM   9475  HN  ASN A 626      -1.525  -1.835  67.708  1.00  0.00      0.163 HD
ATOM   9476  CA  ASN A 626      -0.742  -1.961  69.728  1.00 18.63      0.185 C
ATOM   9478  C   ASN A 626       0.747  -2.064  69.400  1.00 22.60      0.241 C
ATOM   9479  O   ASN A 626       1.413  -2.917  69.978  1.00 19.82     -0.271 OA
ATOM   9480  CB  ASN A 626      -1.353  -3.367  69.931  1.00 25.44      0.137 C
ATOM   9483  CG  ASN A 626      -2.821  -3.257  70.354  1.00 32.97      0.217 C
ATOM   9484  ND2 ASN A 626      -3.732  -3.835  69.574  1.00 31.71     -0.370 N
ATOM   9485 1HD2 ASN A 626      -3.522  -4.371  68.732  1.00  0.00      0.159 HD
ATOM   9486 2HD2 ASN A 626      -4.710  -3.762  69.856  1.00  0.00      0.159 HD
ATOM   9487  OD1 ASN A 626      -3.074  -2.610  71.370  1.00 35.40     -0.274 OA
ATOM   9488  N   GLY A 627       1.206  -1.306  68.405  1.00 17.38     -0.351 N
ATOM   9489  HN  GLY A 627       0.576  -0.656  67.935  1.00  0.00      0.163 HD
ATOM   9490  CA  GLY A 627       2.606  -1.394  67.976  1.00 14.67      0.225 C
ATOM   9493  C   GLY A 627       3.315  -0.096  68.376  1.00 19.36      0.236 C
ATOM   9494  O   GLY A 627       2.867   0.596  69.301  1.00 22.38     -0.272 OA
ATOM   9495  N   ALA A 628       4.501   0.162  67.883  1.00 13.73     -0.347 N
ATOM   9496  HN  ALA A 628       4.916  -0.497  67.224  1.00  0.00      0.163 HD
ATOM   9497  CA  ALA A 628       5.254   1.374  68.251  1.00 13.75      0.172 C
ATOM   9499  C   ALA A 628       5.915   1.911  66.996  1.00 14.97      0.240 C
ATOM   9500  O   ALA A 628       6.169   1.172  66.030  1.00  9.99     -0.271 OA
ATOM   9501  CB  ALA A 628       6.360   1.049  69.253  1.00 14.44      0.042 C
ATOM   9505  N   ILE A 629       6.186   3.212  66.940  1.00 10.55     -0.346 N
ATOM   9506  HN  ILE A 629       5.946   3.827  67.717  1.00  0.00      0.163 HD
ATOM   9507  CA  ILE A 629       6.836   3.743  65.739  1.00  6.63      0.180 C
ATOM   9509  C   ILE A 629       7.998   4.618  66.171  1.00 11.35      0.241 C
ATOM   9510  O   ILE A 629       7.804   5.526  67.015  1.00 10.98     -0.271 OA
ATOM   9511  CB  ILE A 629       5.803   4.652  64.987  1.00 13.81      0.013 C
ATOM   9513  CG1 ILE A 629       4.575   3.849  64.556  1.00 10.34      0.002 C
ATOM   9516  CG2 ILE A 629       6.494   5.322  63.787  1.00  7.27      0.012 C
ATOM   9520  CD1 ILE A 629       3.328   4.709  64.322  1.00 14.84      0.005 C
ATOM   9524  N   VAL A 630       9.167   4.402  65.626  1.00  6.03     -0.346 N
ATOM   9525  HN  VAL A 630       9.274   3.581  65.031  1.00  0.00      0.163 HD
ATOM   9526  CA  VAL A 630      10.321   5.262  65.818  1.00  7.29      0.180 C
ATOM   9528  C   VAL A 630      10.421   6.154  64.565  1.00  9.96      0.241 C
ATOM   9529  O   VAL A 630      10.852   5.686  63.518  1.00  7.58     -0.271 OA
ATOM   9530  CB  VAL A 630      11.598   4.446  66.046  1.00 12.69      0.009 C
ATOM   9532  CG1 VAL A 630      12.798   5.380  66.226  1.00 13.38      0.012 C
ATOM   9536  CG2 VAL A 630      11.379   3.585  67.305  1.00 12.42      0.012 C
ATOM   9540  N   GLY A 631       9.901   7.378  64.693  1.00  9.81     -0.351 N
ATOM   9541  HN  GLY A 631       9.566   7.721  65.593  1.00  0.00      0.163 HD
ATOM   9542  CA  GLY A 631       9.831   8.224  63.464  1.00  7.63      0.225 C
ATOM   9545  C   GLY A 631      10.003   9.683  63.894  1.00 14.99      0.236 C
ATOM   9546  O   GLY A 631      10.400   9.978  65.049  1.00 12.72     -0.272 OA
ATOM   9547  N   MET A 632       9.760  10.576  62.939  1.00 10.73     -0.346 N
ATOM   9548  HN  MET A 632       9.516  10.267  61.998  1.00  0.00      0.163 HD
ATOM   9549  CA  MET A 632       9.845  12.017  63.249  1.00 10.81      0.177 C
ATOM   9551  C   MET A 632       8.440  12.518  63.551  1.00 14.59      0.241 C
ATOM   9552  O   MET A 632       7.428  12.021  63.006  1.00 14.53     -0.271 OA
ATOM   9553  CB  MET A 632      10.410  12.811  62.085  1.00 13.19      0.045 C
ATOM   9556  CG  MET A 632      11.862  12.611  61.603  1.00 13.28      0.076 C
ATOM   9559  SD  MET A 632      12.988  13.330  62.830  1.00 21.15     -0.173 SA
ATOM   9560  CE  MET A 632      12.880  15.087  62.352  1.00 13.42      0.089 C
ATOM   9564  N   THR A 633       8.328  13.469  64.498  1.00 10.36     -0.344 N
ATOM   9565  HN  THR A 633       9.139  13.742  65.054  1.00  0.00      0.163 HD
ATOM   9566  CA  THR A 633       7.035  14.103  64.719  1.00 11.92      0.205 C
ATOM   9568  C   THR A 633       7.208  15.627  64.657  1.00 16.41      0.243 C
ATOM   9569  O   THR A 633       6.256  16.364  64.896  1.00 13.00     -0.271 OA
ATOM   9570  CB  THR A 633       6.432  13.753  66.093  1.00 24.67      0.146 C
ATOM   9572  OG1 THR A 633       6.189  12.253  66.277  1.00 23.84      0.042 C
ATOM   9576  OG1 THR A 633       7.422  14.132  67.044  1.00 18.15     -0.393 OA
ATOM   9577  HG1 THR A 633       7.050  13.916  67.891  1.00  0.00      0.210 HD
ATOM   9578  N   THR A 634       8.357  16.170  64.270  1.00 11.28     -0.344 N
ATOM   9579  HN  THR A 634       9.127  15.553  64.011  1.00  0.00      0.163 HD
ATOM   9580  CA  THR A 634       8.565  17.620  64.199  1.00 12.17      0.205 C
ATOM   9582  C   THR A 634       9.426  17.935  62.979  1.00 12.29      0.243 C
ATOM   9583  O   THR A 634       9.887  17.035  62.289  1.00  9.96     -0.271 OA
ATOM   9584  CB  THR A 634       9.451  18.110  65.388  1.00 16.81      0.146 C
ATOM   9586  CG2 THR A 634       8.930  17.757  66.767  1.00 23.67      0.042 C
ATOM   9590  OG1 THR A 634      10.723  17.416  65.305  1.00 19.83     -0.393 OA
ATOM   9591  HG1 THR A 634      11.262  17.714  66.028  1.00  0.00      0.210 HD
ATOM   9592  N   PHE A 635       9.729  19.209  62.737  1.00 11.60     -0.344 N
ATOM   9593  HN  PHE A 635       9.294  19.940  63.300  1.00  0.00      0.163 HD
ATOM   9594  CA  PHE A 635      10.675  19.586  61.679  1.00 11.34      0.180 C
ATOM   9596  C   PHE A 635      12.095  19.246  62.177  1.00 14.67      0.241 C
ATOM   9597  O   PHE A 635      12.236  18.969  63.386  1.00 13.07     -0.271 OA
ATOM   9598  CB  PHE A 635      10.563  21.104  61.469  1.00 11.38      0.073 C
ATOM   9601  CG  PHE A 635       9.211  21.462  60.839  1.00 10.99     -0.056 A
ATOM   9602  CD1 PHE A 635       8.875  20.984  59.604  1.00 14.52      0.007 A
ATOM   9604  CD2 PHE A 635       8.315  22.235  61.559  1.00 11.73      0.007 A
ATOM   9606  CE1 PHE A 635       7.644  21.335  59.031  1.00 13.95      0.001 A
ATOM   9608  CE2 PHE A 635       7.092  22.596  60.991  1.00 13.16      0.001 A
ATOM   9610  CZ  PHE A 635       6.748  22.136  59.729  1.00 12.23      0.000 A
ATOM   9612  N   GLY A 636      13.046  19.291  61.270  1.00 10.15     -0.351 N
ATOM   9613  HN  GLY A 636      12.795  19.576  60.323  1.00  0.00      0.163 HD
ATOM   9614  CA  GLY A 636      14.438  18.956  61.542  1.00  9.24      0.225 C
ATOM   9617  C   GLY A 636      15.189  20.158  62.114  1.00 13.29      0.236 C
ATOM   9618  O   GLY A 636      14.585  21.090  62.653  1.00 15.16     -0.272 OA
ATOM   9619  N   GLU A 637      16.529  20.111  62.113  1.00 15.01     -0.346 N
ATOM   9620  HN  GLU A 637      16.980  19.289  61.712  1.00  0.00      0.163 HD
ATOM   9621  CA  GLU A 637      17.381  21.168  62.653  1.00 11.79      0.177 C
ATOM   9623  C   GLU A 637      18.679  21.214  61.856  1.00  9.19      0.241 C
ATOM   9624  O   GLU A 637      19.021  20.189  61.272  1.00 11.51     -0.271 OA
ATOM   9625  CB  GLU A 637      17.848  20.897  64.102  1.00 19.41      0.045 C
ATOM   9628  CG  GLU A 637      16.757  20.567  65.079  1.00 34.57      0.116 C
ATOM   9631  CD  GLU A 637      16.767  21.601  66.200  1.00 54.79      0.172 C
ATOM   9632  OE1 GLU A 637      17.767  21.568  66.949  1.00 55.25     -0.648 OA
ATOM   9633  OE2 GLU A 637      15.760  22.340  66.189  1.00 53.61     -0.648 OA
ATOM   9634  N   SER A 638      19.380  22.354  61.865  1.00 10.76     -0.344 N
ATOM   9635  HN  SER A 638      19.027  23.157  62.385  1.00  0.00      0.163 HD
ATOM   9636  CA  SER A 638      20.636  22.465  61.145  1.00 11.38      0.200 C
ATOM   9638  C   SER A 638      21.801  21.950  61.995  1.00 16.04      0.243 C
ATOM   9639  O   SER A 638      22.140  22.583  63.017  1.00 16.84     -0.271 OA
ATOM   9640  CB  SER A 638      20.903  23.969  60.827  1.00 12.67      0.199 C
ATOM   9643  OG  SER A 638      22.141  24.028  60.131  1.00 16.42     -0.398 OA
ATOM   9644  HG  SER A 638      22.304  24.944  59.937  1.00  0.00      0.209 HD
ATOM   9645  N   ALA A 639      22.399  20.838  61.632  1.00 10.62     -0.346 N
ATOM   9646  HN  ALA A 639      22.049  20.344  60.811  1.00  0.00      0.163 HD
ATOM   9647  CA  ALA A 639      23.548  20.271  62.353  1.00 12.35      0.172 C
ATOM   9649  C   ALA A 639      24.098  19.102  61.547  1.00 12.26      0.243 C
ATOM   9650  O   ALA A 639      23.374  18.577  60.699  1.00 15.40     -0.271 OA
ATOM   9651  CB  ALA A 639      23.064  19.738  63.708  1.00 12.09      0.042 C
ATOM   9655  N   PRO A 640      25.308  18.630  61.769  1.00 13.68     -0.337 N
ATOM   9656  CA  PRO A 640      25.820  17.435  61.133  1.00 13.22      0.179 C
ATOM   9658  C   PRO A 640      24.870  16.245  61.322  1.00 13.43      0.241 C
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ATOM   9659  O   PRO A 640      24.251  16.037  62.376  1.00 13.50      -0.271 OA
ATOM   9660  CB  PRO A 640      27.151  17.166  61.861  1.00 16.21       0.037 C
ATOM   9663  CG  PRO A 640      27.553  18.537  62.363  1.00 18.17       0.022 C
ATOM   9666  CD  PRO A 640      26.246  19.176  62.800  1.00 16.57       0.127 C
ATOM   9669  N   ALA A 641      24.753  15.416  60.279  1.00 14.38      -0.346 N
ATOM   9670  HN  ALA A 641      25.337  15.548  59.454  1.00  0.00       0.163 HD
ATOM   9671  CA  ALA A 641      23.780  14.313  60.324  1.00 16.60       0.172 C
ATOM   9673  C   ALA A 641      23.927  13.394  61.511  1.00 16.43       0.240 C
ATOM   9674  O   ALA A 641      22.932  12.964  62.096  1.00 17.29      -0.271 OA
ATOM   9675  CB  ALA A 641      23.839  13.508  59.019  1.00 18.97       0.042 C
ATOM   9679  N   GLU A 642      25.156  12.976  61.838  1.00 15.48      -0.346 N
ATOM   9680  HN  GLU A 642      25.976  13.296  61.324  1.00  0.00       0.163 HD
ATOM   9681  CA  GLU A 642      25.284  12.027  62.979  1.00 20.34       0.177 C
ATOM   9683  C   GLU A 642      24.638  12.547  64.243  1.00 18.31       0.241 C
ATOM   9684  O   GLU A 642      24.000  11.801  65.027  1.00 19.05      -0.271 OA
ATOM   9685  CB  GLU A 642      26.763  11.690  63.222  1.00 30.97       0.045 C
ATOM   9688  CG  GLU A 642      27.103  10.912  64.466  1.00 65.49       0.116 C
ATOM   9691  CD  GLU A 642      28.521  11.023  64.993  1.00 80.68       0.172 C
ATOM   9692  OE1 GLU A 642      29.480  11.037  64.187  1.00 88.22      -0.648 OA
ATOM   9693  OE2 GLU A 642      28.704  11.086  66.237  1.00 86.90      -0.648 OA
ATOM   9694  N   LEU A 643      24.796  13.844  64.529  1.00 11.42      -0.346 N
ATOM   9695  HN  LEU A 643      25.344  14.443  63.911  1.00  0.00       0.163 HD
ATOM   9696  CA  LEU A 643      24.182  14.396  65.727  1.00 11.41       0.177 C
ATOM   9698  C   LEU A 643      22.676  14.479  65.616  1.00 16.29       0.241 C
ATOM   9699  O   LEU A 643      22.003  14.399  66.639  1.00 14.17      -0.271 OA
ATOM   9700  CB  LEU A 643      24.715  15.842  65.927  1.00 18.23       0.038 C
ATOM   9703  CG  LEU A 643      26.217  15.978  66.206  1.00 22.96      -0.020 C
ATOM   9705  CD1 LEU A 643      26.560  17.400  66.648  1.00 29.45       0.009 C
ATOM   9709  CD2 LEU A 643      26.690  15.026  67.296  1.00 30.96       0.009 C
ATOM   9713  N   LEU A 644      22.105  14.679  64.412  1.00 12.35      -0.346 N
ATOM   9714  HN  LEU A 644      22.677  14.774  63.573  1.00  0.00       0.163 HD
ATOM   9715  CA  LEU A 644      20.637  14.757  64.334  1.00 10.70       0.177 C
ATOM   9717  C   LEU A 644      20.021  13.388  64.575  1.00 10.65       0.241 C
ATOM   9718  O   LEU A 644      18.951  13.250  65.183  1.00 13.10      -0.271 OA
ATOM   9719  CB  LEU A 644      20.212  15.302  62.953  1.00 11.88       0.038 C
ATOM   9722  CG  LEU A 644      20.683  16.736  62.647  1.00 12.62      -0.020 C
ATOM   9724  CD1 LEU A 644      20.328  17.080  61.194  1.00 11.34       0.009 C
ATOM   9728  CD2 LEU A 644      19.993  17.719  63.624  1.00 12.08       0.009 C
ATOM   9732  N   PHE A 645      20.675  12.324  64.036  1.00 12.01      -0.346 N
ATOM   9733  HN  PHE A 645      21.542  12.433  63.510  1.00  0.00       0.163 HD
ATOM   9734  CA  PHE A 645      20.051  10.993  64.260  1.00 11.32       0.180 C
ATOM   9736  C   PHE A 645      19.984  10.692  65.758  1.00 12.17       0.241 C
ATOM   9737  O   PHE A 645      18.957  10.214  66.273  1.00 13.86      -0.271 OA
ATOM   9738  CB  PHE A 645      20.860   9.920  63.534  1.00 16.21       0.073 C
ATOM   9741  CG  PHE A 645      20.532   9.851  62.061  1.00 20.91      -0.056 A
ATOM   9742  CD1 PHE A 645      19.226   9.671  61.639  1.00 21.93       0.007 A
ATOM   9744  CD2 PHE A 645      21.520   9.984  61.104  1.00 24.81       0.007 A
ATOM   9746  CE1 PHE A 645      18.921   9.595  60.285  1.00 23.80       0.001 A
ATOM   9748  CE2 PHE A 645      21.222   9.956  59.756  1.00 18.43       0.001 A
ATOM   9750  CZ  PHE A 645      19.904   9.745  59.344  1.00 22.14       0.000 A
ATOM   9752  N   GLU A 646      21.035  11.092  66.457  1.00 13.59      -0.346 N
ATOM   9753  HN  GLU A 646      21.833  11.517  65.985  1.00  0.00       0.163 HD
ATOM   9754  CA  GLU A 646      21.046  10.919  67.923  1.00 18.84       0.177 C
ATOM   9756  C   GLU A 646      19.985  11.747  68.594  1.00 19.01       0.241 C
ATOM   9757  O   GLU A 646      19.168  11.288  69.411  1.00 16.54      -0.271 OA
ATOM   9758  CB  GLU A 646      22.431  11.325  68.449  1.00 26.62       0.045 C
ATOM   9761  CG  GLU A 646      23.094  10.388  69.436  1.00 50.81       0.116 C
ATOM   9764  CD  GLU A 646      24.607  10.602  69.374  1.00 58.48       0.172 C
ATOM   9765  OE1 GLU A 646      25.025  11.731  69.714  1.00 61.86      -0.648 OA
ATOM   9766  OE2 GLU A 646      25.310   9.657  68.966  1.00 61.63      -0.648 OA
ATOM   9767  N   GLU A 647      19.933  13.046  68.289  1.00 16.57      -0.346 N
ATOM   9768  HN  GLU A 647      20.605  13.424  67.621  1.00  0.00       0.163 HD
ATOM   9769  CA  GLU A 647      18.943  13.945  68.883  1.00 20.20       0.177 C
ATOM   9771  C   GLU A 647      17.501  13.520  68.672  1.00 17.38       0.241 C
ATOM   9772  O   GLU A 647      16.635  13.734  69.543  1.00 18.30      -0.271 OA
ATOM   9773  CB  GLU A 647      19.143  15.305  68.166  1.00 24.68       0.045 C
ATOM   9776  CG  GLU A 647      18.300  16.413  68.694  1.00 42.33       0.116 C
ATOM   9779  CD  GLU A 647      18.985  17.201  69.807  1.00 46.20       0.172 C
ATOM   9780  OE1 GLU A 647      19.976  16.742  70.408  1.00 47.50      -0.648 OA
ATOM   9781  OE2 GLU A 647      18.460  18.319  70.023  1.00 54.46      -0.648 OA
ATOM   9782  N   PHE A 648      17.173  12.887  67.544  1.00 13.41      -0.346 N
ATOM   9783  HN  PHE A 648      17.910  12.626  66.889  1.00  0.00       0.163 HD
ATOM   9784  CA  PHE A 648      15.789  12.559  67.224  1.00 15.31       0.180 C
ATOM   9786  C   PHE A 648      15.445  11.104  67.519  1.00 19.37       0.241 C
ATOM   9787  O   PHE A 648      14.371  10.628  67.134  1.00 17.68      -0.271 OA
ATOM   9788  CB  PHE A 648      15.411  12.901  65.765  1.00 15.72       0.073 C
ATOM   9791  CG  PHE A 648      15.287  14.390  65.542  1.00 15.55      -0.056 A
ATOM   9792  CD1 PHE A 648      14.241  15.124  66.047  1.00 18.54       0.007 A
ATOM   9794  CD2 PHE A 648      16.283  15.036  64.802  1.00 15.16       0.007 A
ATOM   9796  CE1 PHE A 648      14.174  16.502  65.836  1.00 20.55       0.001 A
ATOM   9798  CE2 PHE A 648      16.220  16.396  64.563  1.00 19.66       0.001 A
ATOM   9800  CZ  PHE A 648      15.157  17.140  65.075  1.00 21.41       0.000 A
ATOM   9802  N   GLY A 649      16.358  10.373  68.162  1.00 19.72      -0.351 N
ATOM   9803  HN  GLY A 649      17.273  10.781  68.354  1.00  0.00       0.163 HD
ATOM   9804  CA  GLY A 649      16.088   9.016  68.596  1.00 16.29       0.225 C
ATOM   9807  C   GLY A 649      16.349   7.862  67.665  1.00 12.71       0.236 C
ATOM   9808  O   GLY A 649      15.931   6.713  67.957  1.00 14.34      -0.272 OA
ATOM   9809  N   PHE A 650      17.106   8.057  66.621  1.00 11.40      -0.346 N
ATOM   9810  HN  PHE A 650      17.474   8.995  66.465  1.00  0.00       0.163 HD
ATOM   9811  CA  PHE A 650      17.456   7.022  65.670  1.00  8.90       0.180 C
ATOM   9813  C   PHE A 650      18.765   6.421  66.179  1.00 13.37       0.241 C
ATOM   9814  O   PHE A 650      19.811   6.618  65.606  1.00 12.47      -0.271 OA
ATOM   9815  CB  PHE A 650      17.536   7.514  64.229  1.00  9.72       0.073 C
ATOM   9818  CG  PHE A 650      16.141   7.976  63.810  1.00 11.21      -0.056 A
ATOM   9819  CD1 PHE A 650      15.194   7.040  63.374  1.00 13.18       0.007 A
ATOM   9821  CD2 PHE A 650      15.802   9.293  63.889  1.00 12.86       0.007 A
ATOM   9823  CE1 PHE A 650      13.911   7.460  63.008  1.00  9.90       0.001 A
ATOM   9825  CE2 PHE A 650      14.523   9.735  63.526  1.00 13.85       0.001 A
ATOM   9827  CZ  PHE A 650      13.594   8.806  63.119  1.00 11.06       0.000 A
ATOM   9829  N   THR A 651      18.663   5.705  67.321  1.00 16.11      -0.344 N
ATOM   9830  HN  THR A 651      17.758   5.633  67.785  1.00  0.00       0.163 HD
ATOM   9831  CA  THR A 651      19.812   5.037  67.901  1.00 15.41       0.205 C
ATOM   9833  C   THR A 651      19.348   3.609  68.243  1.00 12.40       0.243 C
ATOM   9834  O   THR A 651      18.175   3.376  68.544  1.00 12.03      -0.271 OA
ATOM   9835  CB  THR A 651      20.339   5.671  69.220  1.00 16.25       0.146 C
ATOM   9837  CG2 THR A 651      20.671   7.159  69.071  1.00 17.61       0.042 C
ATOM   9841  OG1 THR A 651      19.277   5.601  70.173  1.00 15.28      -0.393 OA
ATOM   9842  HG1 THR A 651      19.599   5.988  70.979  1.00  0.00       0.210 HD
ATOM   9843  N   VAL A 652      20.292   2.681  68.188  1.00 15.16      -0.346 N
ATOM   9844  HN  VAL A 652      21.237   2.938  67.902  1.00  0.00       0.163 HD
ATOM   9845  CA  VAL A 652      19.989   1.277  68.537  1.00 17.24       0.180 C
ATOM   9847  C   VAL A 652      19.332   1.211  69.899  1.00 20.05       0.241 C
ATOM   9848  O   VAL A 652      18.317   0.538  70.133  1.00 17.07      -0.271 OA
ATOM   9849  CB  VAL A 652      21.263   0.417  68.476  1.00 16.78       0.009 C
ATOM   9851  CG1 VAL A 652      21.025  -1.026  68.914  1.00 21.50       0.012 C
ATOM   9855  CG2 VAL A 652      21.836   0.423  67.064  1.00 26.65       0.012 C
ATOM   9859  N   ASP A 653      19.916   1.921  70.887  1.00 13.78      -0.345 N
ATOM   9860  HN  ASP A 653      20.734   2.500  70.700  1.00  0.00       0.163 HD
ATOM   9861  CA  ASP A 653      19.348   1.840  72.230  1.00 18.43       0.186 C
ATOM   9863  C   ASP A 653      17.917   2.315  72.340  1.00 18.01       0.241 C
ATOM   9864  O   ASP A 653      17.171   1.774  73.155  1.00 21.66      -0.271 OA
ATOM   9865  CB  ASP A 653      20.206   2.600  73.251  1.00 31.43       0.147 C
ATOM   9868  CG  ASP A 653      21.599   1.992  73.313  1.00 37.74       0.175 C
ATOM   9869  OD1 ASP A 653      21.724   0.754  73.224  1.00 43.73      -0.648 OA
ATOM   9870  OD2 ASP A 653      22.564   2.769  73.410  1.00 45.03      -0.648 OA
ATOM   9871  N   ASN A 654      17.516   3.345  71.587  1.00 15.04      -0.346 N
ATOM   9872  HN  ASN A 654      18.160   3.798  70.939  1.00  0.00       0.163 HD
ATOM   9873  CA  ASN A 654      16.139   3.806  71.713  1.00 12.58       0.185 C
ATOM   9875  C   ASN A 654      15.188   2.828  70.987  1.00 15.37       0.244 C
ATOM   9876  O   ASN A 654      14.050   2.627  71.416  1.00 15.10      -0.271 OA
ATOM   9877  CB  ASN A 654      16.015   5.184  71.051  1.00 18.22       0.137 C
ATOM   9880  CG  ASN A 654      14.619   5.756  71.167  1.00 23.12       0.217 C
ATOM   9881  ND2 ASN A 654      14.007   6.209  70.075  1.00 24.25      -0.370 N
ATOM   9882 1HD2 ASN A 654      14.456   6.192  69.159  1.00  0.00       0.159 HD
ATOM   9883 2HD2 ASN A 654      13.066   6.595  70.153  1.00  0.00       0.159 HD
ATOM   9884  OD1 ASN A 654      14.077   5.777  72.273  1.00 24.54      -0.274 OA
ATOM   9885  N   VAL A 655      15.673   2.289  69.876  1.00 15.30      -0.346 N
ATOM   9886  HN  VAL A 655      16.612   2.519  69.551  1.00  0.00       0.163 HD
ATOM   9887  CA  VAL A 655      14.818   1.343  69.116  1.00 14.02       0.180 C
ATOM   9889  C   VAL A 655      14.616   0.096  69.983  1.00 17.24       0.241 C
ATOM   9890  O   VAL A 655      13.517  -0.445  70.084  1.00 11.99      -0.271 OA
ATOM   9891  CB  VAL A 655      15.446   1.013  67.772  1.00 16.28       0.009 C
ATOM   9893  CG1 VAL A 655      14.655  -0.089  67.082  1.00  9.93       0.012 C
ATOM   9897  CG2 VAL A 655      15.503   2.227  66.802  1.00 13.24       0.012 C
ATOM   9901  N   VAL A 656      15.696  -0.369  70.621  1.00 15.78      -0.346 N
ATOM   9902  HN  VAL A 656      16.606   0.072  70.489  1.00  0.00       0.163 HD
ATOM   9903  CA  VAL A 656      15.549  -1.529  71.518  1.00 14.98       0.180 C
ATOM   9905  C   VAL A 656      14.584  -1.222  72.633  1.00 14.89       0.241 C
ATOM   9906  O   VAL A 656      13.730  -2.019  73.031  1.00 13.40      -0.271 OA
ATOM   9907  CB  VAL A 656      16.925  -1.911  72.096  1.00 11.93       0.009 C
ATOM   9909  CG1 VAL A 656      16.750  -2.974  73.193  1.00 17.56       0.012 C
ATOM   9913  CG2 VAL A 656      17.774  -2.515  70.961  1.00 17.26       0.012 C
ATOM   9917  N   ALA A 657      14.682  -0.038  73.244  1.00 16.96      -0.346 N
ATOM   9918  HN  ALA A 657      15.386   0.632  72.936  1.00  0.00       0.163 HD
ATOM   9919  CA  ALA A 657      13.784   0.309  74.358  1.00 19.31       0.172 C
ATOM   9921  C   ALA A 657      12.332   0.356  73.962  1.00 19.60       0.240 C
ATOM   9922  O   ALA A 657      11.423  -0.087  74.682  1.00 16.91      -0.271 OA
ATOM   9923  CB  ALA A 657      14.164   1.700  74.935  1.00 13.06       0.042 C
ATOM   9927  N   LYS A 658      12.009   0.928  72.787  1.00 19.42      -0.346 N
ATOM   9928  HN  LYS A 658      12.734   1.328  72.191  1.00  0.00       0.163 HD
ATOM   9929  CA  LYS A 658      10.603   0.970  72.373  1.00 18.84       0.176 C
ATOM   9931  C   LYS A 658      10.091  -0.435  72.098  1.00 15.42       0.241 C
ATOM   9932  O   LYS A 658       8.920  -0.706  72.325  1.00 20.71      -0.271 OA
ATOM   9933  CB  LYS A 658      10.379   1.814  71.120  1.00 19.71       0.035 C
ATOM   9936  CG  LYS A 658      10.735   3.274  71.180  1.00 31.71       0.004 C
ATOM   9939  CD  LYS A 658      10.059   3.997  72.323  1.00 39.90       0.027 C
ATOM   9942  CE  LYS A 658      10.982   5.087  72.855  1.00 58.68       0.229 C
ATOM   9945  NZ  LYS A 658      10.229   6.255  73.387  1.00 65.76      -0.079 N
ATOM   9946  HZ1 LYS A 658      10.847   6.985  73.742  1.00  0.00       0.274 HD
ATOM   9947  HZ2 LYS A 658       9.554   5.967  74.095  1.00  0.00       0.274 HD
ATOM   9948  HZ3 LYS A 658       9.584   6.626  72.689  1.00  0.00       0.274 HD
ATOM   9949  N   ALA A 659      10.934  -1.260  71.472  1.00 12.62      -0.346 N
ATOM   9950  HN  ALA A 659      11.865  -0.941  71.202  1.00  0.00       0.163 HD
ATOM   9951  CA  ALA A 659      10.505  -2.627  71.178  1.00 16.47       0.172 C
ATOM   9953  C   ALA A 659      10.181  -3.369  72.472  1.00 15.16       0.240 C
ATOM   9954  O   ALA A 659       9.163  -4.057  72.554  1.00 16.46      -0.271 OA
ATOM   9955  CB  ALA A 659      11.647  -3.422  70.556  1.00 13.59       0.042 C
ATOM   9959  N   LYS A 660      11.060  -3.228  73.488  1.00 16.35      -0.346 N
ATOM   9960  HN  LYS A 660      11.879  -2.632  73.366  1.00  0.00       0.163 HD
ATOM   9961  CA  LYS A 660      10.856  -3.912  74.749  1.00 17.57       0.176 C
ATOM   9963  C   LYS A 660       9.602  -3.513  75.484  1.00 19.63       0.241 C
ATOM   9964  O   LYS A 660       9.020  -4.310  76.246  1.00 20.71      -0.271 OA
ATOM   9965  CB  LYS A 660      12.061  -3.624  75.688  1.00 19.22       0.035 C
ATOM   9968  CG  LYS A 660      13.245  -4.509  75.307  1.00 16.29       0.004 C
ATOM   9971  CD  LYS A 660      14.388  -4.199  76.311  1.00 30.00       0.027 C
ATOM   9974  CE  LYS A 660      15.522  -5.167  75.965  1.00 30.29       0.229 C
ATOM   9977  NZ  LYS A 660      16.602  -5.172  76.995  1.00 35.75      -0.079 N
ATOM   9978  HZ1 LYS A 660      17.358  -5.817  76.764  1.00  0.00       0.274 HD
ATOM   9979  HZ2 LYS A 660      16.224  -5.365  77.922  1.00  0.00       0.274 HD
ATOM   9980  HZ3 LYS A 660      16.959  -4.230  77.157  1.00  0.00       0.274 HD
ATOM   9981  N   GLU A 661       9.065  -2.332  75.295  1.00 19.01      -0.346 N
ATOM   9982  HN  GLU A 661       9.562  -1.662  74.708  1.00  0.00       0.163 HD
ATOM   9983  CA  GLU A 661       7.801  -1.932  75.879  1.00 20.63       0.177 C
ATOM   9985  C   GLU A 661       6.630  -2.746  75.337  1.00 25.88       0.241 C
ATOM   9986  O   GLU A 661       5.583  -2.708  76.004  1.00 25.44      -0.271 OA
ATOM   9987  CB  GLU A 661       7.496  -0.458  75.536  1.00 26.66       0.045 C
ATOM   9990  CG  GLU A 661       8.364   0.543  76.275  1.00 36.24       0.116 C
ATOM   9993  CD  GLU A 661       8.221   1.976  75.802  1.00 40.26       0.172 C
ATOM   9994  OE1 GLU A 661       7.216   2.326  75.143  1.00 43.64      -0.648 OA
ATOM   9995  OE2 GLU A 661       9.124   2.799  76.089  1.00 51.64      -0.648 OA
ATOM   9996  N   LEU A 662       6.753  -3.451  74.198  1.00 18.69      -0.346 N
ATOM   9997  HN  LEU A 662       7.639  -3.469  73.694  1.00  0.00       0.163 HD
ATOM   9998  CA  LEU A 662       5.597  -4.191  73.694  1.00 17.32       0.177 C
ATOM  10000  C   LEU A 662       5.602  -5.622  74.228  1.00 23.14       0.241 C
ATOM  10001  O   LEU A 662       4.626  -6.346  74.062  1.00 25.47      -0.271 OA
ATOM  10002  CB  LEU A 662       5.736  -4.281  72.164  1.00 17.73       0.038 C
ATOM  10005  CG  LEU A 662       5.793  -2.907  71.465  1.00 17.55      -0.020 C
ATOM  10007  CD1 LEU A 662       5.781  -3.161  69.954  1.00 17.89       0.009 C
ATOM  10011  CD2 LEU A 662       4.597  -2.051  71.877  1.00 15.11       0.009 C
ATOM  10015  N   LEU A 663       6.715  -6.012  74.825  1.00 22.37      -0.345 N
ATOM  10016  HN  LEU A 663       7.448  -5.328  75.016  1.00  0.00       0.163 HD
ATOM  10017  CA  LEU A 663       6.913  -7.403  75.215  1.00 34.15       0.186 C
ATOM  10019  C   LEU A 663       6.541  -7.705  76.664  1.00 40.91       0.196 C
ATOM  10020  O   LEU A 663       6.387  -6.758  77.468  1.00 40.04      -0.646 OA
ATOM  10022  CB  LEU A 663       8.367  -7.771  74.956  1.00 28.83       0.040 C
ATOM  10024  CG  LEU A 663       8.859  -7.804  73.505  1.00 33.53      -0.020 C
ATOM  10026  CD1 LEU A 663      10.305  -8.260  73.534  1.00 34.21       0.009 C
ATOM  10030  CD2 LEU A 663       8.050  -8.726  72.606  1.00 31.03       0.009 C
ATOM  10034  N   LEU A 664       6.076  -8.851  76.892  1.00 47.30      -0.640 OA
ATOM  10035  HN  SER B   2      38.529  53.617  57.205  1.00 30.28      -0.064 N
ATOM  10038  HN1 SER B   2      38.792  54.532  56.838  1.00  0.00       0.275 HD
ATOM  10039  HN2 SER B   2      38.963  53.425  58.108  1.00  0.00       0.275 HD
ATOM  10040  HN3 SER B   2      37.554  53.587  57.502  1.00  0.00       0.275 HD
ATOM  10041  CA  SER B   2      38.842  52.564  56.194  1.00 32.90       0.297 C
ATOM  10043  C   SER B   2      38.073  52.838  54.916  1.00 31.56       0.251 C
ATOM  10044  O   SER B   2      37.113  53.608  54.968  1.00 36.26      -0.271 OA
ATOM  10045  CB  SER B   2      38.450  51.199  56.741  1.00 32.69       0.206 C
ATOM  10048  OG  SER B   2      38.913  51.028  58.053  1.00 38.71      -0.398 OA
ATOM  10049  HG  SER B   2      38.668  50.176  58.394  1.00  0.00       0.209 HD
ATOM  10050  N   SER B   3      38.513  52.290  53.793  1.00 32.65      -0.344 N
ATOM  10051  HN  SER B   3      39.350  51.707  53.797  1.00  0.00       0.163 HD
ATOM  10052  CA  SER B   3      37.786  52.530  52.550  1.00 30.07       0.200 C
ATOM  10054  C   SER B   3      36.557  51.607  52.626  1.00 27.16       0.243 C
ATOM  10055  O   SER B   3      36.523  50.683  53.439  1.00 21.70      -0.271 OA
ATOM  10056  CB  SER B   3      38.637  52.176  51.332  1.00 32.32       0.199 C
ATOM  10059  OG  SER B   3      39.076  50.826  51.481  1.00 28.94      -0.398 OA
ATOM  10060  HG  SER B   3      39.605  50.606  50.723  1.00  0.00       0.209 HD
ATOM  10061  N   ARG B   4      35.608  51.868  51.739  1.00 23.91      -0.346 N
ATOM  10062  HN  ARG B   4      35.725  52.652  51.097  1.00  0.00       0.163 HD
ATOM  10063  CA  ARG B   4      34.394  51.052  51.662  1.00 19.94       0.176 C
ATOM  10065  C   ARG B   4      34.793  49.631  51.292  1.00 20.20       0.241 C
ATOM  10066  O   ARG B   4      34.175  48.710  51.785  1.00 18.18      -0.271 OA
ATOM  10067  CB  ARG B   4      33.463  51.632  50.571  1.00 18.32       0.036 C
ATOM  10070  CG  ARG B   4      33.078  53.049  50.975  1.00 27.02       0.023 C
ATOM  10073  CD  ARG B   4      31.841  53.499  50.193  1.00 32.15       0.138 C
ATOM  10076  NE  ARG B   4      30.724  52.988  50.974  1.00 36.00      -0.227 N
ATOM  10077  HE  ARG B   4      30.816  52.020  51.282  1.00  0.00       0.177 HD
ATOM  10078  CZ  ARG B   4      29.615  53.589  51.341  1.00 32.57       0.665 C
ATOM  10079  NH1 ARG B   4      29.336  54.850  51.000  1.00 35.49      -0.235 N
ATOM  10080 1HH1 ARG B   4      29.967  55.418  50.434  1.00  0.00       0.174 HD
ATOM  10081 2HH1 ARG B   4      28.475  55.317  51.285  1.00  0.00       0.174 HD
ATOM  10082  NH2 ARG B   4      28.797  52.853  52.075  1.00 25.62      -0.235 N
ATOM  10083 1HH2 ARG B   4      29.010  51.890  52.335  1.00  0.00       0.174 HD
ATOM  10084 2HH2 ARG B   4      27.936  53.320  52.360  1.00  0.00       0.174 HD
ATOM  10085  N   LYS B   5      35.817  49.479  50.425  1.00 18.36      -0.346 N
ATOM  10086  HN  LYS B   5      36.305  50.287  50.037  1.00  0.00       0.163 HD
ATOM  10087  CA  LYS B   5      36.203  48.111  50.060  1.00 19.84       0.176 C
ATOM  10089  C   LYS B   5      36.713  47.318  51.243  1.00 20.42       0.241 C
ATOM  10090  O   LYS B   5      36.413  46.135  51.356  1.00 16.91      -0.271 OA
ATOM  10091  CB  LYS B   5      37.274  48.080  48.970  1.00 30.23       0.035 C
ATOM  10094  CG  LYS B   5      36.819  48.856  47.726  1.00 50.18       0.004 C
ATOM  10097  CD  LYS B   5      37.150  50.332  47.886  1.00 70.31       0.027 C
ATOM  10100  CE  LYS B   5      36.080  51.279  47.394  1.00 75.22       0.229 C
ATOM  10103  NZ  LYS B   5      36.232  52.654  47.952  1.00 71.59      -0.079 N
ATOM  10104  HZ1 LYS B   5      35.510  53.293  47.620  1.00  0.00       0.274 HD
ATOM  10105  HZ2 LYS B   5      37.164  53.025  47.765  1.00  0.00       0.274 HD
ATOM  10106  HZ3 LYS B   5      36.264  52.635  48.971  1.00  0.00       0.274 HD
ATOM  10107  N   GLU B   6      37.511  47.972  52.084  1.00 15.10      -0.346 N
ATOM  10108  HN  GLU B   6      37.779  48.939  51.900  1.00  0.00       0.163 HD
ATOM  10109  CA  GLU B   6      37.996  47.280  53.275  1.00 19.00       0.177 C
ATOM  10111  C   GLU B   6      36.830  46.920  54.180  1.00 14.48       0.241 C
ATOM  10112  O   GLU B   6      36.822  45.812  54.744  1.00 15.00      -0.271 OA
ATOM  10113  CB  GLU B   6      38.979  48.220  54.013  1.00 26.22       0.045 C
ATOM  10116  CG  GLU B   6      39.254  47.714  55.418  1.00 41.76       0.116 C
ATOM  10119  CD  GLU B   6      40.621  48.023  55.993  1.00 54.77       0.172 C
ATOM  10120  OE1 GLU B   6      40.939  49.223  56.120  1.00 52.92      -0.648 OA
ATOM  10121  OE2 GLU B   6      41.349  47.061  56.336  1.00 56.14      -0.648 OA
ATOM  10122  N   LEU B   7      35.862  47.849  54.352  1.00 14.34      -0.346 N
ATOM  10123  HN  LEU B   7      35.934  48.775  53.930  1.00  0.00       0.163 HD
ATOM  10124  CA  LEU B   7      34.695  47.469  55.176  1.00 11.91       0.177 C
ATOM  10126  C   LEU B   7      33.906  46.309  54.584  1.00 14.66       0.241 C
ATOM  10127  O   LEU B   7      33.420  45.436  55.338  1.00 13.18      -0.271 OA
ATOM  10128  CB  LEU B   7      33.746  48.645  55.410  1.00 14.53       0.038 C
ATOM  10131  CG  LEU B   7      34.529  49.840  56.056  1.00 16.36      -0.020 C
ATOM  10133  CD1 LEU B   7      33.648  51.076  55.982  1.00 24.06       0.009 C
ATOM  10137  CD2 LEU B   7      34.915  49.448  57.463  1.00 14.90       0.009 C
ATOM  10141  N   ALA B   8      33.745  46.300  53.258  1.00 10.83      -0.346 N
ATOM  10142  HN  ALA B   8      34.111  47.063  52.688  1.00  0.00       0.163 HD
ATOM  10143  CA  ALA B   8      33.031  45.173  52.628  1.00 16.09       0.172 C
ATOM  10145  C   ALA B   8      33.853  43.900  52.700  1.00 14.57       0.240 C
ATOM  10146  O   ALA B   8      33.341  42.774  52.828  1.00 14.10      -0.271 OA
ATOM  10147  CB  ALA B   8      32.688  45.497  51.173  1.00 12.12       0.042 C
ATOM  10151  N   ASN B   9      35.205  43.997  52.706  1.00 11.96      -0.348 N
ATOM  10152  HN  ASN B   9      35.651  44.911  52.631  1.00  0.00       0.163 HD
ATOM  10153  CA  ASN B   9      36.017  42.799  52.819  1.00 12.53       0.185 C
ATOM  10155  C   ASN B   9      35.844  42.126  54.181  1.00 13.70       0.241 C
ATOM  10156  O   ASN B   9      36.165  40.919  54.258  1.00 13.19      -0.271 OA
ATOM  10157  CB  ASN B   9      37.509  43.047  52.545  1.00 13.80       0.137 C
ATOM  10160  CG  ASN B   9      37.734  43.247  51.063  1.00 18.35       0.217 C
ATOM  10161  ND2 ASN B   9      38.870  43.880  50.734  1.00 17.90      -0.370 N
ATOM  10162 1HD2 ASN B   9      39.508  44.161  51.478  1.00  0.00       0.159 HD
ATOM  10163 2HD2 ASN B   9      39.022  44.015  49.734  1.00  0.00       0.159 HD
ATOM  10164  OD1 ASN B   9      36.961  42.907  50.162  1.00 18.04      -0.274 OA
ATOM  10165  N   ALA B  10      35.378  42.818  55.214  1.00 14.50      -0.346 N
ATOM  10166  HN  ALA B  10      35.170  43.811  55.112  1.00  0.00       0.163 HD
ATOM  10167  CA  ALA B  10      35.164  42.153  56.498  1.00 14.04       0.172 C
ATOM  10169  C   ALA B  10      34.051  41.106  56.352  1.00 15.17       0.240 C
ATOM  10170  O   ALA B  10      34.152  40.013  56.928  1.00 15.10      -0.271 OA
ATOM  10171  CB  ALA B  10      34.779  43.154  57.583  1.00 13.57       0.042 C
ATOM  10175  N   ILE B  11      33.040  41.383  55.511  1.00 10.60      -0.346 N
ATOM  10176  HN  ILE B  11      33.002  42.291  55.047  1.00  0.00       0.163 HD
ATOM  10177  CA  ILE B  11      31.995  40.396  55.256  1.00 10.35       0.180 C
ATOM  10179  C   ILE B  11      32.576  39.186  54.543  1.00 11.94       0.241 C
ATOM  10180  O   ILE B  11      32.289  38.010  54.844  1.00 13.81      -0.271 OA
ATOM  10181  CB  ILE B  11      30.870  41.015  54.343  1.00 11.77       0.013 C
ATOM  10183  CG1 ILE B  11      30.107  42.096  55.095  1.00 12.30       0.002 C
ATOM  10186  CG2 ILE B  11      29.934  39.889  53.888  1.00 10.18       0.012 C
ATOM  10190  CD1 ILE B  11      29.355  43.071  54.179  1.00 14.02       0.005 C
ATOM  10194  N   ARG B  12      33.475  39.431  53.580  1.00 12.21      -0.346 N
ATOM  10195  HN  ARG B  12      33.714  40.396  53.352  1.00  0.00       0.163 HD
ATOM  10196  CA  ARG B  12      34.113  38.351  52.858  1.00 13.30       0.176 C
ATOM  10198  C   ARG B  12      34.973  37.484  53.791  1.00 15.58       0.241 C
ATOM  10199  O   ARG B  12      34.903  36.250  53.715  1.00 15.79      -0.271 OA
ATOM  10200  CB  ARG B  12      34.952  38.907  51.685  1.00 10.41       0.036 C
ATOM  10203  CG  ARG B  12      34.140  39.698  50.669  1.00 10.05       0.023 C
ATOM  10206  CD  ARG B  12      35.008  40.037  49.424  1.00 17.76       0.138 C
ATOM  10209  NE  ARG B  12      34.065  40.454  48.380  1.00 17.49      -0.227 N
ATOM  10210  HE  ARG B  12      33.558  39.722  47.883  1.00  0.00       0.177 HD
ATOM  10211  CZ  ARG B  12      33.821  41.718  48.032  1.00 14.83       0.665 C
ATOM  10212  NH1 ARG B  12      34.464  42.762  48.554  1.00 16.68      -0.235 N
ATOM  10213 1HH1 ARG B  12      34.277  43.729  48.288  1.00  0.00       0.174 HD
ATOM  10214 2HH1 ARG B  12      35.169  42.597  49.272  1.00  0.00       0.174 HD
ATOM  10215  NH2 ARG B  12      32.900  41.933  47.094  1.00 15.02      -0.235 N
ATOM  10216 1HH2 ARG B  12      32.713  42.900  46.828  1.00  0.00       0.174 HD
ATOM  10217 2HH2 ARG B  12      32.408  41.134  46.694  1.00  0.00       0.174 HD
ATOM  10218  N   ALA B  13      35.760  38.097  54.657  1.00 12.77      -0.346 N
ATOM  10219  HN  ALA B  13      35.762  39.116  54.693  1.00  0.00       0.163 HD
ATOM  10220  CA  ALA B  13      36.636  37.343  55.572  1.00 12.54       0.172 C
ATOM  10222  C   ALA B  13      35.801  36.500  56.517  1.00 11.43       0.240 C
ATOM  10223  O   ALA B  13      35.946  35.266  56.552  1.00 12.01      -0.271 OA
ATOM  10224  CB  ALA B  13      37.544  38.332  56.313  1.00 14.26       0.042 C
ATOM  10228  N   LEU B  14      34.743  37.085  57.142  1.00 11.24      -0.346 N
ATOM  10229  HN  LEU B  14      34.511  38.066  56.984  1.00  0.00       0.163 HD
ATOM  10230  CA  LEU B  14      33.949  36.253  58.050  1.00 11.74       0.177 C
ATOM  10232  C   LEU B  14      33.216  35.133  57.307  1.00 13.76       0.241 C
ATOM  10233  O   LEU B  14      33.091  34.049  57.862  1.00 12.52      -0.271 OA
ATOM  10234  CB  LEU B  14      32.898  37.116  58.763  1.00 12.13       0.038 C
ATOM  10237  CG  LEU B  14      33.459  38.143  59.756  1.00 16.76      -0.020 C
ATOM  10239  CD1 LEU B  14      32.359  39.104  60.198  1.00 11.52       0.009 C
ATOM  10243  CD2 LEU B  14      34.053  37.446  60.974  1.00 17.05       0.009 C
ATOM  10247  N   SER B  15      32.704  35.448  56.100  1.00 11.82      -0.344 N
ATOM  10248  HN  SER B  15      32.829  36.373  55.689  1.00  0.00       0.163 HD
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ATOM  10249  CA  SER B  15      31.958  34.390  55.410  1.00 13.27      0.200 C
ATOM  10251  C   SER B  15      32.852  33.221  55.040  1.00 15.09      0.243 C
ATOM  10252  O   SER B  15      32.531  32.060  55.257  1.00 14.80     -0.271 OA
ATOM  10253  CB  SER B  15      31.333  35.024  54.138  1.00 10.84      0.199 C
ATOM  10256  OG  SER B  15      30.331  35.983  54.517  1.00 14.33     -0.398 OA
ATOM  10257  HG  SER B  15      29.949  36.371  53.739  1.00  0.00      0.209 HD
ATOM  10258  N   MET B  16      34.009  33.490  54.405  1.00 10.98     -0.346 N
ATOM  10259  HN  MET B  16      34.304  34.452  54.236  1.00  0.00      0.163 HD
ATOM  10260  CA  MET B  16      34.841  32.348  53.960  1.00 13.74      0.177 C
ATOM  10262  C   MET B  16      35.395  31.603  55.150  1.00 11.81      0.241 C
ATOM  10263  O   MET B  16      35.593  30.366  55.054  1.00 11.79     -0.271 OA
ATOM  10264  CB  MET B  16      35.926  32.737  52.950  1.00 15.48      0.045 C
ATOM  10267  CG  MET B  16      37.095  33.540  53.490  1.00 19.23      0.076 C
ATOM  10270  SD  MET B  16      38.165  34.191  52.132  1.00 22.00     -0.173 SA
ATOM  10271  CE  MET B  16      39.300  35.142  53.134  1.00 20.66      0.089 C
ATOM  10275  N   ASP B  17      35.711  32.310  56.239  1.00 11.88     -0.346 N
ATOM  10276  HN  ASP B  17      35.553  33.317  56.273  1.00  0.00      0.163 HD
ATOM  10277  CA  ASP B  17      36.292  31.600  57.385  1.00 12.15      0.186 C
ATOM  10279  C   ASP B  17      35.222  30.791  58.130  1.00 15.22      0.241 C
ATOM  10280  O   ASP B  17      35.522  29.698  58.615  1.00 13.77     -0.271 OA
ATOM  10281  CB  ASP B  17      36.933  32.614  58.359  1.00  9.03      0.147 C
ATOM  10284  CG  ASP B  17      38.181  33.304  57.815  1.00 16.62      0.175 C
ATOM  10285  OD1 ASP B  17      38.841  32.822  56.850  1.00 19.77     -0.648 OA
ATOM  10286  OD2 ASP B  17      38.514  34.373  58.353  1.00 17.50     -0.648 OA
ATOM  10287  N   ALA B  18      33.970  31.297  58.201  1.00 12.24     -0.346 N
ATOM  10288  HN  ALA B  18      33.731  32.187  57.764  1.00  0.00      0.163 HD
ATOM  10289  CA  ALA B  18      32.963  30.508  58.937  1.00 13.25      0.172 C
ATOM  10291  C   ALA B  18      32.583  29.269  58.132  1.00 15.51      0.240 C
ATOM  10292  O   ALA B  18      32.433  28.182  58.733  1.00 13.10     -0.271 OA
ATOM  10293  CB  ALA B  18      31.765  31.385  59.308  1.00 13.36      0.042 C
ATOM  10297  N   VAL B  19      32.540  29.367  56.795  1.00 14.80     -0.346 N
ATOM  10298  HN  VAL B  19      32.692  30.275  56.355  1.00  0.00      0.163 HD
ATOM  10299  CA  VAL B  19      32.278  28.194  55.952  1.00 14.14      0.180 C
ATOM  10301  C   VAL B  19      33.410  27.185  56.095  1.00 15.21      0.241 C
ATOM  10302  O   VAL B  19      33.174  25.968  56.155  1.00 15.20     -0.271 OA
ATOM  10303  CB  VAL B  19      32.127  28.594  54.465  1.00 17.45      0.009 C
ATOM  10305  CG1 VAL B  19      32.042  27.392  53.541  1.00 12.49      0.012 C
ATOM  10309  CG2 VAL B  19      30.818  29.413  54.311  1.00 14.03      0.012 C
ATOM  10313  N   GLN B  20      34.658  27.639  56.132  1.00 14.41     -0.346 N
ATOM  10314  HN  GLN B  20      34.828  28.642  56.063  1.00  0.00      0.163 HD
ATOM  10315  CA  GLN B  20      35.792  26.728  56.270  1.00 11.01      0.177 C
ATOM  10317  C   GLN B  20      35.746  25.989  57.600  1.00 14.32      0.241 C
ATOM  10318  O   GLN B  20      35.938  24.742  57.630  1.00 14.60     -0.271 OA
ATOM  10319  CB  GLN B  20      37.117  27.512  56.124  1.00 17.25      0.044 C
ATOM  10322  CG  GLN B  20      38.319  26.594  55.863  1.00 17.36      0.105 C
ATOM  10325  CD  GLN B  20      38.129  25.814  54.574  1.00 22.45      0.215 C
ATOM  10326  NE2 GLN B  20      38.466  24.523  54.569  1.00 21.27     -0.370 N
ATOM  10327 1HE2 GLN B  20      38.852  24.080  55.403  1.00  0.00      0.159 HD
ATOM  10328 2HE2 GLN B  20      38.338  23.999  53.703  1.00  0.00      0.159 HD
ATOM  10329  OE1 GLN B  20      37.658  26.355  53.556  1.00 21.04     -0.274 OA
ATOM  10330  N   LYS B  21      35.476  26.696  58.690  1.00 11.91     -0.346 N
ATOM  10331  HN  LYS B  21      35.287  27.695  58.613  1.00  0.00      0.163 HD
ATOM  10332  CA  LYS B  21      35.448  26.044  60.009  1.00 15.16      0.176 C
ATOM  10334  C   LYS B  21      34.348  25.004  60.117  1.00 19.25      0.241 C
ATOM  10335  O   LYS B  21      34.504  23.926  60.703  1.00 16.22     -0.271 OA
ATOM  10336  CB  LYS B  21      35.359  27.093  61.128  1.00 18.04      0.035 C
ATOM  10339  CG  LYS B  21      35.299  26.474  62.534  1.00 18.23      0.004 C
ATOM  10342  CD  LYS B  21      35.780  27.424  63.598  1.00 26.73      0.027 C
ATOM  10345  CE  LYS B  21      35.743  26.731  64.966  1.00 25.41      0.229 C
ATOM  10348  NZ  LYS B  21      34.373  26.301  65.359  1.00 30.76     -0.079 N
ATOM  10349  HZ1 LYS B  21      34.348  25.840  66.268  1.00  0.00      0.274 HD
ATOM  10350  HZ2 LYS B  21      33.954  25.712  64.640  1.00  0.00      0.274 HD
ATOM  10351  HZ3 LYS B  21      33.722  27.086  65.330  1.00  0.00      0.274 HD
ATOM  10352  N   ALA B  22      33.184  25.254  59.504  1.00 13.28     -0.346 N
ATOM  10353  HN  ALA B  22      33.067  26.136  59.004  1.00  0.00      0.163 HD
ATOM  10354  CA  ALA B  22      32.078  24.304  59.529  1.00 12.88      0.172 C
ATOM  10356  C   ALA B  22      32.261  23.164  58.522  1.00 16.85      0.240 C
ATOM  10357  O   ALA B  22      31.540  22.156  58.551  1.00 20.14     -0.271 OA
ATOM  10358  CB  ALA B  22      30.793  25.022  59.093  1.00 15.21      0.042 C
ATOM  10362  N   LYS B  23      33.121  23.367  57.550  1.00 13.42     -0.346 N
ATOM  10363  HN  LYS B  23      33.687  24.214  57.606  1.00  0.00      0.163 HD
ATOM  10364  CA  LYS B  23      33.345  22.504  56.403  1.00 16.08      0.176 C
ATOM  10366  C   LYS B  23      32.063  22.251  55.642  1.00 16.93      0.241 C
ATOM  10367  O   LYS B  23      31.770  21.158  55.144  1.00 13.57     -0.271 OA
ATOM  10368  CB  LYS B  23      33.957  21.172  56.852  1.00 24.48      0.035 C
ATOM  10371  CG  LYS B  23      35.441  21.350  57.218  1.00 32.18      0.004 C
ATOM  10374  CD  LYS B  23      36.076  19.985  57.467  1.00 44.51      0.027 C
ATOM  10377  CE  LYS B  23      37.326  20.118  58.324  1.00 57.85      0.229 C
ATOM  10380  NZ  LYS B  23      37.001  19.900  59.766  1.00 58.85     -0.079 N
ATOM  10381  HZ1 LYS B  23      37.839  19.989  60.341  1.00  0.00      0.274 HD
ATOM  10382  HZ2 LYS B  23      36.531  19.007  59.917  1.00  0.00      0.274 HD
ATOM  10383  HZ3 LYS B  23      36.256  20.520  60.084  1.00  0.00      0.274 HD
ATOM  10384  N   SER B  24      31.204  23.279  55.574  1.00 14.42     -0.344 N
ATOM  10385  HN  SER B  24      31.468  24.183  55.965  1.00  0.00      0.163 HD
ATOM  10386  CA  SER B  24      29.884  23.118  54.942  1.00 14.31      0.200 C
ATOM  10388  C   SER B  24      29.369  24.537  54.662  1.00 18.32      0.242 C
ATOM  10389  O   SER B  24      29.623  25.430  55.513  1.00 12.57     -0.271 OA
ATOM  10390  CB  SER B  24      28.967  22.491  56.025  1.00 15.40      0.199 C
ATOM  10393  OG  SER B  24      27.653  22.258  55.480  1.00 15.69     -0.398 OA
ATOM  10394  HG  SER B  24      27.091  21.874  56.143  1.00  0.00      0.209 HD
ATOM  10395  N   GLY B  25      28.616  24.712  53.571  1.00 15.20     -0.350 N
ATOM  10396  HN  GLY B  25      28.416  23.959  52.913  1.00  0.00      0.163 HD
ATOM  10397  CA  GLY B  25      28.099  26.078  53.397  1.00 16.65      0.225 C
ATOM  10400  C   GLY B  25      28.551  26.699  52.086  1.00 15.87      0.236 C
ATOM  10401  O   GLY B  25      29.187  26.069  51.254  1.00 17.13     -0.272 OA
ATOM  10402  N   HIS B  26      28.088  27.928  51.883  1.00 14.91     -0.346 N
ATOM  10403  HN  HIS B  26      27.635  28.414  52.657  1.00  0.00      0.163 HD
ATOM  10404  CA  HIS B  26      28.201  28.613  50.595  1.00 13.77      0.182 C
ATOM  10406  C   HIS B  26      28.889  29.971  50.695  1.00 15.01      0.243 C
ATOM  10407  O   HIS B  26      28.296  30.964  51.127  1.00 14.72     -0.271 OA
ATOM  10408  CB  HIS B  26      26.760  28.860  50.073  1.00 19.35      0.093 C
ATOM  10411  CG  HIS B  26      25.879  27.666  50.019  1.00 21.17      0.028 A
ATOM  10412  CD2 HIS B  26      25.430  26.919  48.969  1.00 18.30      0.114 A
ATOM  10414  ND1 HIS B  26      25.383  27.085  51.179  1.00 12.92     -0.354 N
ATOM  10415  HD1 HIS B  26      25.553  27.417  52.128  1.00  0.00      0.166 HD
ATOM  10416  CE1 HIS B  26      24.650  26.025  50.850  1.00 23.73      0.180 A
ATOM  10418  NE2 HIS B  26      24.656  25.913  49.537  1.00 22.43     -0.360 N
ATOM  10419  HE2 HIS B  26      24.163  25.191  49.012  1.00  0.00      0.160 HD
ATOM  10420  N   PRO B  27      30.147  30.005  50.279  1.00 16.37     -0.337 N
ATOM  10421  CA  PRO B  27      30.940  31.220  50.345  1.00 13.45      0.179 C
ATOM  10423  C   PRO B  27      30.702  32.163  49.172  1.00 12.81      0.241 C
ATOM  10424  O   PRO B  27      30.938  33.363  49.277  1.00 12.49     -0.271 OA
ATOM  10425  CB  PRO B  27      32.381  30.674  50.315  1.00 16.18      0.037 C
ATOM  10428  CG  PRO B  27      32.330  29.360  49.625  1.00 18.24      0.022 C
ATOM  10431  CD  PRO B  27      30.938  28.809  49.855  1.00 16.78      0.127 C
ATOM  10434  N   GLY B  28      30.321  31.581  48.034  1.00 13.62     -0.351 N
ATOM  10435  HN  GLY B  28      30.089  30.588  48.047  1.00  0.00      0.163 HD
ATOM  10436  CA  GLY B  28      30.221  32.309  46.764  1.00 13.45      0.225 C
ATOM  10439  C   GLY B  28      29.391  33.577  46.769  1.00 14.96      0.236 C
ATOM  10440  O   GLY B  28      29.900  34.672  46.448  1.00 15.30     -0.272 OA
ATOM  10442  N   ALA B  29      28.088  33.480  47.073  1.00 14.45     -0.347 N
ATOM  10442  HN  ALA B  29      27.713  32.566  47.325  1.00  0.00      0.163 HD
ATOM  10443  CA  ALA B  29      27.178  34.632  47.059  1.00 15.33      0.172 C
ATOM  10445  C   ALA B  29      27.490  35.718  48.074  1.00 10.67      0.243 C
ATOM  10446  O   ALA B  29      27.539  36.917  47.742  1.00 10.99     -0.271 OA
ATOM  10447  CB  ALA B  29      25.730  34.151  47.182  1.00 18.24      0.042 C
ATOM  10451  N   PRO B  30      27.861  35.387  49.309  1.00 12.33     -0.337 N
ATOM  10452  CA  PRO B  30      28.280  36.385  50.299  1.00 10.90      0.179 C
ATOM  10454  C   PRO B  30      29.516  37.137  49.813  1.00 14.35      0.241 C
ATOM  10455  O   PRO B  30      29.622  38.352  49.957  1.00 15.01     -0.271 OA
ATOM  10456  CB  PRO B  30      28.718  35.540  51.526  1.00 12.42      0.037 C
ATOM  10459  CG  PRO B  30      27.739  34.384  51.433  1.00 15.72      0.022 C
ATOM  10462  CD  PRO B  30      27.701  34.052  49.940  1.00 11.07      0.127 C
ATOM  10465  N   MET B  31      30.481  36.449  49.165  1.00 14.35     -0.346 N
ATOM  10466  HN  MET B  31      30.392  35.443  49.023  1.00  0.00      0.163 HD
ATOM  10467  CA  MET B  31      31.665  37.173  48.666  1.00 12.00      0.177 C
ATOM  10469  C   MET B  31      31.284  38.031  47.452  1.00 11.38      0.240 C
ATOM  10470  O   MET B  31      31.851  39.106  47.277  1.00 14.31     -0.271 OA
ATOM  10471  CB  MET B  31      32.796  36.188  48.296  1.00 13.03      0.045 C
ATOM  10474  CG  MET B  31      33.299  35.461  49.579  1.00 15.23      0.076 C
ATOM  10477  SD  MET B  31      34.344  34.076  49.109  1.00 21.81     -0.173 SA
ATOM  10478  CE  MET B  31      35.864  34.915  48.614  1.00 24.26      0.089 C
ATOM  10482  N   GLY B  32      30.343  37.565  46.616  1.00 10.99     -0.351 N
ATOM  10483  HN  GLY B  32      29.874  36.680  46.809  1.00  0.00      0.163 HD
ATOM  10484  CA  GLY B  32      29.992  38.353  45.407  1.00 11.71      0.225 C
ATOM  10487  C   GLY B  32      29.088  39.528  45.768  1.00 14.22      0.236 C
ATOM  10488  O   GLY B  32      29.184  40.582  45.123  1.00 13.00     -0.272 OA
ATOM  10489  N   MET B  33      28.285  39.483  46.838  1.00  9.58     -0.346 N
ATOM  10490  HN  MET B  33      28.296  38.658  47.438  1.00  0.00      0.163 HD
ATOM  10491  CA  MET B  33      27.402  40.584  47.159  1.00 10.08      0.177 C
ATOM  10493  C   MET B  33      27.866  41.492  48.308  1.00 13.59      0.241 C
ATOM  10494  O   MET B  33      27.117  42.424  48.617  1.00 11.58     -0.271 OA
ATOM  10495  CB  MET B  33      26.007  39.997  47.455  1.00 11.06      0.045 C
ATOM  10498  CG  MET B  33      25.367  39.252  46.362  1.00 14.95      0.076 C
ATOM  10501  SD  MET B  33      23.557  39.045  46.697  1.00 20.11     -0.173 SA
ATOM  10502  CE  MET B  33      23.077  40.706  46.154  1.00 21.66      0.089 C
ATOM  10506  N   ALA B  34      29.058  41.309  48.856  1.00  9.78     -0.346 N
ATOM  10507  HN  ALA B  34      29.679  40.588  48.488  1.00  0.00      0.163 HD
ATOM  10508  CA  ALA B  34      29.495  42.143  49.998  1.00 10.03      0.172 C
ATOM  10510  C   ALA B  34      29.575  43.634  49.714  1.00 12.17      0.240 C
ATOM  10511  O   ALA B  34      29.237  44.426  50.599  1.00  9.04     -0.271 OA
ATOM  10512  CB  ALA B  34      30.872  41.645  50.453  1.00 10.20      0.042 C
ATOM  10516  N   ASP B  35      29.950  44.069  48.511  1.00  9.02     -0.346 N
ATOM  10517  HN  ASP B  35      30.200  43.406  47.778  1.00  0.00      0.163 HD
ATOM  10518  CA  ASP B  35      29.999  45.517  48.253  1.00 13.02      0.186 C
ATOM  10520  C   ASP B  35      28.601  46.143  48.224  1.00 16.62      0.241 C
ATOM  10521  O   ASP B  35      28.387  47.277  48.714  1.00 13.15     -0.271 OA
ATOM  10522  CB  ASP B  35      30.790  45.843  46.977  1.00  9.02      0.147 C
ATOM  10525  CG  ASP B  35      32.164  45.198  46.925  1.00 16.91      0.175 C
ATOM  10526  OD1 ASP B  35      32.958  45.529  47.848  1.00 16.15     -0.648 OA
ATOM  10527  OD2 ASP B  35      32.500  44.389  46.029  1.00 16.66     -0.648 OA
ATOM  10528  N   ILE B  36      27.637  45.408  47.639  1.00  8.48     -0.346 N
ATOM  10529  HN  ILE B  36      27.871  44.505  47.227  1.00  0.00      0.163 HD
ATOM  10530  CA  ILE B  36      26.259  45.892  47.587  1.00 13.06      0.180 C
ATOM  10532  C   ILE B  36      25.692  46.018  48.999  1.00 11.59      0.241 C
ATOM  10533  O   ILE B  36      25.029  46.993  49.375  1.00 11.44     -0.271 OA
ATOM  10534  CB  ILE B  36      25.399  44.919  46.747  1.00 14.12      0.013 C
ATOM  10536  CG1 ILE B  36      25.845  44.935  45.276  1.00 11.35      0.002 C
ATOM  10539  CG2 ILE B  36      23.904  45.300  46.761  1.00 11.31      0.012 C
ATOM  10543  CD1 ILE B  36      25.388  43.686  44.518  1.00 14.88      0.005 C
ATOM  10547  N   ALA B  37      25.965  45.004  49.834  1.00  7.64     -0.346 N
ATOM  10548  HN  ALA B  37      26.548  44.228  49.521  1.00  0.00      0.163 HD
ATOM  10549  CA  ALA B  37      25.429  45.012  51.187  1.00 10.44      0.172 C
ATOM  10551  C   ALA B  37      26.063  46.108  52.022  1.00 12.37      0.240 C
ATOM  10552  O   ALA B  37      25.381  46.716  52.831  1.00 11.18     -0.271 OA
ATOM  10553  CB  ALA B  37      25.704  43.645  51.809  1.00 11.28      0.042 C
ATOM  10557  N   GLU B  38      27.319  46.404  51.764  1.00  9.16     -0.346 N
ATOM  10558  HN  GLU B  38      27.832  45.907  51.036  1.00  0.00      0.163 HD
ATOM  10559  CA  GLU B  38      27.977  47.483  52.560  1.00 10.88      0.177 C
ATOM  10561  C   GLU B  38      27.320  48.836  52.299  1.00 11.81      0.241 C
ATOM  10562  O   GLU B  38      26.953  49.557  53.229  1.00 10.97     -0.271 OA
ATOM  10563  CB  GLU B  38      29.495  47.480  52.270  1.00  9.54      0.045 C
ATOM  10566  CG  GLU B  38      30.258  48.496  53.133  1.00 17.12      0.116 C
ATOM  10569  CD  GLU B  38      30.273  49.920  52.622  1.00 23.08      0.172 C
ATOM  10570  OE1 GLU B  38      30.155  50.195  51.414  1.00 16.58     -0.648 OA
ATOM  10571  OE2 GLU B  38      30.406  50.862  53.427  1.00 21.02     -0.648 OA
ATOM  10572  N   VAL B  39      26.984  49.133  51.039  1.00 12.27     -0.346 N
ATOM  10573  HN  VAL B  39      27.193  48.464  50.298  1.00  0.00      0.163 HD
ATOM  10574  CA  VAL B  39      26.327  50.387  50.697  1.00  8.80      0.180 C
ATOM  10576  C   VAL B  39      24.912  50.379  51.278  1.00 12.10      0.241 C
ATOM  10577  O   VAL B  39      24.530  51.366  51.897  1.00 12.78     -0.271 OA
ATOM  10578  CB  VAL B  39      26.244  50.576  49.161  1.00 13.37      0.009 C
ATOM  10580  CG1 VAL B  39      25.265  51.696  48.813  1.00 15.18      0.012 C
ATOM  10584  CG2 VAL B  39      27.645  50.887  48.613  1.00 15.72      0.012 C
ATOM  10588  N   LEU B  40      24.175  49.272  51.021  1.00 12.12     -0.346 N
ATOM  10589  HN  LEU B  40      24.567  48.475  50.520  1.00  0.00      0.163 HD
ATOM  10590  CA  LEU B  40      22.790  49.271  51.495  1.00 10.71      0.177 C
ATOM  10592  C   LEU B  40      22.733  49.452  53.010  1.00 11.45      0.241 C
ATOM  10593  O   LEU B  40      21.982  50.293  53.506  1.00  9.29     -0.271 OA
ATOM  10594  CB  LEU B  40      22.070  47.970  51.056  1.00  8.27      0.038 C
ATOM  10597  CG  LEU B  40      20.633  47.803  51.606  1.00 16.36     -0.020 C
ATOM  10599  CD1 LEU B  40      19.751  48.945  51.131  1.00 17.86      0.009 C
ATOM  10603  CD2 LEU B  40      20.026  46.459  51.202  1.00 17.79      0.009 C
ATOM  10607  N   TRP B  41      23.453  48.587  53.736  1.00  8.67     -0.346 N
ATOM  10608  HN  TRP B  41      24.064  47.907  53.283  1.00  0.00      0.163 HD
ATOM  10609  CA  TRP B  41      23.343  48.641  55.186  1.00 11.36      0.181 C
ATOM  10611  C   TRP B  41      23.942  49.889  55.838  1.00 14.72      0.241 C
ATOM  10612  O   TRP B  41      23.314  50.410  56.782  1.00 12.33     -0.271 OA
ATOM  10613  CB  TRP B  41      23.939  47.346  55.793  1.00 10.68      0.075 C
ATOM  10616  CG  TRP B  41      22.933  46.202  55.720  1.00 11.61     -0.028 A
ATOM  10617  CD1 TRP B  41      22.407  45.686  54.567  1.00 11.67      0.096 A
ATOM  10619  CD2 TRP B  41      22.366  45.463  56.801  1.00 11.15     -0.002 A
ATOM  10621  NE1 TRP B  41      21.500  44.508  56.250  1.00 14.34     -0.042 A
ATOM  10623  CE3 TRP B  41      22.536  45.522  58.202  1.00 11.58      0.014 A
ATOM  10624  NE1 TRP B  41      21.520  44.650  54.890  1.00 14.64     -0.365 N
ATOM  10624  HE1 TRP B  41      20.981  44.096  54.224  1.00  0.00      0.165 HD
ATOM  10625  CZ2 TRP B  41      20.758  43.597  57.028  1.00 15.67      0.030 A
ATOM  10627  CZ3 TRP B  41      21.787  44.624  58.982  1.00 14.42      0.001 A
ATOM  10629  CH2 TRP B  41      20.923  43.671  58.394  1.00 12.57      0.002 A
ATOM  10631  N   ARG B  42      25.077  50.379  55.403  1.00 12.33     -0.346 N
ATOM  10632  HN  ARG B  42      25.532  49.956  54.594  1.00  0.00      0.163 HD
ATOM  10633  CA  ARG B  42      25.705  51.536  56.071  1.00 13.10      0.176 C
ATOM  10635  C   ARG B  42      25.067  52.832  55.635  1.00 13.30      0.241 C
ATOM  10636  O   ARG B  42      24.938  53.760  56.412  1.00 14.30     -0.271 OA
ATOM  10637  CB  ARG B  42      27.242  51.546  55.820  1.00  9.96      0.036 C
ATOM  10640  CG  ARG B  42      27.889  50.298  56.472  1.00 11.44      0.023 C
ATOM  10643  CD  ARG B  42      29.412  50.349  56.413  1.00 19.18      0.138 C
ATOM  10646  NE  ARG B  42      29.865  51.504  57.185  1.00 20.86     -0.227 N
ATOM  10648  HE  ARG B  42      29.762  51.458  58.199  1.00  0.00      0.177 HD
ATOM  10648  CZ  ARG B  42      30.400  52.609  56.676  1.00 25.06      0.665 C
ATOM  10649  NH1 ARG B  42      30.640  52.763  55.391  1.00 16.48     -0.235 N
ATOM  10650 1HH1 ARG B  42      31.051  53.611  55.000  1.00  0.00      0.174 HD
ATOM  10651 2HH1 ARG B  42      30.382  52.021  54.740  1.00  0.00      0.174 HD
ATOM  10652  NH2 ARG B  42      30.737  53.579  57.527  1.00 19.08     -0.235 N
ATOM  10653 1HH2 ARG B  42      31.148  54.427  57.136  1.00  0.00      0.174 HD
ATOM  10654 2HH2 ARG B  42      30.551  53.460  58.523  1.00  0.00      0.174 HD
ATOM  10655  N   ASP B  43      24.602  52.978  54.377  1.00 11.00     -0.346 N
ATOM  10656  HN  ASP B  43      24.598  52.202  53.715  1.00  0.00      0.163 HD
ATOM  10657  CA  ASP B  43      24.099  54.316  54.003  1.00 14.34      0.186 C
ATOM  10659  C   ASP B  43      22.589  54.439  53.975  1.00 18.11      0.241 C
ATOM  10660  O   ASP B  43      22.136  55.588  53.974  1.00 14.56     -0.271 OA
ATOM  10661  CB  ASP B  43      24.625  54.672  52.611  1.00 15.14      0.147 C
ATOM  10664  CG  ASP B  43      26.099  55.031  52.591  1.00 26.45      0.175 C
ATOM  10665  OD1 ASP B  43      26.826  54.854  53.578  1.00 33.49     -0.648 OA
ATOM  10666  OD2 ASP B  43      26.602  55.497  51.563  1.00 36.18     -0.648 OA
ATOM  10667  N   PHE B  44      21.832  53.342  53.806  1.00 10.92     -0.346 N
ATOM  10668  HN  PHE B  44      22.245  52.410  53.795  1.00  0.00      0.163 HD
ATOM  10669  CA  PHE B  44      20.393  53.537  53.639  1.00 12.23      0.180 C
ATOM  10671  C   PHE B  44      19.513  52.843  54.663  1.00 14.34      0.241 C
ATOM  10672  O   PHE B  44      18.487  53.381  55.062  1.00 14.00     -0.271 OA
ATOM  10673  CB  PHE B  44      20.048  53.015  52.231  1.00 11.10      0.073 C
ATOM  10676  CG  PHE B  44      20.640  53.869  51.121  1.00 11.86     -0.056 A
ATOM  10677  CD1 PHE B  44      20.026  55.064  50.764  1.00 18.10      0.007 A
ATOM  10679  CD2 PHE B  44      21.776  53.435  50.452  1.00 13.00      0.007 A
ATOM  10681  CE1 PHE B  44      20.588  55.833  49.731  1.00 19.36      0.001 A
ATOM  10683  CE2 PHE B  44      22.345  54.217  49.456  1.00 16.47      0.001 A
ATOM  10685  CZ  PHE B  44      21.718  55.398  49.089  1.00 17.20      0.000 A
ATOM  10687  N   LEU B  45      19.839  51.635  55.100  1.00 10.56     -0.346 N
ATOM  10688  HN  LEU B  45      20.755  51.250  54.869  1.00  0.00      0.163 HD
ATOM  10689  CA  LEU B  45      18.918  50.848  55.901  1.00 11.25      0.177 C
ATOM  10691  C   LEU B  45      18.522  51.507  57.199  1.00 15.17      0.241 C
ATOM  10692  O   LEU B  45      19.404  52.003  57.908  1.00 14.22     -0.271 OA
ATOM  10693  CB  LEU B  45      19.579  49.463  56.128  1.00 10.41      0.038 C
ATOM  10696  CG  LEU B  45      18.531  48.463  56.730  1.00 10.10     -0.020 C
ATOM  10698  CD1 LEU B  45      17.590  47.967  55.681  1.00  9.71      0.009 C
ATOM  10702  CD2 LEU B  45      19.351  47.306  57.360  1.00  9.93      0.009 C
ATOM  10706  N   LYS B  46      17.229  51.619  57.479  1.00 10.94     -0.346 N
ATOM  10707  HN  LYS B  46      16.545  51.253  56.817  1.00  0.00      0.163 HD
ATOM  10708  CA  LYS B  46      16.757  52.254  58.714  1.00 10.96      0.176 C
ATOM  10710  C   LYS B  46      16.441  51.164  59.737  1.00 12.06      0.241 C
ATOM  10711  O   LYS B  46      15.458  50.443  59.575  1.00 10.13     -0.271 OA
ATOM  10712  CB  LYS B  46      15.468  53.055  58.435  1.00 14.28      0.035 C
ATOM  10715  CG  LYS B  46      14.995  53.878  59.650  1.00 16.82      0.004 C
ATOM  10718  CD  LYS B  46      13.803  54.783  59.278  1.00 18.07      0.027 C
ATOM  10721  CE  LYS B  46      12.552  53.932  59.131  1.00 19.20      0.229 C
ATOM  10724  NZ  LYS B  46      11.275  54.669  58.944  1.00 16.09     -0.079 N
ATOM  10725  HZ1 LYS B  46      10.436  54.098  58.845  1.00  0.00      0.274 HD
ATOM  10726  HZ2 LYS B  46      11.356  55.303  58.149  1.00  0.00      0.274 HD
ATOM  10727  HZ3 LYS B  46      11.149  55.339  59.703  1.00  0.00      0.274 HD
ATOM  10728  N   HIS B  47      17.283  50.988  60.746  1.00 10.13     -0.346 N
ATOM  10729  HN  HIS B  47      18.087  51.603  60.870  1.00  0.00      0.163 HD
ATOM  10730  CA  HIS B  47      17.026  49.885  61.679  1.00  8.52      0.182 C
ATOM  10732  C   HIS B  47      17.699  50.210  63.011  1.00 12.98      0.241 C
ATOM  10733  O   HIS B  47      18.563  51.101  63.063  1.00 13.45     -0.271 OA
ATOM  10734  CB  HIS B  47      17.644  48.568  61.099  1.00  8.00      0.093 C
ATOM  10737  CG  HIS B  47      19.134  48.596  60.939  1.00 10.33      0.028 A
ATOM  10738  CD2 HIS B  47      19.965  49.472  60.319  1.00 12.23      0.114 A
ATOM  10740  ND1 HIS B  47      19.967  47.627  61.481  1.00 12.94     -0.354 N
ATOM  10741  HD1 HIS B  47      19.646  46.816  62.010  1.00  0.00      0.166 HD
ATOM  10742  CE1 HIS B  47      21.221  47.898  61.220  1.00 15.43      0.180 A
ATOM  10744  NE2 HIS B  47      21.255  49.014  60.475  1.00 14.47     -0.360 N
ATOM  10745  HE2 HIS B  47      22.093  49.449  60.090  1.00  0.00      0.166 HD
ATOM  10746  N   ASN B  48      17.363  49.442  64.038  1.00  9.85     -0.346 N
ATOM  10747  HN  ASN B  48      16.635  48.738  63.913  1.00  0.00      0.163 HD
ATOM  10748  CA  ASN B  48      18.001  49.574  65.336  1.00 13.31      0.185 C
ATOM  10750  C   ASN B  48      18.398  48.173  65.793  1.00  9.01      0.243 C
ATOM  10751  O   ASN B  48      17.574  47.336  66.218  1.00 11.38     -0.271 OA
ATOM  10752  CB  ASN B  48      17.037  50.157  66.397  1.00 13.04      0.137 C
ATOM  10755  CG  ASN B  48      17.705  50.366  67.755  1.00 15.56      0.217 C
ATOM  10756  ND2 ASN B  48      16.960  50.770  68.765  1.00 11.78     -0.370 N
ATOM  10757 1HD2 ASN B  48      17.406  50.910  69.672  1.00  0.00      0.159 HD
ATOM  10758 2HD2 ASN B  48      15.960  50.930  68.639  1.00  0.00      0.159 HD
ATOM  10759  OD1 ASN B  48      18.914  50.173  67.907  1.00 14.41     -0.274 OA
ATOM  10760  N   PRO B  49      19.693  47.886  65.805  1.00 11.85     -0.337 N
ATOM  10761  CA  PRO B  49      20.220  46.600  66.236  1.00 11.50      0.179 C
ATOM  10763  C   PRO B  49      19.814  46.250  67.650  1.00 13.27      0.241 C
ATOM  10764  O   PRO B  49      19.721  45.078  67.984  1.00 15.78     -0.271 OA
ATOM  10765  CB  PRO B  49      21.736  46.735  66.175  1.00 14.23      0.037 C
ATOM  10768  CG  PRO B  49      21.959  47.891  65.237  1.00 18.74      0.022 C
ATOM  10771  CD  PRO B  49      20.781  48.816  65.427  1.00 11.19      0.127 C
ATOM  10774  N   GLN B  50      19.577  47.269  68.492  1.00  9.09     -0.346 N
ATOM  10775  HN  GLN B  50      19.691  48.238  68.196  1.00  0.00      0.163 HD
ATOM  10776  CA  GLN B  50      19.145  46.931  69.864  1.00 13.41      0.177 C
ATOM  10778  C   GLN B  50      17.657  46.721  69.986  1.00 16.54      0.241 C
ATOM  10779  O   GLN B  50      17.220  46.391  71.105  1.00 15.75     -0.271 OA
ATOM  10780  CB  GLN B  50      19.609  48.047  70.841  1.00 14.07      0.044 C
ATOM  10783  CG  GLN B  50      21.155  47.972  70.797  1.00 23.19      0.105 C
ATOM  10786  CD  GLN B  50      21.740  48.595  72.054  1.00 33.89      0.215 C
ATOM  10787  NE2 GLN B  50      21.805  47.783  73.096  1.00 33.59     -0.370 N
ATOM  10788 1HE2 GLN B  50      22.198  48.201  73.940  1.00  0.00      0.159 HD
ATOM  10789 2HE2 GLN B  50      21.538  46.799  73.132  1.00  0.00      0.159 HD
ATOM  10790  OE1 GLN B  50      22.064  49.787  72.010  1.00 33.32     -0.274 OA
ATOM  10791  N   ASN B  51      16.862  46.912  68.925  1.00 12.29     -0.346 N
ATOM  10792  HN  ASN B  51      17.261  47.268  68.056  1.00  0.00      0.163 HD
ATOM  10793  CA  ASN B  51      15.436  46.619  68.993  1.00  9.31      0.185 C
ATOM  10795  C   ASN B  51      14.992  46.137  67.586  1.00 12.60      0.243 C
ATOM  10796  O   ASN B  51      14.460  46.843  66.755  1.00 14.64     -0.271 OA
ATOM  10797  CB  ASN B  51      14.521  47.773  69.452  1.00 14.56      0.137 C
ATOM  10800  CG  ASN B  51      13.083  47.325  69.545  1.00 18.35      0.217 C
ATOM  10801  ND2 ASN B  51      12.108  48.230  69.602  1.00 15.59     -0.370 N
ATOM  10802 1HD2 ASN B  51      11.136  47.927  69.665  1.00  0.00      0.159 HD
ATOM  10803 2HD2 ASN B  51      12.386  49.211  69.634  1.00  0.00      0.159 HD
ATOM  10804  OD1 ASN B  51      12.746  46.134  69.506  1.00 13.63     -0.274 OA
ATOM  10805  N   PRO B  52      15.191  44.851  67.324  1.00 13.36     -0.337 N
ATOM  10806  CA  PRO B  52      14.788  44.199  66.085  1.00 11.37      0.179 C
ATOM  10808  C   PRO B  52      13.284  44.126  65.915  1.00 16.29      0.241 C
ATOM  10809  O   PRO B  52      12.840  43.770  64.801  1.00 17.15     -0.271 OA
ATOM  10810  CB  PRO B  52      15.440  42.824  66.120  1.00 12.00      0.037 C
ATOM  10813  CG  PRO B  52      16.162  42.717  67.404  1.00 17.36      0.022 C
ATOM  10816  CD  PRO B  52      15.863  43.898  68.264  1.00 11.47      0.127 C
ATOM  10819  N   SER B  53      12.484  44.467  66.940  1.00 12.22     -0.344 N
ATOM  10820  HN  SER B  53      12.897  44.668  67.851  1.00  0.00      0.163 HD
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ATOM  10821  CA  SER B  53      11.043  44.555  66.777  1.00 14.78      0.200 C
ATOM  10823  C   SER B  53      10.529  45.975  66.525  1.00 14.25      0.243 C
ATOM  10824  O   SER B  53       9.316  46.079  66.390  1.00 14.79     -0.271 OA
ATOM  10825  CB  SER B  53      10.329  44.127  68.096  1.00 18.86      0.199 C
ATOM  10828  OG  SER B  53      10.518  42.724  68.104  1.00 31.11     -0.398 OA
ATOM  10829  HG  SER B  53      10.083  42.463  68.907  1.00  0.00      0.209 HD
ATOM  10830  N   TRP B  54      11.401  46.969  66.400  1.00 10.52     -0.346 N
ATOM  10831  HN  TRP B  54      12.406  46.809  66.471  1.00  0.00      0.163 HD
ATOM  10832  CA  TRP B  54      10.847  48.323  66.153  1.00 10.16      0.181 C
ATOM  10834  C   TRP B  54       9.888  48.269  64.973  1.00  8.83      0.241 C
ATOM  10835  O   TRP B  54      10.242  47.827  63.861  1.00 11.69     -0.271 OA
ATOM  10836  CB  TRP B  54      12.032  49.259  65.912  1.00 10.36      0.075 C
ATOM  10839  CG  TRP B  54      11.688  50.616  65.401  1.00 11.03     -0.028 A
ATOM  10840  CD1 TRP B  54      10.590  51.363  65.732  1.00 12.37      0.096 A
ATOM  10842  CD2 TRP B  54      12.524  51.427  64.580  1.00  8.52     -0.002 A
ATOM  10843  CE2 TRP B  54      11.843  52.647  64.382  1.00  7.75      0.042 A
ATOM  10844  CE3 TRP B  54      13.777  51.233  63.966  1.00  8.90      0.014 A
ATOM  10846  NE1 TRP B  54      10.674  52.597  65.074  1.00  9.86     -0.365 N
ATOM  10847  HE1 TRP B  54       9.973  53.337  65.109  1.00  0.00      0.165 HD
ATOM  10848  CZ2 TRP B  54      12.367  53.678  63.583  1.00 12.34      0.030 A
ATOM  10850  CZ3 TRP B  54      14.305  52.251  63.213  1.00 12.67      0.001 A
ATOM  10852  CH2 TRP B  54      13.603  53.472  63.024  1.00 12.01      0.002 A
ATOM  10854  N   ALA B  55       8.670  48.796  65.194  1.00  9.06     -0.346 N
ATOM  10855  HN  ALA B  55       8.496  49.316  66.054  1.00  0.00      0.163 HD
ATOM  10856  CA  ALA B  55       7.587  48.634  64.215  1.00 10.38      0.172 C
ATOM  10858  C   ALA B  55       7.882  49.288  62.885  1.00 12.38      0.240 C
ATOM  10859  O   ALA B  55       7.428  48.772  61.829  1.00 11.82     -0.271 OA
ATOM  10860  CB  ALA B  55       6.294  49.248  64.770  1.00 10.00      0.042 C
ATOM  10864  N   ASP B  56       8.596  50.435  62.951  1.00  8.44     -0.346 N
ATOM  10865  HN  ASP B  56       8.964  50.793  63.832  1.00  0.00      0.163 HD
ATOM  10866  CA  ASP B  56       8.810  51.135  61.674  1.00  7.95      0.186 C
ATOM  10868  C   ASP B  56      10.142  50.865  61.039  1.00 11.47      0.241 C
ATOM  10869  O   ASP B  56      10.514  51.634  60.122  1.00  9.72     -0.271 OA
ATOM  10870  CB  ASP B  56       8.558  52.668  61.894  1.00 11.58      0.147 C
ATOM  10873  CG  ASP B  56       8.189  53.378  60.603  1.00 14.01      0.175 C
ATOM  10874  OD1 ASP B  56       7.480  52.814  59.729  1.00 10.22     -0.648 OA
ATOM  10875  OD2 ASP B  56       8.618  54.536  60.439  1.00 12.29     -0.648 OA
ATOM  10876  N   ARG B  57      10.895  49.819  61.391  1.00 10.03     -0.346 N
ATOM  10877  HN  ARG B  57      10.575  49.201  62.137  1.00  0.00      0.163 HD
ATOM  10878  CA  ARG B  57      12.167  49.543  60.730  1.00  8.94      0.176 C
ATOM  10880  C   ARG B  57      11.983  49.187  59.238  1.00 10.52      0.241 C
ATOM  10881  O   ARG B  57      10.898  48.698  58.828  1.00  9.82     -0.271 OA
ATOM  10882  CB  ARG B  57      12.874  48.344  61.416  1.00  7.41      0.036 C
ATOM  10885  CG  ARG B  57      12.079  47.027  61.159  1.00  7.41      0.023 C
ATOM  10888  CD  ARG B  57      12.568  45.922  62.107  1.00 11.61      0.138 C
ATOM  10891  NE  ARG B  57      11.886  44.635  61.872  1.00 11.76     -0.227 N
ATOM  10892  HE  ARG B  57      12.365  43.976  61.259  1.00  0.00      0.177 HD
ATOM  10893  CZ  ARG B  57      10.729  44.240  62.364  1.00 15.34      0.665 C
ATOM  10894  NH1 ARG B  57      10.021  45.007  63.193  1.00  8.57     -0.235 N
ATOM  10895 1HH1 ARG B  57      10.413  45.922  63.417  1.00  0.00      0.174 HD
ATOM  10896 2HH1 ARG B  57       9.125  44.701  63.574  1.00  0.00      0.174 HD
ATOM  10897  NH2 ARG B  57      10.211  43.030  62.068  1.00 11.71     -0.235 N
ATOM  10898 1HH2 ARG B  57      10.753  42.443  61.434  1.00  0.00      0.174 HD
ATOM  10899 2HH2 ARG B  57       9.315  42.724  62.449  1.00  0.00      0.174 HD
ATOM  10900  N   ASP B  58      12.994  49.440  58.426  1.00 10.24     -0.346 N
ATOM  10901  HN  ASP B  58      13.775  50.007  58.756  1.00  0.00      0.163 HD
ATOM  10902  CA  ASP B  58      13.008  48.911  57.044  1.00  9.87      0.186 C
ATOM  10904  C   ASP B  58      13.083  47.376  57.183  1.00 13.88      0.241 C
ATOM  10905  O   ASP B  58      13.661  46.871  58.156  1.00  9.80     -0.271 OA
ATOM  10906  CB  ASP B  58      14.188  49.352  56.185  1.00  7.89      0.147 C
ATOM  10909  CG  ASP B  58      14.259  50.822  55.798  1.00 11.01      0.175 C
ATOM  10910  OD1 ASP B  58      13.204  51.461  55.806  1.00 10.13     -0.648 OA
ATOM  10911  OD2 ASP B  58      15.372  51.345  55.518  1.00 11.79     -0.648 OA
ATOM  10912  N   ARG B  59      12.567  46.636  56.223  1.00  8.43     -0.346 N
ATOM  10913  HN  ARG B  59      12.110  47.110  55.444  1.00  0.00      0.163 HD
ATOM  10914  CA  ARG B  59      12.611  45.178  56.208  1.00  9.99      0.176 C
ATOM  10916  C   ARG B  59      13.595  44.722  55.142  1.00 11.48      0.241 C
ATOM  10917  O   ARG B  59      13.576  45.180  53.995  1.00 14.96     -0.271 OA
ATOM  10918  CB  ARG B  59      11.230  44.555  55.892  1.00 10.44      0.036 C
ATOM  10921  CG  ARG B  59      10.345  44.278  57.089  1.00 13.17      0.023 C
ATOM  10924  CD  ARG B  59       9.932  45.433  57.968  1.00 10.16      0.138 C
ATOM  10927  NE  ARG B  59       8.962  44.995  59.031  1.00 11.55     -0.227 N
ATOM  10928  HE  ARG B  59       8.761  44.000  59.135  1.00  0.00      0.177 HD
ATOM  10929  CZ  ARG B  59       8.364  45.851  59.830  1.00 16.08      0.665 C
ATOM  10930  NH1 ARG B  59       8.634  47.147  59.764  1.00 11.54     -0.235 N
ATOM  10931 1HH1 ARG B  59       9.320  47.472  59.083  1.00  0.00      0.174 HD
ATOM  10932 2HH1 ARG B  59       8.170  47.811  60.384  1.00  0.00      0.174 HD
ATOM  10933  NH2 ARG B  59       7.476  45.431  60.712  1.00 11.26     -0.235 N
ATOM  10934 1HH2 ARG B  59       7.268  44.434  60.763  1.00  0.00      0.174 HD
ATOM  10935 2HH2 ARG B  59       7.012  46.095  61.332  1.00  0.00      0.174 HD
ATOM  10936  N   PHE B  60      14.560  43.890  55.547  1.00  9.28     -0.346 N
ATOM  10937  HN  PHE B  60      14.631  43.630  56.531  1.00  0.00      0.163 HD
ATOM  10938  CA  PHE B  60      15.526  43.347  54.563  1.00  6.88      0.180 C
ATOM  10940  C   PHE B  60      15.251  41.875  54.382  1.00  8.62      0.241 C
ATOM  10941  O   PHE B  60      15.094  41.168  55.412  1.00  9.54     -0.271 OA
ATOM  10942  CB  PHE B  60      16.969  43.512  55.137  1.00  8.83      0.073 C
ATOM  10945  CG  PHE B  60      18.015  42.839  54.265  1.00 10.36     -0.056 A
ATOM  10946  CD1 PHE B  60      18.364  43.419  53.038  1.00 16.64      0.007 A
ATOM  10948  CD2 PHE B  60      18.597  41.639  54.643  1.00 10.36      0.007 A
ATOM  10950  CE1 PHE B  60      19.279  42.793  52.209  1.00 13.80      0.001 A
ATOM  10952  CE2 PHE B  60      19.524  41.045  53.818  1.00 19.62      0.001 A
ATOM  10954  CZ  PHE B  60      19.881  41.605  52.593  1.00 14.09      0.000 A
ATOM  10956  N   VAL B  61      15.281  41.339  53.178  1.00  4.79     -0.346 N
ATOM  10957  HN  VAL B  61      15.473  41.940  52.376  1.00  0.00      0.163 HD
ATOM  10958  CA  VAL B  61      15.048  39.912  52.951  1.00  5.52      0.180 C
ATOM  10960  C   VAL B  61      16.169  39.351  52.085  1.00  6.64      0.241 C
ATOM  10961  O   VAL B  61      16.364  39.827  50.953  1.00  8.81     -0.271 OA
ATOM  10962  CB  VAL B  61      13.700  39.655  52.244  1.00 11.57      0.009 C
ATOM  10964  CG1 VAL B  61      13.516  38.171  51.880  1.00  8.49      0.012 C
ATOM  10968  CG2 VAL B  61      12.516  40.060  53.182  1.00  8.80      0.012 C
ATOM  10972  N   LEU B  62      16.804  38.287  52.559  1.00  9.15     -0.346 N
ATOM  10973  HN  LEU B  62      16.586  37.951  53.497  1.00  0.00      0.163 HD
ATOM  10974  CA  LEU B  62      17.809  37.587  51.764  1.00  9.84      0.177 C
ATOM  10976  C   LEU B  62      17.120  36.433  51.041  1.00 11.71      0.241 C
ATOM  10977  O   LEU B  62      16.955  35.329  51.589  1.00 11.97     -0.271 OA
ATOM  10978  CB  LEU B  62      18.905  37.071  52.732  1.00  8.58      0.038 C
ATOM  10981  CG  LEU B  62      20.052  36.370  51.954  1.00 15.76     -0.020 C
ATOM  10983  CD1 LEU B  62      20.860  37.412  51.188  1.00 12.11      0.009 C
ATOM  10987  CD2 LEU B  62      20.942  35.570  52.901  1.00 12.82      0.009 C
ATOM  10991  N   SER B  63      16.665  36.632  49.795  1.00 10.01     -0.344 N
ATOM  10992  HN  SER B  63      16.865  37.511  49.318  1.00  0.00      0.163 HD
ATOM  10993  CA  SER B  63      15.886  35.600  49.115  1.00  7.91      0.200 C
ATOM  10995  C   SER B  63      16.767  34.441  48.652  1.00 13.42      0.243 C
ATOM  10996  O   SER B  63      16.339  33.280  48.572  1.00 13.32     -0.271 OA
ATOM  10997  CB  SER B  63      15.133  36.168  47.904  1.00 12.93      0.199 C
ATOM  11000  OG  SER B  63      14.075  35.310  47.505  1.00 12.40     -0.398 OA
ATOM  11001  HG  SER B  63      13.609  35.662  46.754  1.00  0.00      0.209 HD
ATOM  11002  N   ASN B  64      18.034  34.739  48.347  1.00 13.37     -0.345 N
ATOM  11003  HN  ASN B  64      18.332  35.713  48.390  1.00  0.00      0.163 HD
ATOM  11004  CA  ASN B  64      19.015  33.715  47.952  1.00 14.64      0.185 C
ATOM  11006  C   ASN B  64      19.652  33.278  49.289  1.00 12.63      0.241 C
ATOM  11007  O   ASN B  64      20.828  33.532  49.562  1.00 14.95     -0.271 OA
ATOM  11008  CB  ASN B  64      20.077  34.237  47.003  1.00 13.85      0.137 C
ATOM  11011  CG  ASN B  64      20.587  35.647  47.229  1.00 21.48      0.217 C
ATOM  11012  ND2 ASN B  64      21.619  36.069  46.473  1.00 14.53     -0.370 N
ATOM  11013 1HD2 ASN B  64      21.962  37.017  46.625  1.00  0.00      0.159 HD
ATOM  11014 2HD2 ASN B  64      22.011  35.434  45.778  1.00  0.00      0.159 HD
ATOM  11015  OD1 ASN B  64      20.112  36.417  48.072  1.00 14.93     -0.274 OA
ATOM  11016  N   GLY B  65      18.889  32.581  50.081  1.00 14.17     -0.351 N
ATOM  11017  HN  GLY B  65      18.020  32.232  49.676  1.00  0.00      0.163 HD
ATOM  11018  CA  GLY B  65      19.129  32.241  51.474  1.00 15.62      0.225 C
ATOM  11021  C   GLY B  65      20.283  31.347  51.774  1.00 15.72      0.236 C
ATOM  11022  O   GLY B  65      20.808  31.303  52.900  1.00 13.98     -0.272 OA
ATOM  11023  N   HIS B  66      20.769  30.597  50.755  1.00 11.34     -0.346 N
ATOM  11024  HN  HIS B  66      20.262  30.582  49.870  1.00  0.00      0.163 HD
ATOM  11025  CA  HIS B  66      21.985  29.815  50.878  1.00 12.88      0.182 C
ATOM  11027  C   HIS B  66      23.158  30.739  51.222  1.00 14.17      0.241 C
ATOM  11028  O   HIS B  66      24.058  30.262  51.924  1.00 15.59     -0.271 OA
ATOM  11029  CB  HIS B  66      22.371  29.049  49.598  1.00 11.32      0.093 C
ATOM  11032  CG  HIS B  66      22.419  29.869  48.339  1.00 19.99      0.028 A
ATOM  11033  CD2 HIS B  66      23.468  30.363  47.627  1.00 11.52      0.114 A
ATOM  11035  ND1 HIS B  66      21.275  30.202  47.644  1.00 19.49     -0.354 N
ATOM  11036  HD1 HIS B  66      20.325  29.942  47.908  1.00  0.00      0.166 HD
ATOM  11037  CE1 HIS B  66      21.615  30.922  46.566  1.00 16.17      0.180 A
ATOM  11039  NE2 HIS B  66      22.932  31.034  46.523  1.00 11.81     -0.360 N
ATOM  11040  HE2 HIS B  66      23.466  31.526  45.807  1.00  0.00      0.166 HD
ATOM  11041  N   GLY B  67      23.149  32.019  50.827  1.00 15.27     -0.351 N
ATOM  11042  HN  GLY B  67      22.391  32.368  50.241  1.00  0.00      0.163 HD
ATOM  11043  CA  GLY B  67      24.243  32.927  51.244  1.00 12.60      0.225 C
ATOM  11046  C   GLY B  67      24.049  33.414  52.677  1.00 13.89      0.236 C
ATOM  11047  O   GLY B  67      24.318  34.583  52.984  1.00 12.63     -0.272 OA
ATOM  11048  N   SER B  68      23.676  32.530  53.612  1.00 11.11     -0.344 N
ATOM  11049  HN  SER B  68      23.598  31.545  53.381  1.00  0.00      0.163 HD
ATOM  11050  CA  SER B  68      23.378  32.939  54.979  1.00 11.23      0.200 C
ATOM  11052  C   SER B  68      24.516  33.622  55.711  1.00  9.03      0.243 C
ATOM  11053  O   SER B  68      24.233  34.460  56.596  1.00 11.04     -0.271 OA
ATOM  11054  CB  SER B  68      22.903  31.696  55.775  1.00 14.51      0.199 C
ATOM  11057  OG  SER B  68      23.821  30.639  55.598  1.00 14.51     -0.398 OA
ATOM  11058  HG  SER B  68      23.530  29.877  56.086  1.00  0.00      0.209 HD
ATOM  11059  N   MET B  69      25.789  33.306  55.419  1.00 11.61     -0.346 N
ATOM  11060  HN  MET B  69      26.012  32.592  54.726  1.00  0.00      0.163 HD
ATOM  11061  CA  MET B  69      26.851  34.031  56.139  1.00 11.56      0.177 C
ATOM  11063  C   MET B  69      26.815  35.534  55.785  1.00 13.58      0.241 C
ATOM  11064  O   MET B  69      27.357  36.337  56.545  1.00 10.83     -0.271 OA
ATOM  11065  CB  MET B  69      28.257  33.485  55.852  1.00 10.50      0.045 C
ATOM  11068  CG  MET B  69      28.552  32.278  56.766  1.00  8.91      0.076 C
ATOM  11071  SD  MET B  69      28.399  32.615  58.517  1.00 15.37     -0.173 SA
ATOM  11072  CE  MET B  69      29.479  34.033  58.722  1.00 13.28      0.089 C
ATOM  11076  N   LEU B  70      26.228  35.931  54.655  1.00 10.59     -0.346 N
ATOM  11077  HN  LEU B  70      25.842  35.260  53.991  1.00  0.00      0.163 HD
ATOM  11078  CA  LEU B  70      26.161  37.396  54.407  1.00 14.27      0.177 C
ATOM  11080  C   LEU B  70      25.306  38.025  55.492  1.00 10.58      0.241 C
ATOM  11081  O   LEU B  70      25.695  39.078  56.023  1.00  8.73     -0.271 OA
ATOM  11082  CB  LEU B  70      25.534  37.683  53.057  1.00 14.02      0.038 C
ATOM  11085  CG  LEU B  70      25.305  39.152  52.670  1.00 15.62     -0.020 C
ATOM  11087  CD1 LEU B  70      26.638  39.820  52.419  1.00 21.89      0.009 C
ATOM  11091  CD2 LEU B  70      24.459  39.205  51.384  1.00 24.06      0.009 C
ATOM  11095  N   ILE B  71      24.097  37.467  55.744  1.00  9.31     -0.346 N
ATOM  11096  HN  ILE B  71      23.773  36.630  55.260  1.00  0.00      0.163 HD
ATOM  11097  CA  ILE B  71      23.265  38.165  56.785  1.00 10.13      0.180 C
ATOM  11099  C   ILE B  71      23.861  37.963  58.153  1.00 11.87      0.241 C
ATOM  11100  O   ILE B  71      23.793  38.905  59.000  1.00 12.25     -0.271 OA
ATOM  11101  CB  ILE B  71      21.776  37.756  56.665  1.00 15.83      0.013 C
ATOM  11103  CG1 ILE B  71      20.891  38.730  57.457  1.00 18.15      0.002 C
ATOM  11106  CG2 ILE B  71      21.525  36.317  57.130  1.00 16.59      0.012 C
ATOM  11110  CD1 ILE B  71      19.404  38.629  57.256  1.00 31.29      0.005 C
ATOM  11114  N   TYR B  72      24.431  36.788  58.502  1.00 10.26     -0.346 N
ATOM  11115  HN  TYR B  72      24.432  35.990  57.867  1.00  0.00      0.163 HD
ATOM  11116  CA  TYR B  72      25.047  36.707  59.830  1.00 10.71      0.180 C
ATOM  11118  C   TYR B  72      26.202  37.696  60.005  1.00 10.11      0.241 C
ATOM  11119  O   TYR B  72      26.358  38.240  61.108  1.00 12.15     -0.271 OA
ATOM  11120  CB  TYR B  72      25.567  35.275  60.106  1.00  6.45      0.073 C
ATOM  11123  CG  TYR B  72      24.439  34.267  60.050  1.00  9.35     -0.056 A
ATOM  11124  CD1 TYR B  72      23.166  34.573  60.507  1.00 12.63      0.010 A
ATOM  11126  CD2 TYR B  72      24.679  33.003  59.536  1.00 12.30      0.010 A
ATOM  11128  CE1 TYR B  72      22.136  33.630  60.431  1.00 14.16      0.037 A
ATOM  11130  CE2 TYR B  72      23.678  32.052  59.480  1.00  8.60      0.037 A
ATOM  11132  CZ  TYR B  72      22.417  32.385  59.936  1.00 15.49      0.065 A
ATOM  11133  OH  TYR B  72      21.437  31.427  59.852  1.00 13.24     -0.361 OA
ATOM  11134  HH  TYR B  72      21.632  30.563  59.508  1.00  0.00      0.217 HD
ATOM  11135  N   SER B  73      27.036  37.914  58.984  1.00  9.40     -0.344 N
ATOM  11136  HN  SER B  73      26.920  37.385  58.119  1.00  0.00      0.163 HD
ATOM  11137  CA  SER B  73      28.111  38.898  59.087  1.00 11.67      0.200 C
ATOM  11139  C   SER B  73      27.555  40.305  59.310  1.00 12.07      0.243 C
ATOM  11140  O   SER B  73      28.048  41.104  60.123  1.00 12.20     -0.271 OA
ATOM  11141  CB  SER B  73      28.843  38.955  57.704  1.00 13.26      0.199 C
ATOM  11144  OG  SER B  73      29.608  37.777  57.545  1.00 15.76     -0.398 OA
ATOM  11145  HG  SER B  73      30.052  37.812  56.706  1.00  0.00      0.209 HD
ATOM  11146  N   LEU B  74      26.533  40.631  58.508  1.00  9.28     -0.346 N
ATOM  11147  HN  LEU B  74      26.179  39.977  57.810  1.00  0.00      0.163 HD
ATOM  11148  CA  LEU B  74      25.931  41.989  58.675  1.00  9.42      0.177 C
ATOM  11150  C   LEU B  74      25.360  42.185  60.063  1.00 11.78      0.241 C
ATOM  11151  O   LEU B  74      25.521  43.248  60.693  1.00 12.50     -0.271 OA
ATOM  11152  CB  LEU B  74      24.859  42.243  57.605  1.00 10.01      0.038 C
ATOM  11155  CG  LEU B  74      25.357  42.388  56.148  1.00 14.25     -0.020 C
ATOM  11157  CD1 LEU B  74      24.176  42.284  55.191  1.00  9.21      0.009 C
ATOM  11161  CD2 LEU B  74      26.009  43.771  56.000  1.00 11.74      0.009 C
ATOM  11165  N   LEU B  75      24.587  41.247  60.606  1.00  9.82     -0.346 N
ATOM  11166  HN  LEU B  75      24.397  40.402  60.067  1.00  0.00      0.163 HD
ATOM  11167  CA  LEU B  75      24.000  41.370  61.933  1.00  7.48      0.177 C
ATOM  11169  C   LEU B  75      25.085  41.491  63.009  1.00 12.09      0.241 C
ATOM  11170  O   LEU B  75      24.937  42.332  63.892  1.00 12.93     -0.271 OA
ATOM  11171  CB  LEU B  75      23.085  40.146  62.291  1.00 12.42      0.038 C
ATOM  11174  CG  LEU B  75      21.885  39.991  61.325  1.00 15.96     -0.020 C
ATOM  11176  CD1 LEU B  75      21.169  38.647  61.595  1.00 16.34      0.009 C
ATOM  11180  CD2 LEU B  75      20.866  41.126  61.453  1.00 13.57      0.009 C
ATOM  11184  N   HIS B  76      26.130  40.677  62.889  1.00  8.41     -0.346 N
ATOM  11185  HN  HIS B  76      26.171  39.993  62.133  1.00  0.00      0.163 HD
ATOM  11186  CA  HIS B  76      27.237  40.781  63.876  1.00 10.00      0.182 C
ATOM  11188  C   HIS B  76      27.955  42.118  63.829  1.00 12.65      0.241 C
ATOM  11189  O   HIS B  76      28.120  42.770  64.887  1.00 13.16     -0.271 OA
ATOM  11190  CB  HIS B  76      28.223  39.632  63.623  1.00  9.69      0.093 C
ATOM  11193  CG  HIS B  76      29.437  39.758  64.528  1.00 11.87      0.028 A
ATOM  11194  CD2 HIS B  76      30.694  40.158  64.238  1.00 14.06      0.114 A
ATOM  11196  ND1 HIS B  76      29.368  39.530  65.888  1.00 13.91     -0.354 N
ATOM  11197  HD1 HIS B  76      28.540  39.240  66.408  1.00  0.00      0.166 HD
ATOM  11198  CE1 HIS B  76      30.585  39.758  66.402  1.00 15.93      0.180 A
ATOM  11200  NE2 HIS B  76      31.380  40.163  65.440  1.00 13.70     -0.360 N
ATOM  11202  HE2 HIS B  76      32.355  40.439  65.560  1.00  0.00      0.166 HD
ATOM  11202  N   LEU B  77      28.368  42.520  62.616  1.00  9.84     -0.346 N
ATOM  11203  HN  LEU B  77      28.148  41.950  61.799  1.00  0.00      0.163 HD
ATOM  11204  CA  LEU B  77      29.122  43.751  62.442  1.00 12.16      0.177 C
ATOM  11206  C   LEU B  77      28.327  44.991  62.867  1.00 15.32      0.241 C
ATOM  11207  O   LEU B  77      28.917  45.934  63.464  1.00 13.51     -0.271 OA
ATOM  11208  CB  LEU B  77      29.577  43.934  60.973  1.00 11.84      0.038 C
ATOM  11211  CG  LEU B  77      30.695  42.950  60.529  1.00 13.32     -0.020 C
ATOM  11213  CD1 LEU B  77      30.794  42.893  59.016  1.00 12.91      0.009 C
ATOM  11217  CD2 LEU B  77      32.030  43.324  61.171  1.00 14.25      0.009 C
ATOM  11221  N   THR B  78      27.036  45.056  62.569  1.00 12.15     -0.344 N
ATOM  11222  HN  THR B  78      26.586  44.266  62.108  1.00  0.00      0.163 HD
ATOM  11223  CA  THR B  78      26.248  46.249  62.894  1.00  9.63      0.205 C
ATOM  11225  C   THR B  78      25.810  46.318  64.370  1.00 11.93      0.243 C
ATOM  11226  O   THR B  78      25.239  47.333  64.788  1.00 12.57     -0.271 OA
ATOM  11227  CB  THR B  78      25.044  46.484  61.988  1.00 12.71      0.146 C
ATOM  11229  CG2 THR B  78      25.496  46.668  60.547  1.00 13.36      0.042 C
ATOM  11233  OG1 THR B  78      24.124  45.379  62.054  1.00 11.30     -0.393 OA
ATOM  11234  HG1 THR B  78      23.374  45.525  61.490  1.00  0.00      0.210 HD
ATOM  11235  N   GLY B  79      26.020  45.300  65.155  1.00 10.96     -0.350 N
ATOM  11236  HN  GLY B  79      26.397  44.439  64.760  1.00  0.00      0.163 HD
ATOM  11237  CA  GLY B  79      25.731  45.358  66.580  1.00 11.27      0.225 C
ATOM  11240  C   GLY B  79      24.518  44.615  67.051  1.00 14.00      0.236 C
ATOM  11241  O   GLY B  79      24.175  44.851  68.228  1.00 12.92     -0.272 OA
ATOM  11242  N   TYR B  80      23.930  43.697  66.283  1.00  9.21     -0.346 N
ATOM  11243  HN  TYR B  80      24.254  43.588  65.327  1.00  0.00      0.163 HD
ATOM  11244  CA  TYR B  80      22.812  42.898  66.815  1.00  9.63      0.180 C
ATOM  11246  C   TYR B  80      23.396  41.944  67.870  1.00 11.99      0.241 C
ATOM  11247  O   TYR B  80      24.603  41.668  67.883  1.00 13.03     -0.271 OA
ATOM  11248  CB  TYR B  80      22.148  42.048  65.723  1.00  8.62      0.073 C
ATOM  11251  CG  TYR B  80      21.252  42.925  64.836  1.00 10.30     -0.056 A
ATOM  11252  CD1 TYR B  80      21.795  43.796  63.918  1.00 10.97      0.010 A
ATOM  11254  CD2 TYR B  80      19.865  42.913  64.986  1.00 10.32      0.010 A
ATOM  11256  CE1 TYR B  80      21.004  44.603  63.106  1.00 10.72      0.037 A
ATOM  11258  CE2 TYR B  80      19.029  43.695  64.160  1.00 12.29      0.037 A
ATOM  11260  CZ  TYR B  80      19.625  44.536  63.237  1.00 13.59      0.065 A
ATOM  11261  OH  TYR B  80      18.840  45.365  62.433  1.00 13.36     -0.361 OA
ATOM  11263  HH  TYR B  80      17.895  45.319  62.523  1.00  0.00      0.217 HD
ATOM  11263  N   ASP B  81      22.535  41.277  68.609  1.00 13.09     -0.345 N
ATOM  11264  HN  ASP B  81      21.537  41.452  68.492  1.00  0.00      0.163 HD
ATOM  11265  CA  ASP B  81      22.981  40.281  69.604  1.00 14.81      0.186 C
ATOM  11267  C   ASP B  81      23.351  38.968  68.933  1.00 14.60      0.241 C
ATOM  11268  O   ASP B  81      22.585  38.001  69.047  1.00 16.22     -0.271 OA
ATOM  11269  CB  ASP B  81      21.828  40.101  70.596  1.00 16.38      0.147 C
ATOM  11272  CG  ASP B  81      22.255  39.285  71.812  1.00 31.21      0.175 C
ATOM  11273  OD1 ASP B  81      23.463  39.077  72.006  1.00 26.56     -0.648 OA
ATOM  11274  OD2 ASP B  81      21.370  38.817  72.549  1.00 30.65     -0.648 OA
ATOM  11275  N   LEU B  82      24.464  38.932  68.208  1.00 12.42     -0.346 N
ATOM  11276  HN  LEU B  82      25.020  39.783  68.121  1.00  0.00      0.163 HD
ATOM  11277  CA  LEU B  82      24.926  37.715  67.527  1.00 12.84      0.177 C
ATOM  11279  C   LEU B  82      26.458  37.744  67.682  1.00 13.78      0.243 C
ATOM  11280  O   LEU B  82      27.195  38.329  66.895  1.00 16.00     -0.271 OA
ATOM  11281  CB  LEU B  82      24.473  37.738  66.068  1.00 12.68      0.038 C
ATOM  11284  CG  LEU B  82      24.804  36.429  65.279  1.00 17.25     -0.020 C
ATOM  11286  CD1 LEU B  82      23.925  35.306  65.826  1.00 16.99      0.009 C
ATOM  11290  CD2 LEU B  82      24.483  36.567  63.776  1.00 17.08      0.009 C
ATOM  11294  N   PRO B  83      26.957  37.150  68.757  1.00 16.91     -0.337 N
ATOM  11295  CA  PRO B  83      28.365  37.191  69.108  1.00 17.82      0.179 A
ATOM  11297  C   PRO B  83      29.304  36.420  68.200  1.00 16.21      0.241 C
ATOM  11298  O   PRO B  83      28.858  35.530  67.464  1.00 14.54     -0.271 OA
ATOM  11299  CB  PRO B  83      28.412  36.658  70.528  1.00 18.62      0.037 A
ATOM  11302  CG  PRO B  83      27.067  36.208  70.916  1.00 21.82      0.022 A
ATOM  11305  CD  PRO B  83      26.108  36.479  69.780  1.00 12.41      0.127 A
ATOM  11308  N   MET B  84      30.621  36.749  68.229  1.00 13.63     -0.346 N
ATOM  11309  HN  MET B  84      30.965  37.471  68.862  1.00  0.00      0.163 HD
ATOM  11310  CA  MET B  84      31.538  36.041  67.327  1.00 15.86      0.177 C
ATOM  11312  C   MET B  84      31.485  34.541  67.533  1.00 15.83      0.241 C
ATOM  11313  O   MET B  84      31.597  33.737  66.597  1.00 16.71     -0.271 OA
ATOM  11314  CB  MET B  84      32.984  36.537  67.486  1.00 22.36      0.045 C
ATOM  11317  CG  MET B  84      33.951  35.917  66.473  1.00 23.11      0.076 C
ATOM  11320  SD  MET B  84      33.590  36.509  64.793  1.00 21.63     -0.173 SA
ATOM  11321  CE  MET B  84      34.121  38.214  64.948  1.00 25.08      0.089 C
ATOM  11325  N   GLU B  85      31.285  34.083  68.764  1.00 15.02     -0.346 N
ATOM  11326  HN  GLU B  85      31.173  34.752  69.526  1.00  0.00      0.163 HD
ATOM  11327  CA  GLU B  85      31.220  32.645  69.066  1.00 18.37      0.177 C
ATOM  11329  C   GLU B  85      30.125  31.936  68.279  1.00 17.26      0.241 C
ATOM  11330  O   GLU B  85      30.284  30.791  67.869  1.00 16.80     -0.271 OA
ATOM  11331  CB  GLU B  85      31.033  32.476  70.580  1.00 29.87      0.045 C
ATOM  11334  CG  GLU B  85      31.423  31.126  71.133  1.00 61.97      0.116 C
ATOM  11337  CD  GLU B  85      32.811  30.620  70.795  1.00 79.44      0.172 C
ATOM  11338  OE1 GLU B  85      33.806  31.361  70.983  1.00 86.38     -0.648 OA
ATOM  11339  OE2 GLU B  85      32.941  29.454  70.333  1.00 87.03     -0.648 OA
ATOM  11340  N   GLU B  86      28.977  32.591  68.033  1.00 14.46     -0.346 N
ATOM  11341  HN  GLU B  86      28.817  33.512  68.442  1.00  0.00      0.163 HD
ATOM  11342  CA  GLU B  86      27.951  31.979  67.174  1.00 14.14      0.177 C
ATOM  11344  C   GLU B  86      28.402  31.905  65.740  1.00 13.25      0.241 C
ATOM  11345  O   GLU B  86      28.090  30.891  65.094  1.00 14.32     -0.271 OA
ATOM  11346  CB  GLU B  86      26.622  32.765  67.267  1.00 13.33      0.045 C
ATOM  11349  CG  GLU B  86      26.062  32.717  68.672  1.00 16.04      0.116 C
ATOM  11352  CD  GLU B  86      25.546  31.349  69.086  1.00 26.47      0.172 C
ATOM  11353  OE1 GLU B  86      25.297  30.421  68.300  1.00 20.25     -0.648 OA
ATOM  11354  OE2 GLU B  86      25.354  31.205  70.309  1.00 29.08     -0.648 OA
ATOM  11355  N   LEU B  87      29.160  32.896  65.230  1.00 12.95     -0.346 N
ATOM  11356  HN  LEU B  87      29.378  33.720  65.790  1.00  0.00      0.163 HD
ATOM  11357  CA  LEU B  87      29.669  32.774  63.855  1.00 17.48      0.177 C
ATOM  11359  C   LEU B  87      30.651  31.609  63.748  1.00 18.02      0.241 C
ATOM  11360  O   LEU B  87      30.704  30.920  62.708  1.00 15.71     -0.271 OA
ATOM  11361  CB  LEU B  87      30.407  34.006  63.325  1.00 16.07      0.038 C
ATOM  11364  CG  LEU B  87      29.609  35.311  63.207  1.00 27.07     -0.020 C
ATOM  11366  CD1 LEU B  87      30.298  36.297  62.254  1.00 26.08      0.009 C
ATOM  11370  CD2 LEU B  87      28.195  35.111  62.749  1.00 24.19      0.009 C
ATOM  11374  N   LYS B  88      31.434  31.363  64.805  1.00 17.58     -0.346 N
ATOM  11375  HN  LYS B  88      31.402  31.982  65.615  1.00  0.00      0.163 HD
ATOM  11376  CA  LYS B  88      32.336  30.210  64.804  1.00 15.00      0.176 C
ATOM  11378  C   LYS B  88      31.557  28.900  64.898  1.00 15.47      0.241 C
ATOM  11379  O   LYS B  88      32.176  27.858  64.696  1.00 19.81     -0.271 OA
ATOM  11380  CB  LYS B  88      33.291  30.224  66.028  1.00 14.99      0.035 C
ATOM  11383  CG  LYS B  88      34.306  31.364  65.902  1.00 18.28      0.004 C
ATOM  11386  CD  LYS B  88      35.158  31.324  67.195  1.00 27.50      0.027 C
ATOM  11389  CE  LYS B  88      36.231  32.406  67.091  1.00 44.02      0.229 C
ATOM  11392  NZ  LYS B  88      37.157  32.320  68.266  1.00 48.51     -0.079 N
ATOM  11393  HZ1 LYS B  88      37.874  33.043  68.197  1.00  0.00      0.274 HD
ATOM  11394  HZ2 LYS B  88      37.561  31.389  68.368  1.00  0.00      0.274 HD
ATOM  11395  HZ3 LYS B  88      36.655  32.362  69.153  1.00  0.00      0.274 HD
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ATOM  11396  N   ASN B  89      30.280  28.913  65.256  1.00 13.09    -0.346 N
ATOM  11397  HN  ASN B  89      29.841  29.804  65.487  1.00  0.00     0.163 HD
ATOM  11398  CA  ASN B  89      29.484  27.697  65.330  1.00 12.14     0.185 C
ATOM  11400  C   ASN B  89      28.434  27.652  64.202  1.00 12.51     0.241 C
ATOM  11401  O   ASN B  89      27.348  27.046  64.341  1.00 12.73    -0.271 OA
ATOM  11402  CB  ASN B  89      28.771  27.629  66.695  1.00 16.50     0.137 C
ATOM  11405  CG  ASN B  89      29.810  27.116  67.707  1.00 34.35     0.217 C
ATOM  11406  ND2 ASN B  89      29.830  27.740  68.861  1.00 27.88    -0.370 N
ATOM  11407 1HD2 ASN B  89      30.519  27.400  69.532  1.00  0.00     0.159 HD
ATOM  11408 2HD2 ASN B  89      29.170  28.497  69.040  1.00  0.00     0.159 HD
ATOM  11409  OD1 ASN B  89      30.608  26.200  67.490  1.00 32.17    -0.274 OA
ATOM  11410  N   PHE B  90      28.758  28.253  63.073  1.00 12.86    -0.346 N
ATOM  11411  HN  PHE B  90      29.618  28.800  63.029  1.00  0.00     0.163 HD
ATOM  11412  CA  PHE B  90      27.907  28.152  61.895  1.00 13.22     0.180 C
ATOM  11414  C   PHE B  90      27.615  26.701  61.551  1.00 12.75     0.241 C
ATOM  11415  O   PHE B  90      28.504  25.814  61.579  1.00 12.12    -0.271 OA
ATOM  11416  CB  PHE B  90      28.641  28.821  60.710  1.00 11.38     0.073 C
ATOM  11419  CG  PHE B  90      27.940  28.805  59.370  1.00 17.48    -0.056 A
ATOM  11420  CD1 PHE B  90      26.659  29.316  59.207  1.00  9.59     0.007 A
ATOM  11422  CD2 PHE B  90      28.604  28.298  58.258  1.00 14.61     0.007 A
ATOM  11424  CE1 PHE B  90      26.065  29.377  57.938  1.00 10.02     0.001 A
ATOM  11426  CE2 PHE B  90      28.022  28.347  57.006  1.00 11.51     0.001 A
ATOM  11428  CZ  PHE B  90      26.743  28.869  56.841  1.00 12.81     0.000 A
ATOM  11430  N   ARG B  91      26.326  26.391  61.326  1.00  9.92    -0.346 N
ATOM  11431  HN  ARG B  91      25.639  27.140  61.410  1.00  0.00     0.163 HD
ATOM  11432  CA  ARG B  91      25.837  25.066  60.972  1.00 10.68     0.176 C
ATOM  11434  C   ARG B  91      26.005  24.003  62.045  1.00 16.45     0.241 C
ATOM  11435  O   ARG B  91      25.884  22.807  61.747  1.00 14.85    -0.271 OA
ATOM  11436  CB  ARG B  91      26.505  24.568  59.641  1.00 10.40     0.036 C
ATOM  11439  CG  ARG B  91      25.828  25.347  58.479  1.00 12.62     0.023 C
ATOM  11442  CD  ARG B  91      26.538  25.204  57.123  1.00 12.62     0.138 C
ATOM  11445  NE  ARG B  91      25.593  25.719  56.099  1.00 15.10    -0.227 N
ATOM  11446  HE  ARG B  91      25.439  26.727  56.073  1.00  0.00     0.177 HD
ATOM  11447  CZ  ARG B  91      24.932  24.985  55.216  1.00 15.65     0.665 C
ATOM  11448  NH1 ARG B  91      25.090  23.678  55.006  1.00 13.33    -0.235 N
ATOM  11449 1HH1 ARG B  91      25.759  23.199  55.609  1.00  0.00     0.174 HD
ATOM  11450 2HH1 ARG B  91      24.581  23.113  54.326  1.00  0.00     0.174 HD
ATOM  11451  NH2 ARG B  91      24.060  25.609  54.430  1.00 14.48    -0.235 N
ATOM  11452 1HH2 ARG B  91      23.939  26.609  54.591  1.00  0.00     0.174 HD
ATOM  11453 2HH2 ARG B  91      23.551  25.044  53.750  1.00  0.00     0.174 HD
ATOM  11454  N   GLN B  92      26.218  24.399  63.305  1.00 12.70    -0.346 N
ATOM  11455  HN  GLN B  92      26.289  25.391  63.531  1.00  0.00     0.163 HD
ATOM  11456  CA  GLN B  92      26.349  23.380  64.360  1.00 14.58     0.177 C
ATOM  11458  C   GLN B  92      25.080  23.328  65.181  1.00 14.23     0.241 C
ATOM  11459  O   GLN B  92      24.245  24.251  65.373  1.00 15.62    -0.271 OA
ATOM  11460  CB  GLN B  92      27.601  23.729  65.223  1.00 13.28     0.044 C
ATOM  11463  CG  GLN B  92      28.871  23.947  64.403  1.00 17.78     0.105 C
ATOM  11466  CD  GLN B  92      29.144  22.771  63.484  1.00 19.94     0.215 C
ATOM  11467  NE2 GLN B  92      29.187  22.942  62.171  1.00 15.43    -0.370 N
ATOM  11468 1HE2 GLN B  92      29.371  22.151  61.553  1.00  0.00     0.159 HD
ATOM  11469 2HE2 GLN B  92      29.081  23.868  61.756  1.00  0.00     0.159 HD
ATOM  11470  OE1 GLN B  92      29.272  21.656  63.984  1.00 18.60    -0.274 OA
ATOM  11471  N   LEU B  93      24.930  22.172  65.848  1.00 16.05    -0.346 N
ATOM  11472  HN  LEU B  93      25.667  21.469  65.794  1.00  0.00     0.163 HD
ATOM  11473  CA  LEU B  93      23.741  21.895  66.648  1.00 13.40     0.177 C
ATOM  11475  C   LEU B  93      23.426  22.991  67.646  1.00 15.95     0.241 C
ATOM  11476  O   LEU B  93      24.246  23.382  68.477  1.00 19.28    -0.271 OA
ATOM  11477  CB  LEU B  93      23.941  20.544  67.397  1.00 17.49     0.038 C
ATOM  11480  CG  LEU B  93      22.697  20.059  68.153  1.00 17.17    -0.020 C
ATOM  11482  CD1 LEU B  93      21.577  19.679  67.222  1.00 25.52     0.009 C
ATOM  11486  CD2 LEU B  93      23.149  18.861  68.997  1.00 27.89     0.009 C
ATOM  11490  N   HIS B  94      22.227  23.515  67.578  1.00 14.96    -0.346 N
ATOM  11491  HN  HIS B  94      21.603  23.143  66.863  1.00  0.00     0.163 HD
ATOM  11492  CA  HIS B  94      21.702  24.568  68.416  1.00 21.51     0.182 C
ATOM  11494  C   HIS B  94      22.443  25.903  68.361  1.00 22.24     0.241 C
ATOM  11495  O   HIS B  94      22.267  26.690  69.312  1.00 21.95    -0.271 OA
ATOM  11496  CB  HIS B  94      21.655  24.090  69.894  1.00 26.40     0.093 C
ATOM  11499  CG  HIS B  94      20.820  22.846  70.056  1.00 34.87     0.028 A
ATOM  11500  CD2 HIS B  94      19.664  22.485  69.435  1.00 33.71     0.114 A
ATOM  11502  ND1 HIS B  94      21.190  21.809  70.900  1.00 36.64    -0.354 N
ATOM  11503  HD1 HIS B  94      22.024  21.774  71.486  1.00  0.00     0.166 HD
ATOM  11504  CE1 HIS B  94      20.258  20.874  70.802  1.00 36.10     0.180 A
ATOM  11506  NE2 HIS B  94      19.333  21.247  69.923  1.00 43.52    -0.360 N
ATOM  11507  HE2 HIS B  94      18.513  20.702  69.656  1.00  0.00     0.166 HD
ATOM  11508  N   SER B  95      23.226  26.210  67.331  1.00 18.98    -0.344 N
ATOM  11509  HN  SER B  95      23.396  25.539  66.581  1.00  0.00     0.163 HD
ATOM  11510  CA  SER B  95      23.842  27.551  67.306  1.00 17.52     0.200 C
ATOM  11512  C   SER B  95      22.759  28.534  66.852  1.00 19.15     0.243 C
ATOM  11513  O   SER B  95      21.680  28.116  66.391  1.00 17.27    -0.271 OA
ATOM  11514  CB  SER B  95      24.994  27.601  66.320  1.00 18.81     0.199 C
ATOM  11517  OG  SER B  95      24.450  27.536  64.986  1.00 16.05    -0.398 OA
ATOM  11518  HG  SER B  95      25.171  27.567  64.369  1.00  0.00     0.209 HD
ATOM  11519  N   LYS B  96      23.017  29.844  66.886  1.00 11.60    -0.346 N
ATOM  11520  HN  LYS B  96      23.897  30.167  67.288  1.00  0.00     0.163 HD
ATOM  11521  CA  LYS B  96      22.077  30.819  66.365  1.00 11.97     0.176 C
ATOM  11523  C   LYS B  96      22.420  31.122  64.914  1.00 11.17     0.241 C
ATOM  11524  O   LYS B  96      21.910  32.099  64.366  1.00 12.85    -0.271 OA
ATOM  11525  CB  LYS B  96      22.250  32.149  67.145  1.00 14.37     0.035 C
ATOM  11528  CG  LYS B  96      21.740  31.848  68.578  1.00 26.79     0.004 C
ATOM  11531  CD  LYS B  96      21.595  33.126  69.389  1.00 45.32     0.027 C
ATOM  11534  CE  LYS B  96      20.724  32.869  70.613  1.00 52.00     0.229 C
ATOM  11537  NZ  LYS B  96      20.405  34.111  71.364  1.00 66.91    -0.079 N
ATOM  11538  HZ1 LYS B  96      19.822  33.939  72.183  1.00  0.00     0.274 HD
ATOM  11539  HZ2 LYS B  96      19.980  34.808  70.753  1.00  0.00     0.274 HD
ATOM  11540  HZ3 LYS B  96      21.256  34.612  71.620  1.00  0.00     0.274 HD
ATOM  11541  N   THR B  97      23.267  30.286  64.301  1.00 21.77    -0.344 N
ATOM  11542  HN  THR B  97      23.674  29.508  64.820  1.00  0.00     0.163 HD
ATOM  11543  CA  THR B  97      23.617  30.479  62.884  1.00 10.33     0.205 C
ATOM  11545  C   THR B  97      23.405  29.184  62.095  1.00 11.25     0.246 C
ATOM  11546  O   THR B  97      24.356  28.590  61.547  1.00 14.30    -0.271 OA
ATOM  11547  CB  THR B  97      25.098  30.885  62.746  1.00 17.29     0.146 C
ATOM  11549  CG2 THR B  97      25.372  32.283  63.282  1.00 12.51     0.042 C
ATOM  11553  OG1 THR B  97      25.867  29.959  63.562  1.00 14.26    -0.393 OA
ATOM  11554  HG1 THR B  97      26.780  30.209  63.307  1.00  0.00     0.210 HD
ATOM  11555  N   PRO B  98      22.152  28.779  61.892  1.00 10.97    -0.337 N
ATOM  11556  CA  PRO B  98      21.803  27.625  61.070  1.00 10.17     0.179 C
ATOM  11558  C   PRO B  98      22.142  27.837  59.613  1.00 12.90     0.241 C
ATOM  11559  O   PRO B  98      22.397  28.947  59.147  1.00 11.52    -0.271 OA
ATOM  11560  CB  PRO B  98      20.294  27.422  61.267  1.00 13.03     0.037 C
ATOM  11563  CG  PRO B  98      19.804  28.768  61.691  1.00 11.37     0.022 C
ATOM  11566  CD  PRO B  98      20.932  29.367  62.504  1.00 14.37     0.127 C
ATOM  11569  N   GLY B  99      22.210  26.729  58.840  1.00  9.45    -0.351 N
ATOM  11570  HN  GLY B  99      21.943  25.829  59.239  1.00  0.00     0.163 HD
ATOM  11571  CA  GLY B  99      22.651  26.784  57.463  1.00  9.98     0.225 C
ATOM  11574  C   GLY B  99      21.840  27.735  56.600  1.00 14.04     0.236 C
ATOM  11575  O   GLY B  99      22.377  28.262  55.633  1.00 11.53    -0.272 OA
ATOM  11576  N   HIS B 100      20.554  27.899  56.871  1.00 11.46    -0.346 N
ATOM  11577  HN  HIS B 100      20.120  27.318  57.588  1.00  0.00     0.163 HD
ATOM  11578  CA  HIS B 100      19.736  28.894  56.168  1.00  9.60     0.182 C
ATOM  11580  C   HIS B 100      19.103  29.719  57.283  1.00 12.36     0.243 C
ATOM  11581  O   HIS B 100      18.904  29.150  58.348  1.00 12.55    -0.271 OA
ATOM  11582  CB  HIS B 100      18.674  28.221  55.275  1.00 10.40     0.093 C
ATOM  11585  CG  HIS B 100      19.312  27.576  54.069  1.00 13.22     0.028 A
ATOM  11586  CD2 HIS B 100      19.583  28.020  52.836  1.00 15.74     0.114 A
ATOM  11588  ND1 HIS B 100      19.740  26.260  54.073  1.00 11.78    -0.354 N
ATOM  11589  HD1 HIS B 100      19.661  25.620  54.863  1.00  0.00     0.166 HD
ATOM  11590  CE1 HIS B 100      20.266  25.958  52.901  1.00 13.39     0.180 A
ATOM  11592  NE2 HIS B 100      20.179  27.004  52.129  1.00 15.30    -0.360 N
ATOM  11593  HE2 HIS B 100      20.500  27.059  51.162  1.00  0.00     0.166 HD
ATOM  11594  N   PRO B 101      18.842  30.987  57.074  1.00 13.81    -0.337 N
ATOM  11595  CA  PRO B 101      18.386  31.870  58.135  1.00 14.81     0.179 C
ATOM  11597  C   PRO B 101      16.980  31.505  58.581  1.00 15.29     0.241 C
ATOM  11598  O   PRO B 101      16.189  31.146  57.705  1.00 11.09    -0.271 OA
ATOM  11599  CB  PRO B 101      18.448  33.273  57.543  1.00 13.23     0.037 C
ATOM  11602  CG  PRO B 101      19.140  33.161  56.215  1.00 13.82     0.022 C
ATOM  11605  CD  PRO B 101      18.997  31.714  55.782  1.00 13.11     0.127 C
ATOM  11608  N   GLU B 102      16.759  31.511  59.898  1.00 11.54    -0.346 N
ATOM  11609  HN  GLU B 102      17.518  31.770  60.529  1.00  0.00     0.163 HD
ATOM  11610  CA  GLU B 102      15.472  31.160  60.451  1.00 13.24     0.177 C
ATOM  11612  C   GLU B 102      14.854  32.282  61.292  1.00 14.99     0.241 C
ATOM  11613  O   GLU B 102      15.512  32.740  62.218  1.00 15.22    -0.271 OA
ATOM  11614  CB  GLU B 102      15.556  29.893  61.342  1.00 14.04     0.045 C
ATOM  11617  CG  GLU B 102      16.019  28.675  60.503  1.00 14.94     0.116 C
ATOM  11620  CD  GLU B 102      16.188  27.466  61.424  1.00 20.28     0.172 C
ATOM  11621  OE1 GLU B 102      15.571  27.454  62.515  1.00 21.14    -0.648 OA
ATOM  11622  OE2 GLU B 102      16.925  26.532  61.094  1.00 18.53    -0.648 OA
ATOM  11623  N   VAL B 103      13.657  32.742  60.920  1.00 13.36    -0.346 N
ATOM  11624  HN  VAL B 103      13.185  32.346  60.107  1.00  0.00     0.163 HD
ATOM  11625  CA  VAL B 103      13.028  33.813  61.683  1.00 14.36     0.180 C
ATOM  11627  C   VAL B 103      12.677  33.257  63.059  1.00 18.21     0.241 C
ATOM  11628  O   VAL B 103      12.356  32.091  63.333  1.00 13.49    -0.271 OA
ATOM  11629  CB  VAL B 103      11.780  34.417  61.014  1.00 16.69     0.009 C
ATOM  11631  CG1 VAL B 103      10.673  33.375  60.880  1.00 12.87     0.012 C
ATOM  11635  CG2 VAL B 103      11.187  35.590  61.809  1.00 15.44     0.012 C
ATOM  11639  N   GLY B 104      12.789  34.144  64.033  1.00 16.49    -0.351 N
ATOM  11640  HN  GLY B 104      13.160  35.064  63.797  1.00  0.00     0.163 HD
ATOM  11641  CA  GLY B 104      12.420  33.898  65.415  1.00 22.07     0.225 C
ATOM  11644  C   GLY B 104      13.579  33.277  66.169  1.00 28.29     0.236 C
ATOM  11645  O   GLY B 104      13.626  33.353  67.388  1.00 35.16    -0.272 OA
ATOM  11646  N   LYS B 105      14.525  32.694  65.484  1.00 26.37    -0.346 N
ATOM  11647  HN  LYS B 105      14.474  32.753  64.467  1.00  0.00     0.163 HD
ATOM  11648  CA  LYS B 105      15.644  31.968  66.057  1.00 27.98     0.176 C
ATOM  11650  C   LYS B 105      16.842  32.878  66.254  1.00 30.21     0.241 C
ATOM  11651  O   LYS B 105      17.483  32.800  67.307  1.00 31.56    -0.271 OA
ATOM  11652  CB  LYS B 105      15.969  30.773  65.161  1.00 39.66     0.035 C
ATOM  11655  CG  LYS B 105      16.432  29.509  65.866  1.00 43.50     0.004 C
ATOM  11658  CD  LYS B 105      17.805  29.079  65.361  1.00 42.39     0.027 C
ATOM  11661  CE  LYS B 105      18.805  28.940  66.478  1.00 44.71     0.229 C
ATOM  11664  NZ  LYS B 105      18.848  27.627  67.183  1.00 46.16    -0.079 N
ATOM  11665  HZ1 LYS B 105      19.525  27.533  67.940  1.00  0.00     0.274 HD
ATOM  11666  HZ2 LYS B 105      18.989  26.879  66.504  1.00  0.00     0.274 HD
ATOM  11667  HZ3 LYS B 105      17.917  27.394  67.528  1.00  0.00     0.274 HD
ATOM  11668  N   THR B 106      17.121  33.743  65.284  1.00 14.63    -0.344 N
ATOM  11669  HN  THR B 106      16.509  33.764  64.468  1.00  0.00     0.163 HD
ATOM  11670  CA  THR B 106      18.241  34.656  65.317  1.00 13.90     0.205 C
ATOM  11672  C   THR B 106      17.740  36.100  65.303  1.00 18.08     0.243 C
ATOM  11673  O   THR B 106      16.953  36.390  64.387  1.00 14.11    -0.271 OA
ATOM  11674  CB  THR B 106      19.075  34.406  64.020  1.00 13.03     0.146 C
ATOM  11676  CG2 THR B 106      20.295  35.337  64.007  1.00 17.08     0.042 C
ATOM  11680  OG1 THR B 106      19.436  33.035  64.079  1.00 16.26    -0.393 OA
ATOM  11681  HG1 THR B 106      18.681  32.459  64.087  1.00  0.00     0.210 HD
ATOM  11682  N   ALA B 107      18.201  36.969  66.194  1.00 18.02    -0.346 N
ATOM  11683  HN  ALA B 107      18.884  36.672  66.891  1.00  0.00     0.163 HD
ATOM  11684  CA  ALA B 107      17.732  38.341  66.176  1.00 20.06     0.172 C
ATOM  11686  C   ALA B 107      18.044  39.056  64.859  1.00 15.91     0.240 C
ATOM  11687  O   ALA B 107      19.158  39.014  64.365  1.00 16.60    -0.271 OA
ATOM  11688  CB  ALA B 107      18.393  39.177  67.284  1.00 22.57     0.042 C
ATOM  11692  N   GLY B 108      17.069  39.781  64.302  1.00 11.89    -0.351 N
ATOM  11693  HN  GLY B 108      16.140  39.790  64.723  1.00  0.00     0.163 HD
ATOM  11694  CA  GLY B 108      17.329  40.569  63.080  1.00 11.01     0.225 C
ATOM  11697  C   GLY B 108      16.908  39.797  61.818  1.00 13.63     0.236 C
ATOM  11698  O   GLY B 108      16.807  40.436  60.758  1.00 17.16    -0.272 OA
ATOM  11699  N   VAL B 109      16.663  38.494  61.894  1.00  8.54    -0.346 N
ATOM  11700  HN  VAL B 109      16.743  38.003  62.785  1.00  0.00     0.163 HD
ATOM  11701  CA  VAL B 109      16.272  37.764  60.667  1.00  9.45     0.180 C
ATOM  11703  C   VAL B 109      14.793  37.943  60.443  1.00 12.22     0.241 C
ATOM  11704  O   VAL B 109      14.030  37.656  61.364  1.00 12.33    -0.271 OA
ATOM  11705  CB  VAL B 109      16.678  36.281  60.819  1.00 10.40     0.009 C
ATOM  11707  CG1 VAL B 109      16.131  35.429  59.673  1.00 12.82     0.012 C
ATOM  11711  CG2 VAL B 109      18.196  36.215  60.791  1.00  8.80     0.012 C
ATOM  11715  N   GLU B 110      14.347  38.434  59.282  1.00  8.58    -0.346 N
ATOM  11716  HN  GLU B 110      15.011  38.605  58.527  1.00  0.00     0.163 HD
ATOM  11717  CA  GLU B 110      12.944  38.730  59.070  1.00  7.92     0.177 C
ATOM  11719  C   GLU B 110      12.090  37.578  58.530  1.00  9.85     0.241 C
ATOM  11720  O   GLU B 110      10.865  37.652  58.721  1.00  9.06    -0.271 OA
ATOM  11721  CB  GLU B 110      12.758  39.883  58.061  1.00 11.96     0.045 C
ATOM  11724  CG  GLU B 110      13.497  41.179  58.477  1.00  8.65     0.116 C
ATOM  11727  CD  GLU B 110      12.762  41.897  59.600  1.00 16.15     0.172 C
ATOM  11728  OE1 GLU B 110      11.664  41.535  60.071  1.00 13.34    -0.648 OA
ATOM  11729  OE2 GLU B 110      13.279  42.940  60.078  1.00 17.45    -0.648 OA
ATOM  11730  N   THR B 111      12.695  36.578  57.916  1.00  8.75    -0.344 N
ATOM  11731  HN  THR B 111      13.706  36.568  57.785  1.00  0.00     0.163 HD
ATOM  11732  CA  THR B 111      11.842  35.471  57.426  1.00  7.40     0.205 C
ATOM  11734  C   THR B 111      12.801  34.280  57.307  1.00 12.78     0.243 C
ATOM  11735  O   THR B 111      14.026  34.502  57.337  1.00 12.42    -0.271 OA
ATOM  11736  CB  THR B 111      11.253  35.862  56.068  1.00  9.26     0.146 C
ATOM  11738  CG2 THR B 111      12.245  36.230  54.990  1.00 16.34     0.042 C
ATOM  11742  OG1 THR B 111      10.422  34.762  55.596  1.00  9.21    -0.393 OA
ATOM  11743  HG1 THR B 111       9.788  34.531  56.274  1.00  0.00     0.210 HD
ATOM  11744  N   THR B 112      12.262  33.089  57.127  1.00 10.45    -0.344 N
ATOM  11745  HN  THR B 112      11.248  32.982  57.154  1.00  0.00     0.163 HD
ATOM  11746  CA  THR B 112      13.108  31.923  56.889  1.00  7.10     0.205 C
ATOM  11748  C   THR B 112      13.243  31.672  55.383  1.00 11.03     0.243 C
ATOM  11749  O   THR B 112      12.215  31.507  54.690  1.00 11.19    -0.271 OA
ATOM  11750  CB  THR B 112      12.448  30.698  57.552  1.00 14.43     0.146 C
ATOM  11752  CG2 THR B 112      13.288  29.426  57.372  1.00 11.42     0.042 C
ATOM  11756  OG1 THR B 112      12.402  31.051  58.972  1.00 11.19    -0.393 OA
ATOM  11757  HG1 THR B 112      11.882  31.838  59.083  1.00  0.00     0.210 HD
ATOM  11758  N   THR B 113      14.445  31.633  54.865  1.00  5.24    -0.344 N
ATOM  11759  HN  THR B 113      15.269  31.772  55.450  1.00  0.00     0.163 HD
ATOM  11760  CA  THR B 113      14.585  31.381  53.398  1.00  8.84     0.205 C
ATOM  11762  C   THR B 113      15.417  30.125  53.168  1.00 12.68     0.243 C
ATOM  11763  O   THR B 113      15.788  29.441  54.106  1.00 15.34    -0.271 OA
ATOM  11764  CB  THR B 113      15.133  32.592  52.647  1.00 10.33     0.146 C
ATOM  11766  CG2 THR B 113      14.169  33.794  52.713  1.00 18.09     0.042 C
ATOM  11770  OG1 THR B 113      16.354  33.032  53.278  1.00 13.36    -0.393 OA
ATOM  11771  HG1 THR B 113      16.948  32.292  53.237  1.00  0.00     0.210 HD
ATOM  11772  N   GLY B 114      15.708  29.727  51.915  1.00 14.31    -0.350 N
ATOM  11773  HN  GLY B 114      15.514  30.342  51.124  1.00  0.00     0.163 HD
ATOM  11774  CA  GLY B 114      16.309  28.399  51.690  1.00 12.49     0.225 C
ATOM  11777  C   GLY B 114      15.591  27.816  50.451  1.00 12.09     0.238 C
ATOM  11778  O   GLY B 114      16.174  27.654  49.373  1.00 16.06    -0.272 OA
ATOM  11779  N   PRO B 115      14.282  27.768  50.504  1.00 13.18    -0.337 N
ATOM  11780  CA  PRO B 115      13.479  27.394  49.341  1.00 12.33     0.179 C
ATOM  11782  C   PRO B 115      13.435  28.615  48.424  1.00 11.50     0.241 C
ATOM  11783  O   PRO B 115      12.764  29.625  48.656  1.00  8.62    -0.271 OA
ATOM  11784  CB  PRO B 115      12.114  26.968  49.864  1.00 13.90     0.037 C
ATOM  11787  CG  PRO B 115      12.344  26.807  51.349  1.00 13.34     0.022 C
ATOM  11790  CD  PRO B 115      13.401  27.853  51.711  1.00 14.36     0.127 C
ATOM  11793  N   LEU B 116      14.132  28.487  47.281  1.00  8.83    -0.346 N
ATOM  11794  HN  LEU B 116      14.605  27.610  47.065  1.00  0.00     0.163 HD
ATOM  11795  CA  LEU B 116      14.208  29.615  46.347  1.00 10.24     0.177 C
ATOM  11797  C   LEU B 116      12.878  30.139  45.852  1.00 10.24     0.240 C
ATOM  11798  O   LEU B 116      11.890  29.484  45.614  1.00  8.64    -0.271 OA
ATOM  11799  CB  LEU B 116      15.092  29.246  45.127  1.00 11.56     0.038 C
ATOM  11802  CG  LEU B 116      16.549  28.937  45.481  1.00 11.61    -0.020 C
ATOM  11804  CD1 LEU B 116      17.233  28.172  44.332  1.00 13.12     0.009 C
ATOM  11808  CD2 LEU B 116      17.330  30.208  45.763  1.00 14.56     0.009 C
ATOM  11812  N   GLY B 117      12.822  31.469  45.649  1.00  7.47    -0.351 N
ATOM  11813  HN  GLY B 117      13.670  32.004  45.838  1.00  0.00     0.163 HD
ATOM  11814  CA  GLY B 117      11.661  32.210  45.184  1.00 10.01     0.225 C
ATOM  11817  C   GLY B 117      10.784  32.714  46.307  1.00 10.03     0.236 C
ATOM  11818  O   GLY B 117      10.039  33.697  46.125  1.00  9.73    -0.272 OA
ATOM  11819  N   GLN B 118      10.746  31.994  47.452  1.00  7.12    -0.346 N
ATOM  11820  HN  GLN B 118      11.352  31.188  47.604  1.00  0.00     0.163 HD
ATOM  11821  CA  GLN B 118       9.784  32.442  48.458  1.00  5.02     0.177 C
ATOM  11823  C   GLN B 118      10.229  33.703  49.175  1.00  8.64     0.240 C
ATOM  11824  O   GLN B 118       9.336  34.392  49.708  1.00  7.28    -0.271 OA
ATOM  11825  CB  GLN B 118       9.497  31.320  49.491  1.00  9.44     0.044 C
ATOM  11828  CG  GLN B 118       8.628  30.263  48.778  1.00  9.94     0.105 C
ATOM  11831  CD  GLN B 118       8.152  29.179  49.728  1.00 11.34     0.215 C
ATOM  11832  OE1 GLN B 118       8.557  27.938  49.481  1.00  9.29    -0.370 O
ATOM  11833 1HE2 GLN B 118       9.180  27.697  48.710  1.00  0.00     0.159 HD
ATOM  11834 2HE2 GLN B 118       8.237  27.210  50.119  1.00  0.00     0.159 HD
ATOM  11835  OE1 GLN B 118       7.407  29.467  50.650  1.00  9.46    -0.274 OA
ATOM  11839  N   GLY B 119      11.539  33.958  49.271  1.00  8.07    -0.351 N
ATOM  11837  HN  GLY B 119      12.253  33.338  48.888  1.00  0.00     0.163 HD
ATOM  11838  CA  GLY B 119      11.867  35.225  49.985  1.00  9.32     0.225 C
ATOM  11841  C   GLY B 119      11.400  36.458  49.221  1.00 10.93     0.236 C
ATOM  11842  O   GLY B 119      10.853  37.398  49.830  1.00  7.03    -0.272 OA
ATOM  11843  N   ILE B 120      11.551  36.501  47.881  1.00  7.43    -0.346 N
ATOM  11844  HN  ILE B 120      12.013  35.754  47.363  1.00  0.00     0.163 HD
ATOM  11845  CA  ILE B 120      10.995  37.718  47.202  1.00  5.89     0.180 C
ATOM  11847  C   ILE B 120       9.482  37.753  47.324  1.00  9.83     0.241 C
ATOM  11848  O   ILE B 120       8.878  38.836  47.516  1.00 10.62    -0.271 OA
ATOM  11849  CB  ILE B 120      11.485  37.826  45.741  1.00  9.00     0.013 C
ATOM  11851  CG1 ILE B 120      10.872  39.042  45.001  1.00 12.97     0.002 C
ATOM  11854  CG2 ILE B 120      11.058  36.591  44.971  1.00  9.22     0.012 C
ATOM  11858  CD1 ILE B 120      11.334  40.368  45.589  1.00 13.30     0.005 C
ATOM  11862  N   ALA B 121       8.796  36.602  47.377  1.00  6.23    -0.346 N
ATOM  11863  HN  ALA B 121       9.287  35.717  47.246  1.00  0.00     0.163 HD
ATOM  11864  CA  ALA B 121       7.342  36.598  47.622  1.00  6.72     0.172 C
ATOM  11866  C   ALA B 121       7.009  37.172  48.993  1.00  8.77     0.240 C
ATOM  11867  O   ALA B 121       6.096  38.012  49.129  1.00  5.66    -0.271 OA
ATOM  11868  CB  ALA B 121       6.801  35.158  47.504  1.00  6.17     0.042 C
ATOM  11872  N   ASN B 122       7.782  36.763  50.020  1.00  6.78    -0.346 N
ATOM  11873  HN  ASN B 122       8.533  36.092  49.859  1.00  0.00     0.163 HD
ATOM  11874  CA  ASN B 122       7.540  37.285  51.364  1.00  6.74     0.185 C
ATOM  11876  C   ASN B 122       7.780  38.801  51.363  1.00  7.17     0.241 C
ATOM  11877  O   ASN B 122       7.063  39.525  52.063  1.00  8.72    -0.271 OA
ATOM  11879  CB  ASN B 122       8.468  36.661  52.415  1.00  5.81     0.137 C
ATOM  11881  CG  ASN B 122       8.365  35.165  52.606  1.00 10.67     0.217 C
ATOM  11882  ND2 ASN B 122       7.281  34.465  52.255  1.00  8.10    -0.370 N
ATOM  11883 1HD2 ASN B 122       6.439  34.915  51.895  1.00  0.00     0.159 HD
ATOM  11884 2HD2 ASN B 122       7.212  33.456  52.384  1.00  0.00     0.159 HD
ATOM  11885  OD1 ASN B 122       9.372  34.627  53.037  1.00  8.91    -0.274 OA
ATOM  11886  N   ALA B 123       8.813  39.261  50.679  1.00  6.35    -0.346 N
ATOM  11887  HN  ALA B 123       9.440  38.610  50.207  1.00  0.00     0.163 HD
ATOM  11888  CA  ALA B 123       9.062  40.707  50.596  1.00  8.54     0.172 C
ATOM  11890  C   ALA B 123       7.928  41.445  49.866  1.00  9.28     0.240 C
ATOM  11891  O   ALA B 123       7.610  42.541  50.314  1.00  7.35    -0.271 OA
ATOM  11892  CB  ALA B 123      10.370  40.992  49.861  1.00  8.80     0.042 C
ATOM  11896  N   VAL B 124       7.287  40.885  48.834  1.00  7.11    -0.346 N
ATOM  11897  HN  VAL B 124       7.604  39.992  48.457  1.00  0.00     0.163 HD
ATOM  11898  CA  VAL B 124       6.107  41.572  48.237  1.00  5.48     0.180 C
ATOM  11900  C   VAL B 124       5.033  41.693  49.295  1.00  7.66     0.241 C
ATOM  11901  O   VAL B 124       4.360  42.738  49.431  1.00  7.08    -0.271 OA
ATOM  11902  CB  VAL B 124       5.588  40.786  46.994  1.00  7.19     0.009 C
ATOM  11904  CG1 VAL B 124       4.232  41.295  46.513  1.00  5.41     0.012 C
ATOM  11908  CG2 VAL B 124       6.717  40.874  45.928  1.00  5.04     0.012 C
ATOM  11912  N   GLY B 125       4.826  40.614  50.088  1.00  6.63    -0.351 N
ATOM  11913  HN  GLY B 125       5.349  39.752  49.931  1.00  0.00     0.163 HD
ATOM  11914  CA  GLY B 125       3.844  40.697  51.173  1.00  7.03     0.225 C
ATOM  11917  C   GLY B 125       4.196  41.755  52.227  1.00 11.16     0.236 C
ATOM  11918  O   GLY B 125       3.287  42.492  52.688  1.00  7.22    -0.272 OA
ATOM  11919  N   MET B 126       5.443  41.898  52.623  1.00  5.74    -0.346 N
ATOM  11920  HN  MET B 126       6.153  41.262  52.260  1.00  0.00     0.163 HD
ATOM  11921  CA  MET B 126       5.848  42.954  53.580  1.00  8.18     0.177 C
ATOM  11923  C   MET B 126       5.609  44.349  52.995  1.00 10.48     0.241 C
ATOM  11924  O   MET B 126       5.197  45.278  53.730  1.00  8.17    -0.271 OA
ATOM  11925  CB  MET B 126       7.339  42.796  53.932  1.00  6.45     0.045 C
ATOM  11928  CG  MET B 126       7.560  41.521  54.767  1.00  8.00     0.076 C
ATOM  11931  SD  MET B 126       9.352  41.204  54.897  1.00 11.41    -0.173 SA
ATOM  11932  CE  MET B 126       9.270  39.659  55.842  1.00 13.98     0.089 C
ATOM  11936  N   ALA B 127       5.907  44.547  51.700  1.00  5.34    -0.346 N
ATOM  11937  HN  ALA B 127       6.322  43.791  51.156  1.00  0.00     0.163 HD
ATOM  11938  CA  ALA B 127       5.641  45.838  51.063  1.00  7.26     0.172 C
ATOM  11940  C   ALA B 127       4.152  46.117  50.965  1.00  8.41     0.240 C
ATOM  11941  O   ALA B 127       3.746  47.262  51.144  1.00  8.46    -0.271 OA
ATOM  11942  CB  ALA B 127       6.284  45.938  49.674  1.00  5.57     0.042 C
ATOM  11946  N   ILE B 128       3.295  45.119  50.684  1.00  4.97    -0.346 N
ATOM  11947  HN  ILE B 128       3.653  44.189  50.464  1.00  0.00     0.163 HD
ATOM  11948  CA  ILE B 128       1.847  45.362  50.692  1.00  5.72     0.180 C
ATOM  11950  C   ILE B 128       1.381  45.723  52.088  1.00  7.91     0.241 C
ATOM  11951  O   ILE B 128       0.505  46.587  52.285  1.00  9.31    -0.271 OA
ATOM  11952  CB  ILE B 128       1.142  44.040  50.210  1.00  7.39     0.013 C
ATOM  11954  CG1 ILE B 128       1.319  43.887  48.691  1.00  9.70     0.002 C
ATOM  11957  CG2 ILE B 128      -0.365  44.065  50.615  1.00  6.79     0.012 C
ATOM  11961  CD1 ILE B 128       0.903  42.443  48.253  1.00 11.26     0.005 C
ATOM  11965  N   ALA B 129       1.959  45.058  53.107  1.00  6.44    -0.346 N
ATOM  11966  HN  ALA B 129       2.674  44.353  52.929  1.00  0.00     0.163 HD
ATOM  11967  CA  ALA B 129       1.539  45.368  54.478  1.00  8.45     0.172 C
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ATOM  11969  C   ALA B 129       1.878  46.800  54.843  1.00  8.81      0.240 C
ATOM  11970  O   ALA B 129       1.070  47.488  55.487  1.00  9.72     -0.271 OA
ATOM  11971  CB  ALA B 129       2.155  44.415  55.532  1.00 10.66      0.042 C
ATOM  11975  N   GLU B 130       3.101  47.211  54.492  1.00  6.63     -0.346 N
ATOM  11976  HN  GLU B 130       3.734  46.587  53.991  1.00  0.00      0.163 HD
ATOM  11977  CA  GLU B 130       3.525  48.595  54.844  1.00  6.83      0.177 C
ATOM  11979  C   GLU B 130       2.594  49.604  54.166  1.00  9.21      0.241 C
ATOM  11980  O   GLU B 130       2.117  50.580  54.748  1.00  6.80     -0.271 OA
ATOM  11981  CB  GLU B 130       4.966  48.810  54.313  1.00  4.16      0.045 C
ATOM  11984  CG  GLU B 130       5.573  50.169  54.821  1.00  4.20      0.116 C
ATOM  11987  CD  GLU B 130       5.301  51.374  53.960  1.00 15.54      0.172 C
ATOM  11988  OE1 GLU B 130       4.809  51.307  52.828  1.00 10.78     -0.648 OA
ATOM  11989  OE2 GLU B 130       5.576  52.533  54.352  1.00  8.77     -0.648 OA
ATOM  11990  N   LYS B 131       2.332  49.395  52.853  1.00  7.62     -0.346 N
ATOM  11991  HN  LYS B 131       2.722  48.580  52.380  1.00  0.00      0.163 HD
ATOM  11992  CA  LYS B 131       1.495  50.331  52.115  1.00  8.70      0.176 C
ATOM  11994  C   LYS B 131       0.102  50.439  52.686  1.00  9.58      0.241 C
ATOM  11995  O   LYS B 131      -0.537  51.500  52.718  1.00  8.83     -0.271 OA
ATOM  11996  CB  LYS B 131       1.466  49.883  50.625  1.00  7.60      0.035 C
ATOM  11999  CG  LYS B 131       0.618  50.810  49.746  1.00 11.48      0.004 C
ATOM  12002  CD  LYS B 131       0.535  50.203  48.309  1.00 13.02      0.027 C
ATOM  12005  CE  LYS B 131      -0.193  51.289  47.463  1.00 19.08      0.229 C
ATOM  12008  NZ  LYS B 131      -0.868  50.710  46.280  1.00 20.30     -0.079 N
ATOM  12009  HZ1 LYS B 131      -1.345  51.421  45.726  1.00  0.00      0.274 HD
ATOM  12010  HZ2 LYS B 131      -1.506  49.960  46.548  1.00  0.00      0.274 HD
ATOM  12011  HZ3 LYS B 131      -0.217  50.171  45.709  1.00  0.00      0.274 HD
ATOM  12012  N   THR B 132      -0.489  49.266  52.988  1.00  5.76     -0.344 N
ATOM  12013  HN  THR B 132       0.032  48.399  52.861  1.00  0.00      0.163 HD
ATOM  12014  CA  THR B 132      -1.845  49.208  53.488  1.00  8.97      0.205 C
ATOM  12016  C   THR B 132      -1.939  49.754  54.918  1.00 11.59      0.243 C
ATOM  12017  O   THR B 132      -2.871  50.508  55.277  1.00 11.11     -0.271 OA
ATOM  12018  CB  THR B 132      -2.328  47.719  53.473  1.00 14.76      0.146 C
ATOM  12020  CG2 THR B 132      -3.791  47.666  53.873  1.00 12.63      0.042 C
ATOM  12024  OG1 THR B 132      -2.183  47.223  52.113  1.00 10.48     -0.393 OA
ATOM  12025  HG1 THR B 132      -1.267  47.257  51.863  1.00  0.00      0.210 HD
ATOM  12026  N   LEU B 133      -0.935  49.454  55.743  1.00  8.95     -0.346 N
ATOM  12027  HN  LEU B 133      -0.164  48.860  55.437  1.00  0.00      0.163 HD
ATOM  12028  CA  LEU B 133      -0.971  50.009  57.121  1.00 10.25      0.177 C
ATOM  12030  C   LEU B 133      -0.753  51.527  57.102  1.00 11.35      0.241 C
ATOM  12031  O   LEU B 133      -1.431  52.234  57.913  1.00  9.79     -0.271 OA
ATOM  12032  CB  LEU B 133       0.096  49.329  57.970  1.00 10.92      0.038 C
ATOM  12035  CG  LEU B 133      -0.017  49.253  59.485  1.00 22.01     -0.020 C
ATOM  12037  CD1 LEU B 133      -1.201  48.400  59.907  1.00 19.13      0.009 C
ATOM  12041  CD2 LEU B 133       1.309  48.658  60.000  1.00 21.48      0.009 C
ATOM  12045  N   ALA B 134       0.106  52.032  56.260  1.00  6.90     -0.346 N
ATOM  12046  HN  ALA B 134       0.656  51.402  55.675  1.00  0.00      0.163 HD
ATOM  12047  CA  ALA B 134       0.281  53.489  56.120  1.00 11.95      0.172 C
ATOM  12049  C   ALA B 134      -1.031  54.148  55.687  1.00 11.31      0.240 C
ATOM  12050  O   ALA B 134      -1.484  55.201  56.213  1.00  9.88     -0.271 OA
ATOM  12051  CB  ALA B 134       1.431  53.788  55.152  1.00  6.40      0.042 C
ATOM  12055  N   ALA B 135      -1.732  53.548  54.694  1.00  5.46     -0.346 N
ATOM  12056  HN  ALA B 135      -1.370  52.698  54.263  1.00  0.00      0.163 HD
ATOM  12057  CA  ALA B 135      -3.001  54.108  54.236  1.00  9.93      0.172 C
ATOM  12059  C   ALA B 135      -4.033  54.087  55.361  1.00 16.23      0.240 C
ATOM  12060  O   ALA B 135      -4.866  54.997  55.489  1.00 12.51     -0.271 OA
ATOM  12061  CB  ALA B 135      -3.550  53.325  53.031  1.00 10.04      0.042 C
ATOM  12065  N   GLN B 136      -4.074  53.048  56.180  1.00  8.84     -0.346 N
ATOM  12066  HN  GLN B 136      -3.418  52.278  56.047  1.00  0.00      0.163 HD
ATOM  12067  CA  GLN B 136      -5.046  52.985  57.275  1.00 12.34      0.177 C
ATOM  12069  C   GLN B 136      -4.701  53.879  58.457  1.00 13.39      0.241 C
ATOM  12070  O   GLN B 136      -5.649  54.396  59.074  1.00 13.35     -0.271 OA
ATOM  12071  CB  GLN B 136      -5.238  51.553  57.784  1.00 11.42      0.044 C
ATOM  12074  CG  GLN B 136      -5.841  50.586  56.762  1.00 26.05      0.105 C
ATOM  12077  CD  GLN B 136      -5.915  49.149  57.280  1.00 12.45      0.215 C
ATOM  12078  NE2 GLN B 136      -6.498  48.255  56.488  1.00 10.29     -0.370 N
ATOM  12079 1HE2 GLN B 136      -6.547  47.297  56.833  1.00  0.00      0.159 HD
ATOM  12080 2HE2 GLN B 136      -6.841  48.536  55.570  1.00  0.00      0.159 HD
ATOM  12081  OE1 GLN B 136      -5.498  48.807  58.396  1.00 13.46     -0.274 OA
ATOM  12082  N   PHE B 137      -3.437  54.102  58.789  1.00  9.37     -0.346 N
ATOM  12083  HN  PHE B 137      -2.682  53.765  58.191  1.00  0.00      0.163 HD
ATOM  12084  CA  PHE B 137      -3.130  54.837  60.022  1.00 12.05      0.180 C
ATOM  12086  C   PHE B 137      -2.515  56.209  59.870  1.00 11.32      0.241 C
ATOM  12087  O   PHE B 137      -2.603  57.008  60.821  1.00 15.00     -0.271 OA
ATOM  12088  CB  PHE B 137      -2.140  53.979  60.873  1.00 10.85      0.073 C
ATOM  12091  CG  PHE B 137      -2.869  52.833  61.522  1.00 12.45     -0.056 A
ATOM  12092  CD1 PHE B 137      -3.473  52.996  62.748  1.00 14.96      0.007 A
ATOM  12094  CD2 PHE B 137      -2.949  51.598  60.866  1.00 11.95      0.007 A
ATOM  12096  CE1 PHE B 137      -4.173  51.956  63.355  1.00 15.57      0.001 A
ATOM  12098  CE2 PHE B 137      -3.644  50.558  61.466  1.00 12.22      0.001 A
ATOM  12100  CZ  PHE B 137      -4.256  50.731  62.707  1.00 11.30      0.000 A
ATOM  12102  N   ASN B 138      -1.801  56.502  58.788  1.00 10.24     -0.346 N
ATOM  12103  HN  ASN B 138      -1.740  55.844  58.011  1.00  0.00      0.163 HD
ATOM  12104  CA  ASN B 138      -1.101  57.795  58.735  1.00 11.73      0.185 C
ATOM  12106  C   ASN B 138      -2.115  58.956  58.685  1.00 17.45      0.241 C
ATOM  12107  O   ASN B 138      -3.222  58.850  58.157  1.00 15.48     -0.271 OA
ATOM  12108  CB  ASN B 138      -0.151  57.933  57.525  1.00 11.63      0.137 C
ATOM  12111  CG  ASN B 138       1.109  57.097  57.640  1.00 14.41      0.217 C
ATOM  12112  ND2 ASN B 138       1.908  56.911  56.587  1.00  9.17     -0.370 N
ATOM  12113 1HD2 ASN B 138       2.755  56.349  56.664  1.00  0.00      0.159 HD
ATOM  12114 2HD2 ASN B 138       1.695  57.336  55.684  1.00  0.00      0.159 HD
ATOM  12115  OD1 ASN B 138       1.369  56.577  58.744  1.00 10.04     -0.274 OA
ATOM  12116  N   ARG B 139      -1.693  60.086  59.246  1.00 14.81     -0.346 N
ATOM  12117  HN  ARG B 139      -0.804  60.066  59.745  1.00  0.00      0.163 HD
ATOM  12118  CA  ARG B 139      -2.432  61.379  59.194  1.00 22.95      0.177 C
ATOM  12120  C   ARG B 139      -1.385  62.428  58.835  1.00 23.50      0.243 C
ATOM  12121  O   ARG B 139      -0.149  62.261  58.830  1.00 21.44     -0.271 OA
ATOM  12122  CB  ARG B 139      -3.251  61.653  60.418  1.00 24.47      0.040 C
ATOM  12125  CG  ARG B 139      -3.680  60.572  61.410  1.00 22.51      0.047 C
ATOM  12128  CD  ARG B 139      -4.930  59.946  60.975  1.00 22.43      0.079 C
ATOM  12130  NE  ARG B 139      -6.001  59.172  61.490  1.00 21.44     -0.206 N
ATOM  12131  HE  ARG B 139      -6.447  59.386  62.382  1.00  0.00      0.183 HD
ATOM  12132  CZ  ARG B 139      -6.389  58.135  60.721  1.00 30.20      0.668 C
ATOM  12133  NH1 ARG B 139      -5.743  57.931  59.570  1.00 32.96     -0.235 N
ATOM  12134 1HH1 ARG B 139      -4.999  58.580  59.313  1.00  0.00      0.174 HD
ATOM  12135 2HH1 ARG B 139      -6.037  57.146  58.988  1.00  0.00      0.174 HD
ATOM  12136  NH2 ARG B 139      -7.351  57.296  61.054  1.00 33.19     -0.235 N
ATOM  12137 1HH2 ARG B 139      -7.844  57.452  61.933  1.00  0.00      0.174 HD
ATOM  12138 2HH2 ARG B 139      -7.645  56.511  60.472  1.00  0.00      0.174 HD
ATOM  12139  N   PRO B 140      -1.795  63.520  58.163  1.00 36.44     -0.337 N
ATOM  12140  CA  PRO B 140      -0.866  64.499  57.581  1.00 33.63      0.179 C
ATOM  12142  C   PRO B 140       0.073  65.029  58.643  1.00 26.63      0.241 C
ATOM  12143  O   PRO B 140      -0.455  65.356  59.680  1.00 21.68     -0.271 OA
ATOM  12144  CB  PRO B 140      -1.811  65.547  56.994  1.00 41.57      0.037 C
ATOM  12147  CG  PRO B 140      -3.064  65.425  57.827  1.00 42.60      0.022 C
ATOM  12150  CD  PRO B 140      -3.208  63.934  58.018  1.00 36.02      0.127 C
ATOM  12153  N   GLY B 141       1.399  64.940  58.531  1.00 28.85     -0.351 N
ATOM  12154  HN  GLY B 141       1.808  64.575  57.671  1.00  0.00      0.163 HD
ATOM  12155  CA  GLY B 141       2.280  65.361  59.631  1.00 27.92      0.225 C
ATOM  12158  C   GLY B 141       2.434  64.296  60.722  1.00 30.19      0.236 C
ATOM  12159  O   GLY B 141       3.211  64.443  61.685  1.00 22.96     -0.272 OA
ATOM  12160  N   HIS B 142       1.660  63.197  60.586  1.00 16.68     -0.346 N
ATOM  12161  HN  HIS B 142       1.002  63.131  59.809  1.00  0.00      0.163 HD
ATOM  12162  CA  HIS B 142       1.763  62.100  61.552  1.00 14.91      0.182 C
ATOM  12164  C   HIS B 142       1.942  60.799  60.729  1.00 17.89      0.241 C
ATOM  12165  O   HIS B 142       1.074  59.935  60.698  1.00 11.93     -0.271 OA
ATOM  12166  CB  HIS B 142       0.467  62.055  62.328  1.00 13.51      0.093 C
ATOM  12169  CG  HIS B 142       0.202  63.188  63.292  1.00 20.41      0.028 A
ATOM  12170  CD2 HIS B 142      -0.502  64.342  63.129  1.00 19.29      0.114 A
ATOM  12172  ND1 HIS B 142       0.608  63.188  64.593  1.00 26.67     -0.354 N
ATOM  12173  HD1 HIS B 142       1.162  62.449  65.026  1.00  0.00      0.166 HD
ATOM  12174  CE1 HIS B 142       0.187  64.277  65.220  1.00 25.58      0.180 A
ATOM  12176  NE2 HIS B 142      -0.478  64.997  64.333  1.00 21.28     -0.360 N
ATOM  12177  HE2 HIS B 142      -0.908  65.903  64.517  1.00  0.00      0.166 HD
ATOM  12178  N   ASP B 143       3.007  60.760  59.975  1.00 14.12     -0.345 N
ATOM  12179  HN  ASP B 143       3.652  61.550  59.953  1.00  0.00      0.163 HD
ATOM  12180  CA  ASP B 143       3.272  59.547  59.145  1.00 18.54      0.186 C
ATOM  12182  C   ASP B 143       4.025  58.524  59.986  1.00 26.66      0.241 C
ATOM  12183  O   ASP B 143       5.249  58.406  59.886  1.00 17.76     -0.271 OA
ATOM  12184  CB  ASP B 143       4.101  60.044  57.966  1.00 23.74      0.147 C
ATOM  12187  CG  ASP B 143       3.235  60.716  56.905  1.00 36.46      0.175 C
ATOM  12188  OD1 ASP B 143       1.992  60.849  57.010  1.00 32.82     -0.648 OA
ATOM  12189  OD2 ASP B 143       3.833  61.149  55.895  1.00 57.43     -0.648 OA
ATOM  12190  N   ILE B 144       3.353  57.774  60.840  1.00  9.98     -0.346 N
ATOM  12191  HN  ILE B 144       2.338  57.869  60.865  1.00  0.00      0.163 HD
ATOM  12192  CA  ILE B 144       3.976  56.815  61.752  1.00  0.06      0.180 C
ATOM  12194  C   ILE B 144       4.379  55.519  61.029  1.00  9.48      0.241 C
ATOM  12195  O   ILE B 144       5.149  54.721  61.579  1.00 13.10     -0.271 OA
ATOM  12196  CB  ILE B 144       3.069  56.473  62.947  1.00 13.45      0.013 C
ATOM  12198  CG1 ILE B 144       1.671  55.978  62.580  1.00 13.56      0.002 C
ATOM  12201  CG2 ILE B 144       2.924  57.744  63.815  1.00 18.23      0.012 C
ATOM  12205  CD1 ILE B 144       1.021  55.171  63.707  1.00 16.38      0.005 C
ATOM  12209  N   VAL B 145       3.855  55.331  59.818  1.00 11.47     -0.346 N
ATOM  12210  HN  VAL B 145       3.165  55.984  59.446  1.00  0.00      0.163 HD
ATOM  12211  CA  VAL B 145       4.284  54.171  59.026  1.00  0.88      0.180 C
ATOM  12213  C   VAL B 145       4.994  54.713  57.781  1.00  9.13      0.241 C
ATOM  12214  O   VAL B 145       4.356  55.345  56.929  1.00 10.34     -0.271 OA
ATOM  12215  CB  VAL B 145       3.124  53.266  58.565  1.00 13.42      0.009 C
ATOM  12217  CG1 VAL B 145       3.732  52.055  57.819  1.00  8.27      0.012 C
ATOM  12221  CG2 VAL B 145       2.266  52.781  59.711  1.00 13.56      0.012 C
ATOM  12225  N   ASP B 146       6.254  54.371  57.646  1.00  8.74     -0.345 N
ATOM  12226  HN  ASP B 146       6.704  53.803  58.364  1.00  0.00      0.163 HD
ATOM  12227  CA  ASP B 146       7.023  54.800  56.467  1.00 14.17      0.186 C
ATOM  12229  C   ASP B 146       8.317  54.025  56.432  1.00 13.14      0.241 C
ATOM  12230  O   ASP B 146       9.308  54.447  57.051  1.00 12.00     -0.271 OA
ATOM  12231  CB  ASP B 146       7.327  56.320  56.569  1.00 11.97      0.147 C
ATOM  12234  CG  ASP B 146       8.084  56.818  55.363  1.00 27.72      0.175 C
ATOM  12235  OD1 ASP B 146       8.377  56.122  54.375  1.00 15.15     -0.648 OA
ATOM  12236  OD2 ASP B 146       8.453  58.004  55.375  1.00 22.69     -0.648 OA
ATOM  12237  N   HIS B 147       8.337  52.881  55.741  1.00  9.56     -0.346 N
ATOM  12238  HN  HIS B 147       7.505  52.543  55.257  1.00  0.00      0.163 HD
ATOM  12239  CA  HIS B 147       9.596  52.127  55.701  1.00  9.43      0.182 C
ATOM  12241  C   HIS B 147       9.655  51.380  54.370  1.00  9.20      0.241 C
ATOM  12242  O   HIS B 147       8.623  51.157  53.728  1.00  9.57     -0.271 OA
ATOM  12243  CB  HIS B 147       9.817  51.244  56.910  1.00  6.24      0.093 C
ATOM  12246  CG  HIS B 147       8.674  50.275  57.189  1.00  9.86      0.028 A
ATOM  12247  CD2 HIS B 147       8.386  49.063  56.722  1.00 10.26      0.114 A
ATOM  12249  ND1 HIS B 147       7.691  50.579  58.124  1.00  6.79     -0.354 N
ATOM  12250  HD1 HIS B 147       7.657  51.430  58.685  1.00  0.00      0.166 HD
ATOM  12251  CE1 HIS B 147       6.797  49.585  58.175  1.00 12.74      0.180 A
ATOM  12253  NE2 HIS B 147       7.217  48.652  57.323  1.00  8.84     -0.360 N
ATOM  12254  HE2 HIS B 147       6.744  47.766  57.143  1.00  0.00      0.166 HD
ATOM  12255  N   TYR B 148      10.860  51.047  53.944  1.00  8.31     -0.346 N
ATOM  12256  HN  TYR B 148      11.655  51.288  54.536  1.00  0.00      0.163 HD
ATOM  12257  CA  TYR B 148      11.131  50.367  52.703  1.00  7.16      0.180 C
ATOM  12259  C   TYR B 148      11.268  48.866  52.944  1.00 10.13      0.241 C
ATOM  12260  O   TYR B 148      11.535  48.404  54.063  1.00 13.40     -0.271 OA
ATOM  12261  CB  TYR B 148      12.514  50.837  52.108  1.00  5.63      0.073 C
ATOM  12264  CG  TYR B 148      12.315  52.176  51.417  1.00 14.30     -0.056 A
ATOM  12265  CD1 TYR B 148      12.278  53.368  52.138  1.00 23.35      0.010 A
ATOM  12267  CD2 TYR B 148      12.208  52.225  50.035  1.00 17.30      0.010 A
ATOM  12269  CE1 TYR B 148      12.071  54.585  51.484  1.00 25.91      0.037 A
ATOM  12271  CE2 TYR B 148      11.996  53.422  49.383  1.00 18.99      0.037 A
ATOM  12273  CZ  TYR B 148      11.923  54.587  50.122  1.00 27.19      0.065 A
ATOM  12274  OH  TYR B 148      11.728  55.766  49.425  1.00 35.64     -0.361 OA
ATOM  12275  HH  TYR B 148      11.678  56.567  49.933  1.00  0.00      0.217 HD
ATOM  12276  N   THR B 149      11.176  48.135  51.834  1.00  8.54     -0.344 N
ATOM  12277  HN  THR B 149      10.973  48.595  50.947  1.00  0.00      0.163 HD
ATOM  12278  CA  THR B 149      11.359  46.696  51.865  1.00  7.10      0.205 C
ATOM  12280  C   THR B 149      12.457  46.381  50.846  1.00  6.63      0.243 C
ATOM  12281  O   THR B 149      12.323  46.741  49.652  1.00 10.43     -0.271 OA
ATOM  12282  CB  THR B 149      10.090  45.914  51.447  1.00  8.88      0.146 C
ATOM  12284  CG2 THR B 149      10.361  44.403  51.613  1.00 12.18      0.042 C
ATOM  12288  OG1 THR B 149       9.008  46.271  52.314  1.00 10.54     -0.393 OA
ATOM  12289  HG1 THR B 149       8.229  45.791  52.057  1.00  0.00      0.210 HD
ATOM  12290  N   TYR B 150      13.598  45.860  51.308  1.00  6.73     -0.346 N
ATOM  12291  HN  TYR B 150      13.708  45.663  52.303  1.00  0.00      0.163 HD
ATOM  12292  CA  TYR B 150      14.680  45.577  50.381  1.00  9.17      0.180 C
ATOM  12294  C   TYR B 150      14.885  44.089  50.212  1.00 10.55      0.241 C
ATOM  12295  O   TYR B 150      14.906  43.394  51.236  1.00 10.66     -0.271 OA
ATOM  12296  CB  TYR B 150      16.035  46.147  50.892  1.00 11.58      0.073 C
ATOM  12299  CG  TYR B 150      16.053  47.657  51.067  1.00 10.36     -0.056 A
ATOM  12300  CD1 TYR B 150      16.169  48.439  49.915  1.00 11.18      0.010 A
ATOM  12302  CD2 TYR B 150      15.962  48.291  52.311  1.00 11.60      0.010 A
ATOM  12304  CE1 TYR B 150      16.177  49.825  49.987  1.00 11.16      0.037 A
ATOM  12306  CE2 TYR B 150      16.011  49.681  52.397  1.00 10.89      0.037 A
ATOM  12308  CZ  TYR B 150      16.120  50.423  51.224  1.00  9.19      0.065 A
ATOM  12309  OH  TYR B 150      16.126  51.811  51.319  1.00 14.16     -0.361 OA
ATOM  12310  HH  TYR B 150      16.200  52.317  50.519  1.00  0.00      0.217 HD
ATOM  12311  N   ALA B 151      15.167  43.607  48.982  1.00 10.20     -0.346 N
ATOM  12312  HN  ALA B 151      15.225  44.220  48.169  1.00  0.00      0.163 HD
ATOM  12313  CA  ALA B 151      15.387  42.158  48.871  1.00 12.06      0.172 C
ATOM  12315  C   ALA B 151      16.583  41.859  47.986  1.00 11.52      0.240 C
ATOM  12316  O   ALA B 151      16.847  42.636  47.068  1.00 10.99     -0.271 OA
ATOM  12317  CB  ALA B 151      14.174  41.459  48.250  1.00 10.22      0.042 C
ATOM  12321  N   PHE B 152      17.359  40.841  48.331  1.00  9.83     -0.346 N
ATOM  12322  HN  PHE B 152      17.172  40.371  49.217  1.00  0.00      0.163 HD
ATOM  12323  CA  PHE B 152      18.464  40.357  47.514  1.00  9.60      0.180 C
ATOM  12325  C   PHE B 152      17.984  39.033  46.878  1.00 11.17      0.241 C
ATOM  12326  O   PHE B 152      17.322  38.250  47.568  1.00 10.45     -0.271 OA
ATOM  12327  CB  PHE B 152      19.721  39.993  48.332  1.00 11.52      0.073 C
ATOM  12330  CG  PHE B 152      20.582  41.190  48.735  1.00 13.20     -0.056 A
ATOM  12331  CD1 PHE B 152      20.158  42.479  48.566  1.00 10.40      0.007 A
ATOM  12333  CD2 PHE B 152      21.821  40.967  49.342  1.00 14.37      0.007 A
ATOM  12335  CE1 PHE B 152      20.920  43.582  48.935  1.00 14.99      0.001 A
ATOM  12337  CE2 PHE B 152      22.593  42.056  49.721  1.00 14.24      0.001 A
ATOM  12339  CZ  PHE B 152      22.159  43.361  49.490  1.00 14.09      0.000 A
ATOM  12341  N   MET B 153      18.253  38.852  45.594  1.00  8.85     -0.346 N
ATOM  12342  HN  MET B 153      18.771  39.554  45.066  1.00  0.00      0.163 HD
ATOM  12343  CA  MET B 153      17.788  37.615  44.946  1.00 11.25      0.177 C
ATOM  12345  C   MET B 153      18.802  37.228  43.868  1.00 12.18      0.240 C
ATOM  12346  O   MET B 153      19.614  38.055  43.461  1.00 11.68     -0.271 OA
ATOM  12347  CB  MET B 153      16.378  37.854  44.391  1.00 12.31      0.045 C
ATOM  12350  CG  MET B 153      16.216  38.914  43.338  1.00 20.10      0.076 C
ATOM  12353  SD  MET B 153      14.466  39.379  43.029  1.00 19.93     -0.173 SA
ATOM  12354  CE  MET B 153      13.780  37.795  42.567  1.00 17.64      0.089 C
ATOM  12358  N   GLY B 154      18.804  35.946  43.500  1.00  8.24     -0.351 N
ATOM  12359  HN  GLY B 154      18.106  35.309  43.885  1.00  0.00      0.163 HD
ATOM  12360  CA  GLY B 154      19.799  35.442  42.548  1.00  9.57      0.225 C
ATOM  12363  C   GLY B 154      19.143  34.831  41.308  1.00 12.22      0.236 C
ATOM  12364  O   GLY B 154      17.936  35.001  41.088  1.00 11.00     -0.272 OA
ATOM  12365  N   ASP B 155      19.926  34.108  40.493  1.00  8.07     -0.345 N
ATOM  12366  HN  ASP B 155      20.906  33.947  40.727  1.00  0.00      0.163 HD
ATOM  12367  CA  ASP B 155      19.353  33.549  39.254  1.00  8.53      0.186 C
ATOM  12369  C   ASP B 155      18.315  32.469  39.570  1.00  8.06      0.241 C
ATOM  12370  O   ASP B 155      17.378  32.267  38.784  1.00 10.90     -0.271 OA
ATOM  12371  CB  ASP B 155      20.462  32.871  38.456  1.00  9.15      0.147 C
ATOM  12374  CG  ASP B 155      21.494  33.861  37.938  1.00 16.35      0.175 C
ATOM  12375  OD1 ASP B 155      21.145  34.813  37.218  1.00 13.21     -0.648 OA
ATOM  12376  OD2 ASP B 155      22.659  33.670  38.301  1.00 14.29     -0.648 OA
ATOM  12377  N   GLY B 156      18.598  31.672  40.614  1.00  7.57     -0.351 N
ATOM  12378  HN  GLY B 156      19.466  31.789  41.136  1.00  0.00      0.163 HD
ATOM  12379  CA  GLY B 156      17.624  30.619  40.993  1.00  9.54      0.225 C
ATOM  12382  C   GLY B 156      16.251  31.193  41.291  1.00 11.78      0.236 C
ATOM  12383  O   GLY B 156      15.208  30.649  40.907  1.00  9.95     -0.272 OA
ATOM  12384  N   CYS B 157      16.143  32.293  42.031  1.00  6.44     -0.346 N
ATOM  12385  HN  CYS B 157      16.984  32.706  42.434  1.00  0.00      0.163 HD
ATOM  12386  CA  CYS B 157      14.845  32.928  42.283  1.00  6.22      0.186 C
ATOM  12388  C   CYS B 157      14.221  33.409  40.971  1.00  8.97      0.241 C
ATOM  12389  O   CYS B 157      13.006  33.348  40.852  1.00 10.54     -0.271 OA
ATOM  12390  CB  CYS B 157      15.253  34.173  43.099  1.00  4.31      0.121 C
ATOM  12393  SG  CYS B 157      15.659  33.678  44.864  1.00 14.75     -0.095 SA
ATOM  12394  HG  CYS B 157      15.021  33.978  40.038  1.00  6.62     -0.346 N
ATOM  12395  HN  MET B 158      16.024  34.050  40.207  1.00  0.00      0.163 HD
ATOM  12396  CA  MET B 158      14.454  34.492  38.787  1.00  8.25      0.177 C
ATOM  12398  C   MET B 158      13.920  33.344  37.911  1.00  7.86      0.241 C
ATOM  12399  O   MET B 158      12.961  33.602  37.158  1.00  9.24     -0.271 OA
ATOM  12400  CB  MET B 158      15.572  35.173  37.937  1.00  8.13      0.045 C
ATOM  12403  CG  MET B 158      16.020  36.483  38.603  1.00  8.69      0.076 C
ATOM  12406  SD  MET B 158      14.627  37.633  38.521  1.00 14.59     -0.173 SA
ATOM  12407  CE  MET B 158      15.493  39.193  38.938  1.00 19.05      0.089 C
ATOM  12411  N   MET B 159      14.525  32.178  37.951  1.00  8.79     -0.346 N
ATOM  12412  HN  MET B 159      15.357  32.067  38.530  1.00  0.00      0.163 HD
ATOM  12413  CA  MET B 159      14.029  31.032  37.181  1.00  6.65      0.177 C
ATOM  12415  C   MET B 159      12.729  30.453  37.734  1.00  8.08      0.241 C
ATOM  12416  O   MET B 159      11.854  30.011  36.943  1.00  8.18     -0.271 OA
ATOM  12417  CB  MET B 159      15.072  29.872  37.122  1.00  8.07      0.045 C
ATOM  12420  CG  MET B 159      16.211  30.272  36.121  1.00 10.89      0.076 C
ATOM  12423  SD  MET B 159      17.386  28.883  35.927  1.00 11.99     -0.173 SA
ATOM  12424  CE  MET B 159      18.781  29.545  36.842  1.00 12.77      0.089 C
ATOM  12428  N   GLU B 160      12.560  30.418  39.057  1.00  4.94     -0.346 N
ATOM  12429  HN  GLU B 160      13.284  30.819  39.653  1.00  0.00      0.163 HD
ATOM  12430  CA  GLU B 160      11.383  29.831  39.686  1.00  6.22      0.177 C
ATOM  12432  C   GLU B 160      10.116  30.559  39.241  1.00  9.75      0.240 C
ATOM  12433  O   GLU B 160      10.034  31.803  39.196  1.00  7.09     -0.271 OA
ATOM  12434  CB  GLU B 160      11.453  29.911  41.251  1.00  6.10      0.045 C
ATOM  12437  CG  GLU B 160      12.429  28.861  41.829  1.00  8.53      0.116 C
ATOM  12440  CD  GLU B 160      11.898  27.434  41.776  1.00  8.05      0.172 C
ATOM  12441  OE1 GLU B 160      10.784  27.218  41.277  1.00 10.23     -0.648 OA
ATOM  12442  OE2 GLU B 160      12.593  26.472  42.228  1.00  8.22     -0.648 OA
ATOM  12443  N   GLY B 161       9.094  29.773  38.970  1.00  5.85     -0.351 N
ATOM  12444  HN  GLY B 161       9.194  28.761  39.044  1.00  0.00      0.163 HD
ATOM  12445  CA  GLY B 161       7.789  30.367  38.555  1.00 11.25      0.225 C
ATOM  12448  C   GLY B 161       7.195  31.326  39.564  1.00  6.72      0.236 C
ATOM  12449  O   GLY B 161       6.505  32.308  39.227  1.00  6.90     -0.272 OA
ATOM  12450  N   ILE B 162       7.447  31.130  40.885  1.00  6.71     -0.346 N
ATOM  12451  HN  ILE B 162       8.028  30.355  41.204  1.00  0.00      0.163 HD
ATOM  12452  CA  ILE B 162       6.849  32.078  41.835  1.00  6.95      0.180 C
ATOM  12454  C   ILE B 162       7.337  33.511  41.708  1.00  7.55      0.241 C
ATOM  12455  O   ILE B 162       6.556  34.468  41.982  1.00  6.50     -0.271 OA
ATOM  12456  CB  ILE B 162       7.061  31.545  43.287  1.00  4.95      0.013 C
ATOM  12458  CG1 ILE B 162       6.247  32.401  44.293  1.00  8.32      0.002 C
ATOM  12461  CG2 ILE B 162       8.551  31.581  43.653  1.00  4.97      0.012 C
ATOM  12465  CD1 ILE B 162       6.409  31.668  45.682  1.00  5.26      0.005 C
ATOM  12469  N   SER B 163       8.550  33.713  41.174  1.00  5.21     -0.344 N
ATOM  12470  HN  SER B 163       9.151  32.923  40.940  1.00  0.00      0.163 HD
ATOM  12471  CA  SER B 163       9.004  35.106  40.929  1.00  6.26      0.200 C
ATOM  12473  C   SER B 163       8.096  35.768  39.897  1.00  9.06      0.243 C
ATOM  12474  O   SER B 163       7.793  36.950  40.042  1.00  6.73     -0.271 OA
ATOM  12475  CB  SER B 163      10.473  35.133  40.482  1.00 10.14      0.199 C
ATOM  12478  OG  SER B 163      10.601  34.609  39.172  1.00  8.12     -0.398 OA
ATOM  12479  HG  SER B 163      11.510  34.626  38.895  1.00  0.00      0.209 HD
ATOM  12480  N   HIS B 164       7.647  35.025  38.882  1.00  6.49     -0.346 N
ATOM  12481  HN  HIS B 164       7.958  34.060  38.770  1.00  0.00      0.163 HD
ATOM  12482  CA  HIS B 164       6.688  35.626  37.919  1.00  7.46      0.182 C
ATOM  12484  C   HIS B 164       5.374  35.951  38.609  1.00 11.65      0.241 C
ATOM  12485  O   HIS B 164       4.842  37.059  38.397  1.00  9.86     -0.271 OA
ATOM  12486  CB  HIS B 164       6.421  34.624  36.776  1.00  7.05      0.093 C
ATOM  12489  CG  HIS B 164       5.223  34.970  35.945  1.00  7.84      0.028 A
ATOM  12490  CD2 HIS B 164       4.036  34.364  35.767  1.00  8.56      0.114 A
ATOM  12492  ND1 HIS B 164       5.207  36.084  35.117  1.00  9.14     -0.354 N
ATOM  12493  HD1 HIS B 164       5.984  36.734  34.998  1.00  0.00      0.166 HD
ATOM  12494  CE1 HIS B 164       4.053  36.180  34.513  1.00  9.30      0.180 A
ATOM  12496  NE2 HIS B 164       3.306  35.106  34.873  1.00  8.26     -0.360 N
ATOM  12497  HE2 HIS B 164       2.367  34.889  34.538  1.00  0.00      0.166 HD
ATOM  12498  N   GLU B 165       4.849  35.066  39.461  1.00  5.93     -0.346 N
ATOM  12499  HN  GLU B 165       5.323  34.183  39.648  1.00  0.00      0.163 HD
ATOM  12500  CA  GLU B 165       3.578  35.385  40.124  1.00  5.02      0.177 C
ATOM  12502  C   GLU B 165       3.697  36.670  40.944  1.00  7.62      0.241 C
ATOM  12503  O   GLU B 165       2.806  37.540  40.868  1.00  8.30     -0.271 OA
ATOM  12504  CB  GLU B 165       3.153  34.223  41.073  1.00  5.45      0.045 C
ATOM  12507  CG  GLU B 165       2.875  32.984  40.188  1.00  7.52      0.116 C
ATOM  12510  CD  GLU B 165       2.279  31.810  40.956  1.00 14.94      0.172 C
ATOM  12511  OE1 GLU B 165       1.905  31.934  42.139  1.00 12.47     -0.648 OA
ATOM  12512  OE2 GLU B 165       2.136  30.715  40.346  1.00 10.49     -0.648 OA
ATOM  12513  N   VAL B 166       4.655  36.726  41.859  1.00  5.87     -0.346 N
ATOM  12514  HN  VAL B 166       5.363  35.993  41.901  1.00  0.00      0.163 HD
ATOM  12515  CA  VAL B 166       4.698  37.853  42.822  1.00  5.97      0.180 C
ATOM  12517  C   VAL B 166       5.198  39.141  42.176  1.00  8.07      0.241 C
ATOM  12518  O   VAL B 166       4.708  40.192  42.603  1.00  6.89     -0.271 OA
ATOM  12519  CB  VAL B 166       5.448  37.484  44.115  1.00  7.01      0.009 C
ATOM  12521  CG1 VAL B 166       4.777  36.218  44.668  1.00  6.98      0.012 C
ATOM  12525  CG2 VAL B 166       6.931  37.248  43.926  1.00  7.11      0.012 C
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ATOM  12529  N   CYS B 167       6.133  39.067  41.218  1.00  5.41    -0.345 N
ATOM  12530  HN  CYS B 167       6.483  38.173  40.874  1.00  0.00     0.163 HD
ATOM  12531  CA  CYS B 167       6.640  40.386  40.676  1.00  6.65     0.186 C
ATOM  12533  C   CYS B 167       5.643  40.992  39.705  1.00 11.75     0.242 C
ATOM  12534  O   CYS B 167       5.456  42.213  39.598  1.00  7.14    -0.271 OA
ATOM  12535  CB  CYS B 167       8.012  40.134  40.035  1.00  8.00     0.121 C
ATOM  12538  SG  CYS B 167       9.262  39.697  41.320  1.00 10.32    -0.095 SA
ATOM  12539  N   SER B 168       4.864  40.093  39.037  1.00  4.93    -0.344 N
ATOM  12540  HN  SER B 168       5.017  39.090  39.138  1.00  0.00     0.163 HD
ATOM  12541  CA  SER B 168       3.798  40.612  38.168  1.00  7.79     0.200 C
ATOM  12543  C   SER B 168       2.794  41.359  39.035  1.00  7.78     0.243 C
ATOM  12544  O   SER B 168       2.387  42.511  38.738  1.00  8.86    -0.271 OA
ATOM  12545  CB  SER B 168       3.125  39.415  37.464  1.00 12.42     0.199 C
ATOM  12548  OG  SER B 168       1.873  39.850  36.897  1.00 12.92    -0.398 OA
ATOM  12549  HG  SER B 168       1.459  39.113  36.464  1.00  0.00     0.209 HD
ATOM  12550  N   LEU B 169       2.304  40.763  40.141  1.00  6.51    -0.346 N
ATOM  12551  HN  LEU B 169       2.627  39.828  40.389  1.00  0.00     0.163 HD
ATOM  12552  CA  LEU B 169       1.323  41.426  40.989  1.00  6.95     0.177 C
ATOM  12554  C   LEU B 169       1.869  42.671  41.675  1.00  6.73     0.241 C
ATOM  12555  O   LEU B 169       1.180  43.689  41.836  1.00 10.68    -0.271 OA
ATOM  12556  CB  LEU B 169       0.825  40.465  42.103  1.00  7.79     0.038 C
ATOM  12559  CG  LEU B 169      -0.327  40.909  43.013  1.00 11.39    -0.020 C
ATOM  12561  CD1 LEU B 169      -1.561  41.313  42.222  1.00 13.25     0.009 C
ATOM  12565  CD2 LEU B 169      -0.707  39.725  43.940  1.00 15.85     0.009 C
ATOM  12569  N   ALA B 170       3.152  42.664  42.051  1.00 10.03    -0.346 N
ATOM  12570  HN  ALA B 170       3.708  41.822  41.902  1.00  0.00     0.163 HD
ATOM  12571  CA  ALA B 170       3.784  43.838  42.674  1.00  9.42     0.172 C
ATOM  12573  C   ALA B 170       3.755  45.027  41.709  1.00 10.20     0.240 C
ATOM  12574  O   ALA B 170       3.666  46.166  42.138  1.00 10.10    -0.271 OA
ATOM  12575  CB  ALA B 170       5.255  43.503  43.051  1.00  9.38     0.042 C
ATOM  12579  N   GLY B 171       3.907  44.820  40.411  1.00 16.65    -0.351 N
ATOM  12580  HN  GLY B 171       4.080  43.865  40.096  1.00  0.00     0.163 HD
ATOM  12581  CA  GLY B 171       3.842  45.882  39.392  1.00 11.58     0.225 C
ATOM  12584  C   GLY B 171       2.439  46.449  39.279  1.00 13.34     0.236 C
ATOM  12585  O   GLY B 171       2.218  47.675  39.263  1.00 12.66    -0.272 OA
ATOM  12586  N   THR B 172       1.441  45.551  39.328  1.00  7.06    -0.344 N
ATOM  12587  HN  THR B 172       1.660  44.555  39.353  1.00  0.00     0.163 HD
ATOM  12588  CA  THR B 172       0.048  45.984  39.346  1.00  8.88     0.205 C
ATOM  12590  C   THR B 172      -0.251  46.852  40.559  1.00 16.14     0.243 C
ATOM  12591  O   THR B 172      -0.978  47.850  40.431  1.00 10.00    -0.271 OA
ATOM  12592  CB  THR B 172      -0.919  44.778  39.387  1.00 15.42     0.146 C
ATOM  12594  CG2 THR B 172      -2.360  45.223  39.507  1.00 14.19     0.042 C
ATOM  12598  OG1 THR B 172      -0.720  44.026  38.144  1.00 14.00    -0.393 OA
ATOM  12599  HG1 THR B 172       0.185  43.747  38.071  1.00  0.00     0.210 HD
ATOM  12600  N   LEU B 173       0.260  46.460  41.744  1.00  6.61    -0.346 N
ATOM  12601  HN  LEU B 173       0.879  45.651  41.799  1.00  0.00     0.163 HD
ATOM  12602  CA  LEU B 173      -0.089  47.218  42.955  1.00 10.17     0.177 C
ATOM  12604  C   LEU B 173       0.850  48.381  43.240  1.00 12.92     0.241 C
ATOM  12605  O   LEU B 173       0.720  49.036  44.281  1.00 11.58    -0.271 OA
ATOM  12606  CB  LEU B 173      -0.036  46.246  44.177  1.00 10.27     0.038 C
ATOM  12609  CG  LEU B 173      -1.138  45.160  44.157  1.00 14.89    -0.020 C
ATOM  12611  CD1 LEU B 173      -0.897  44.155  45.293  1.00 16.31     0.009 C
ATOM  12615  CD2 LEU B 173      -2.520  45.736  44.352  1.00 11.69     0.009 C
ATOM  12619  N   LYS B 174       1.725  48.743  42.320  1.00  7.91    -0.346 N
ATOM  12620  HN  LYS B 174       1.822  48.132  41.509  1.00  0.00     0.163 HD
ATOM  12621  CA  LYS B 174       2.558  49.923  42.354  1.00  7.85     0.176 C
ATOM  12623  C   LYS B 174       3.380  50.071  43.624  1.00 10.29     0.241 C
ATOM  12624  O   LYS B 174       3.295  51.105  44.307  1.00  9.42    -0.271 OA
ATOM  12625  CB  LYS B 174       1.600  51.119  42.184  1.00 14.53     0.035 C
ATOM  12628  CG  LYS B 174       0.905  50.994  40.801  1.00 16.37     0.004 C
ATOM  12631  CD  LYS B 174       0.147  52.307  40.612  1.00 29.05     0.027 C
ATOM  12634  CE  LYS B 174      -0.409  52.342  39.192  1.00 51.45     0.229 C
ATOM  12637  NZ  LYS B 174      -0.365  53.716  38.621  1.00 31.99    -0.079 N
ATOM  12638  HZ1 LYS B 174      -0.737  53.739  37.671  1.00  0.00     0.274 HD
ATOM  12639  HZ2 LYS B 174       0.576  54.107  38.663  1.00  0.00     0.274 HD
ATOM  12640  HZ3 LYS B 174      -0.842  54.386  39.225  1.00  0.00     0.274 HD
ATOM  12641  N   LEU B 175       4.093  49.013  44.028  1.00  8.27    -0.346 N
ATOM  12642  HN  LEU B 175       4.157  48.184  43.438  1.00  0.00     0.163 HD
ATOM  12643  CA  LEU B 175       4.790  49.050  45.338  1.00 12.54     0.177 C
ATOM  12645  C   LEU B 175       6.126  49.738  45.197  1.00  8.35     0.240 C
ATOM  12646  O   LEU B 175       7.190  49.145  45.104  1.00 10.10    -0.271 OA
ATOM  12647  CB  LEU B 175       4.991  47.581  45.780  1.00 10.90     0.038 C
ATOM  12650  CG  LEU B 175       3.650  46.842  45.925  1.00  8.87    -0.020 C
ATOM  12652  CD1 LEU B 175       3.919  45.367  46.266  1.00  9.21     0.009 C
ATOM  12656  CD2 LEU B 175       2.794  47.442  47.083  1.00 13.12     0.009 C
ATOM  12660  N   GLY B 176       6.095  51.063  45.192  1.00 10.17    -0.351 N
ATOM  12661  HN  GLY B 176       5.195  51.528  45.315  1.00  0.00     0.163 HD
ATOM  12662  CA  GLY B 176       7.282  51.887  45.020  1.00  9.29     0.225 C
ATOM  12665  C   GLY B 176       8.298  51.714  46.124  1.00 12.14     0.236 C
ATOM  12666  O   GLY B 176       9.462  52.080  45.925  1.00 12.16    -0.272 OA
ATOM  12667  N   LYS B 177       7.893  51.202  47.326  1.00  9.62    -0.346 N
ATOM  12668  HN  LYS B 177       6.927  50.924  47.500  1.00  0.00     0.163 HD
ATOM  12669  CA  LYS B 177       8.942  51.078  48.353  1.00  9.88     0.176 C
ATOM  12671  C   LYS B 177       9.594  49.690  48.347  1.00 10.15     0.241 C
ATOM  12672  O   LYS B 177      10.357  49.369  49.258  1.00 13.84    -0.271 OA
ATOM  12673  CB  LYS B 177       8.375  51.475  49.720  1.00 13.53     0.035 C
ATOM  12676  CG  LYS B 177       7.877  52.948  49.717  1.00 15.08     0.004 C
ATOM  12679  CD  LYS B 177       7.738  53.332  51.208  1.00 11.89     0.027 C
ATOM  12682  CE  LYS B 177       6.716  54.417  51.426  1.00 26.56     0.229 C
ATOM  12685  NZ  LYS B 177       6.558  54.677  52.888  1.00 17.88    -0.079 N
ATOM  12686  HZ1 LYS B 177       5.866  55.412  53.036  1.00  0.00     0.274 HD
ATOM  12687  HZ2 LYS B 177       7.448  54.892  53.338  1.00  0.00     0.274 HD
ATOM  12688  HZ3 LYS B 177       6.332  53.828  53.406  1.00  0.00     0.274 HD
ATOM  12689  N   LEU B 178       9.253  48.849  47.351  1.00  8.69    -0.346 N
ATOM  12690  HN  LEU B 178       8.520  49.105  46.690  1.00  0.00     0.163 HD
ATOM  12691  CA  LEU B 178       9.950  47.556  47.226  1.00 11.27     0.177 C
ATOM  12693  C   LEU B 178      11.138  47.719  46.288  1.00 11.03     0.241 C
ATOM  12694  O   LEU B 178      10.970  48.186  45.154  1.00  7.24    -0.271 OA
ATOM  12695  CB  LEU B 178       9.013  46.493  46.650  1.00  6.96     0.038 C
ATOM  12698  CG  LEU B 178       9.646  45.143  46.272  1.00 13.76    -0.020 C
ATOM  12700  CD1 LEU B 178      10.156  44.486  47.571  1.00 16.98     0.009 C
ATOM  12704  CD2 LEU B 178       8.575  44.248  45.616  1.00  9.44     0.009 C
ATOM  12708  N   ILE B 179      12.348  47.471  46.763  1.00  5.51    -0.346 N
ATOM  12709  HN  ILE B 179      12.444  47.139  47.723  1.00  0.00     0.163 HD
ATOM  12710  CA  ILE B 179      13.557  47.659  45.951  1.00  9.22     0.180 C
ATOM  12712  C   ILE B 179      14.339  46.355  45.998  1.00 12.27     0.241 C
ATOM  12713  O   ILE B 179      14.732  45.930  47.074  1.00 12.01    -0.271 OA
ATOM  12714  CB  ILE B 179      14.417  48.821  46.517  1.00 10.45     0.013 C
ATOM  12716  CG1 ILE B 179      13.635  50.141  46.224  1.00 12.02     0.002 C
ATOM  12719  CG2 ILE B 179      15.759  48.906  45.799  1.00  8.23     0.012 C
ATOM  12723  CD1 ILE B 179      14.304  51.395  46.706  1.00 16.42     0.005 C
ATOM  12727  N   ALA B 180      14.518  45.709  44.854  1.00  9.82    -0.346 N
ATOM  12728  HN  ALA B 180      14.202  46.126  43.979  1.00  0.00     0.163 HD
ATOM  12729  CA  ALA B 180      15.170  44.396  44.846  1.00 11.22     0.172 C
ATOM  12731  C   ALA B 180      16.505  44.459  44.105  1.00 12.46     0.240 C
ATOM  12732  O   ALA B 180      16.569  45.153  43.103  1.00 13.36    -0.271 OA
ATOM  12733  CB  ALA B 180      14.293  43.381  44.107  1.00 12.33     0.042 C
ATOM  12737  N   PHE B 181      17.491  43.782  44.646  1.00  9.98    -0.346 N
ATOM  12738  HN  PHE B 181      17.330  43.254  45.504  1.00  0.00     0.163 HD
ATOM  12739  CA  PHE B 181      18.827  43.777  44.026  1.00 11.10     0.180 C
ATOM  12741  C   PHE B 181      19.057  42.375  43.475  1.00 12.05     0.241 C
ATOM  12742  O   PHE B 181      18.913  41.414  44.221  1.00 10.28    -0.271 OA
ATOM  12743  CB  PHE B 181      19.901  44.026  45.087  1.00 11.39     0.073 C
ATOM  12746  CG  PHE B 181      19.829  45.334  45.818  1.00 13.26    -0.056 A
ATOM  12747  CD1 PHE B 181      18.855  45.649  46.724  1.00 12.08     0.007 A
ATOM  12749  CD2 PHE B 181      20.814  46.280  45.514  1.00 11.09     0.007 A
ATOM  12751  CE1 PHE B 181      18.840  46.886  47.373  1.00 16.15     0.001 A
ATOM  12753  CE2 PHE B 181      20.833  47.500  46.168  1.00 10.75     0.001 A
ATOM  12755  CZ  PHE B 181      19.849  47.765  47.110  1.00 16.43     0.000 A
ATOM  12757  N   TYR B 182      19.350  42.292  42.189  1.00  8.00    -0.346 N
ATOM  12758  HN  TYR B 182      19.430  43.147  41.638  1.00  0.00     0.163 HD
ATOM  12759  CA  TYR B 182      19.562  40.996  41.540  1.00 10.19     0.180 C
ATOM  12761  C   TYR B 182      21.050  40.735  41.383  1.00 12.08     0.241 C
ATOM  12762  O   TYR B 182      21.795  41.537  40.806  1.00 15.15    -0.271 OA
ATOM  12763  CB  TYR B 182      18.893  41.010  40.153  1.00  9.19     0.073 C
ATOM  12766  CG  TYR B 182      19.177  39.847  39.215  1.00  9.49    -0.056 A
ATOM  12767  CD1 TYR B 182      18.529  39.561  38.023  1.00 11.53     0.010 A
ATOM  12769  CD2 TYR B 182      19.342  40.117  37.854  1.00 16.21     0.010 A
ATOM  12771  CE1 TYR B 182      19.541  37.481  38.761  1.00  9.21     0.037 A
ATOM  12773  CE2 TYR B 182      19.570  39.082  36.949  1.00 12.13     0.037 A
ATOM  12775  CZ  TYR B 182      19.660  37.783  37.411  1.00 12.65     0.065 A
ATOM  12776  OH  TYR B 182      19.922  36.781  36.476  1.00 15.28    -0.361 OA
ATOM  12777  HH  TYR B 182      19.984  35.888  36.794  1.00  0.00     0.217 HD
ATOM  12778  N   ASP B 183      21.516  39.617  41.914  1.00  9.46    -0.345 N
ATOM  12779  HN  ASP B 183      20.850  39.012  42.394  1.00  0.00     0.163 HD
ATOM  12780  CA  ASP B 183      22.907  39.180  41.868  1.00 10.95     0.186 C
ATOM  12782  C   ASP B 183      23.176  38.519  40.527  1.00 12.58     0.241 C
ATOM  12783  O   ASP B 183      22.961  37.309  40.352  1.00 13.24    -0.271 OA
ATOM  12784  CB  ASP B 183      23.157  38.207  43.031  1.00 11.49     0.147 C
ATOM  12787  CG  ASP B 183      24.633  37.870  43.213  1.00 20.12     0.175 C
ATOM  12788  OD1 ASP B 183      25.485  38.606  42.732  1.00 21.66    -0.648 OA
ATOM  12789  OD2 ASP B 183      24.961  36.847  43.844  1.00 19.64    -0.648 OA
ATOM  12790  N   ASP B 184      23.491  39.345  39.539  1.00  9.51    -0.345 N
ATOM  12791  HN  ASP B 184      23.640  40.336  39.729  1.00  0.00     0.163 HD
ATOM  12792  CA  ASP B 184      23.628  38.821  38.146  1.00 14.92     0.186 C
ATOM  12794  C   ASP B 184      25.043  38.337  37.889  1.00 16.67     0.241 C
ATOM  12795  O   ASP B 184      25.907  39.072  37.405  1.00 13.71    -0.271 OA
ATOM  12796  CB  ASP B 184      23.237  39.992  37.246  1.00 10.72     0.147 C
ATOM  12799  CG  ASP B 184      23.188  39.625  35.759  1.00 20.71     0.175 C
ATOM  12800  OD1 ASP B 184      23.462  38.484  35.397  1.00 17.12    -0.648 OA
ATOM  12801  OD2 ASP B 184      22.822  40.516  34.985  1.00 20.55    -0.648 OA
ATOM  12802  N   ASN B 185      25.325  37.106  38.354  1.00 11.93    -0.346 N
ATOM  12803  HN  ASN B 185      24.584  36.531  38.754  1.00  0.00     0.163 HD
ATOM  12804  CA  ASN B 185      26.683  36.594  38.287  1.00 13.79     0.185 C
ATOM  12806  C   ASN B 185      26.881  35.471  37.281  1.00 16.31     0.241 C
ATOM  12807  O   ASN B 185      27.995  34.965  37.131  1.00 16.57    -0.271 OA
ATOM  12808  CB  ASN B 185      27.121  36.144  39.684  1.00  9.33     0.137 C
ATOM  12811  CG  ASN B 185      26.314  34.994  40.270  1.00 16.54     0.217 C
ATOM  12812  ND2 ASN B 185      26.404  34.823  41.588  1.00 13.83    -0.370 N
ATOM  12813 1HD2 ASN B 185      26.958  35.458  42.163  1.00  0.00     0.159 HD
ATOM  12814 2HD2 ASN B 185      25.863  34.052  41.981  1.00  0.00     0.159 HD
ATOM  12815  OD1 ASN B 185      25.651  34.233  39.582  1.00 12.90    -0.274 OA
ATOM  12816  N   GLY B 186      25.893  35.143  36.459  1.00 14.72    -0.351 N
ATOM  12817  HN  GLY B 186      24.988  35.591  36.599  1.00  0.00     0.163 HD
ATOM  12818  CA  GLY B 186      26.017  34.179  35.363  1.00 16.74     0.225 C
ATOM  12821  C   GLY B 186      26.249  32.726  35.694  1.00 15.18     0.236 C
ATOM  12822  O   GLY B 186      26.589  31.896  34.818  1.00 12.67    -0.272 OA
ATOM  12823  N   ILE B 187      26.181  32.350  36.979  1.00 13.57    -0.346 N
ATOM  12824  HN  ILE B 187      25.880  33.029  37.678  1.00  0.00     0.163 HD
ATOM  12825  CA  ILE B 187      26.527  30.990  37.410  1.00 15.07     0.180 C
ATOM  12827  C   ILE B 187      25.395  30.368  38.219  1.00 17.42     0.241 C
ATOM  12828  O   ILE B 187      24.757  31.106  38.995  1.00 15.18    -0.271 OA
ATOM  12829  CB  ILE B 187      27.758  31.138  38.353  1.00 18.25     0.013 C
ATOM  12831  CG1 ILE B 187      29.027  31.488  37.544  1.00 18.52     0.002 C
ATOM  12834  CG2 ILE B 187      27.955  29.923  39.242  1.00 20.90     0.012 C
ATOM  12838  CD1 ILE B 187      29.335  30.475  36.463  1.00 25.30     0.005 C
ATOM  12842  N   SER B 188      25.139  29.076  38.037  1.00 14.91    -0.344 N
ATOM  12843  HN  SER B 188      25.602  28.551  37.295  1.00  0.00     0.163 HD
ATOM  12844  CA  SER B 188      24.162  28.416  38.941  1.00 15.13     0.200 C
ATOM  12846  C   SER B 188      24.840  27.106  39.325  1.00 14.63     0.243 C
ATOM  12847  O   SER B 188      26.019  26.906  38.953  1.00 16.33    -0.271 OA
ATOM  12848  CB  SER B 188      22.761  28.253  38.395  1.00 15.51     0.199 C
ATOM  12851  OG  SER B 188      22.683  27.381  37.267  1.00 16.10    -0.398 OA
ATOM  12852  HG  SER B 188      21.803  27.279  36.924  1.00  0.00     0.209 HD
ATOM  12853  N   ILE B 189      24.147  26.157  39.955  1.00 13.80    -0.346 N
ATOM  12854  HN  ILE B 189      23.151  26.263  40.150  1.00  0.00     0.163 HD
ATOM  12855  CA  ILE B 189      24.888  24.948  40.356  1.00 12.66     0.180 C
ATOM  12857  C   ILE B 189      25.391  24.116  39.186  1.00 15.83     0.241 C
ATOM  12858  O   ILE B 189      26.518  23.589  39.211  1.00 16.53    -0.271 OA
ATOM  12859  CB  ILE B 189      23.954  24.105  41.266  1.00 11.03     0.013 C
ATOM  12861  CG1 ILE B 189      23.896  24.782  42.661  1.00 13.29     0.002 C
ATOM  12864  CG2 ILE B 189      24.478  22.677  41.377  1.00 13.49     0.012 C
ATOM  12868  CD1 ILE B 189      22.943  24.062  43.624  1.00 18.78     0.005 C
ATOM  12872  N   ASP B 190      24.609  23.941  38.127  1.00 14.32    -0.345 N
ATOM  12873  HN  ASP B 190      23.680  24.361  38.102  1.00  0.00     0.163 HD
ATOM  12874  CA  ASP B 190      25.093  23.132  36.980  1.00 15.25     0.186 C
ATOM  12876  C   ASP B 190      26.223  23.810  36.213  1.00 20.19     0.241 C
ATOM  12877  O   ASP B 190      26.856  23.156  35.344  1.00 18.60    -0.271 OA
ATOM  12878  CB  ASP B 190      23.922  22.883  36.020  1.00 13.98     0.147 C
ATOM  12881  CG  ASP B 190      23.044  21.707  36.368  1.00 21.12     0.175 C
ATOM  12882  OD1 ASP B 190      23.252  21.137  37.456  1.00 16.06    -0.648 OA
ATOM  12883  OD2 ASP B 190      22.121  21.354  35.590  1.00 16.54    -0.648 OA
ATOM  12884  N   GLY B 191      26.489  25.095  36.411  1.00 15.32    -0.351 N
ATOM  12885  HN  GLY B 191      25.958  25.634  37.095  1.00  0.00     0.163 HD
ATOM  12886  CA  GLY B 191      27.572  25.736  35.622  1.00 14.27     0.225 C
ATOM  12889  C   GLY B 191      27.113  27.104  35.094  1.00 16.16     0.236 C
ATOM  12890  O   GLY B 191      26.362  27.852  35.735  1.00 15.68    -0.272 OA
ATOM  12891  N   HIS B 192      27.628  27.508  33.937  1.00 12.79    -0.346 N
ATOM  12892  HN  HIS B 192      28.311  26.904  33.479  1.00  0.00     0.163 HD
ATOM  12893  CA  HIS B 192      27.277  28.756  33.287  1.00 16.90     0.182 C
ATOM  12895  C   HIS B 192      25.814  28.736  32.865  1.00 17.61     0.241 C
ATOM  12896  O   HIS B 192      25.380  27.869  32.092  1.00 17.00    -0.271 OA
ATOM  12897  CB  HIS B 192      28.142  28.954  32.025  1.00 24.02     0.093 C
ATOM  12900  CG  HIS B 192      29.501  29.390  32.530  1.00 35.89     0.028 A
ATOM  12901  CD2 HIS B 192      30.625  28.691  32.784  1.00 39.56     0.114 A
ATOM  12903  ND1 HIS B 192      29.749  30.708  32.864  1.00 42.40    -0.354 N
ATOM  12904  HD1 HIS B 192      29.085  31.479  32.792  1.00  0.00     0.166 HD
ATOM  12905  CE1 HIS B 192      30.998  30.795  33.294  1.00 47.54     0.180 A
ATOM  12907  NE2 HIS B 192      31.550  29.596  33.250  1.00 43.93    -0.360 N
ATOM  12908  HE2 HIS B 192      32.509  29.376  33.519  1.00  0.00     0.166 HD
ATOM  12909  N   VAL B 193      25.057  29.724  33.329  1.00 12.50    -0.346 N
ATOM  12910  HN  VAL B 193      25.481  30.510  33.821  1.00  0.00     0.163 HD
ATOM  12911  CA  VAL B 193      23.613  29.673  33.128  1.00 17.17     0.180 C
ATOM  12913  C   VAL B 193      23.099  29.791  31.712  1.00 18.79     0.241 C
ATOM  12914  O   VAL B 193      21.937  29.434  31.516  1.00 16.04    -0.271 OA
ATOM  12915  CB  VAL B 193      22.842  30.735  33.943  1.00 19.28     0.009 C
ATOM  12917  CG1 VAL B 193      23.162  30.549  35.419  1.00 18.22     0.012 C
ATOM  12921  CG2 VAL B 193      23.133  32.123  33.444  1.00 17.48     0.012 C
ATOM  12925  N   GLU B 194      23.906  30.235  30.755  1.00 17.94    -0.346 N
ATOM  12926  HN  GLU B 194      24.887  30.442  30.945  1.00  0.00     0.163 HD
ATOM  12927  CA  GLU B 194      23.334  30.418  29.408  1.00 20.31     0.177 C
ATOM  12929  C   GLU B 194      22.902  29.112  28.795  1.00 20.32     0.240 C
ATOM  12930  O   GLU B 194      22.153  29.152  27.826  1.00 16.05    -0.271 OA
ATOM  12931  CB  GLU B 194      24.275  31.219  28.484  1.00 23.77     0.045 C
ATOM  12934  CG  GLU B 194      25.738  30.803  28.672  1.00 43.30     0.116 C
ATOM  12937  CD  GLU B 194      26.399  31.690  29.719  1.00 54.33     0.172 C
ATOM  12938  OE1 GLU B 194      26.807  32.823  29.368  1.00 72.10    -0.648 OA
ATOM  12939  OE2 GLU B 194      26.507  31.323  30.904  1.00 48.61    -0.648 OA
ATOM  12940  N   GLY B 195      23.234  27.916  29.284  1.00 15.62    -0.351 N
ATOM  12941  HN  GLY B 195      23.870  27.844  30.078  1.00  0.00     0.163 HD
ATOM  12942  CA  GLY B 195      22.683  26.720  28.677  1.00 16.41     0.225 C
ATOM  12945  C   GLY B 195      21.224  26.463  29.083  1.00 15.64     0.236 C
ATOM  12946  O   GLY B 195      20.618  25.556  28.514  1.00 16.61    -0.272 OA
ATOM  12947  N   TRP B 196      20.725  27.135  30.128  1.00 12.63    -0.346 N
ATOM  12948  HN  TRP B 196      21.305  27.806  30.631  1.00  0.00     0.163 HD
ATOM  12949  CA  TRP B 196      19.355  26.903  30.540  1.00 14.62     0.181 C
ATOM  12951  C   TRP B 196      18.626  28.190  30.932  1.00 11.36     0.241 C
ATOM  12952  O   TRP B 196      17.469  28.106  31.363  1.00 11.44    -0.271 OA
ATOM  12953  CB  TRP B 196      19.360  25.932  31.753  1.00 14.02     0.075 C
ATOM  12956  CG  TRP B 196      20.405  26.187  32.797  1.00 12.00    -0.028 A
ATOM  12957  CD1 TRP B 196      20.268  26.940  33.942  1.00 12.09     0.096 A
ATOM  12959  CD2 TRP B 196      21.754  25.691  32.812  1.00 16.38    -0.002 A
ATOM  12960  CE2 TRP B 196      22.374  26.178  33.970  1.00 10.80     0.042 A
ATOM  12961  CD3 TRP B 196      22.484  24.882  31.930  1.00 14.39     0.014 A
ATOM  12963  NE1 TRP B 196      21.456  26.972  34.641  1.00 11.37    -0.365 N
ATOM  12964  HE1 TRP B 196      21.630  27.490  35.502  1.00  0.00     0.165 HD
ATOM  12965  CZ2 TRP B 196      23.705  25.896  34.275  1.00 16.03     0.030 A
ATOM  12967  CZ3 TRP B 196      23.809  24.580  32.232  1.00 17.85     0.001 A
ATOM  12969  CH2 TRP B 196      24.402  25.113  33.390  1.00 13.29     0.002 A
ATOM  12971  N   PHE B 197      19.263  29.368  30.847  1.00 11.51    -0.346 N
ATOM  12972  HN  PHE B 197      20.206  29.433  30.464  1.00  0.00     0.163 HD
ATOM  12973  CA  PHE B 197      18.546  30.569  31.329  1.00 10.07     0.180 C
ATOM  12975  C   PHE B 197      19.010  31.740  30.480  1.00 10.91     0.241 C
ATOM  12976  O   PHE B 197      20.152  32.200  30.714  1.00 12.65    -0.271 OA
ATOM  12977  CB  PHE B 197      18.881  30.787  32.822  1.00  7.22     0.073 C
ATOM  12980  CG  PHE B 197      18.212  32.018  33.414  1.00 10.90    -0.056 A
ATOM  12981  CD1 PHE B 197      16.893  32.324  33.152  1.00 15.28     0.007 A
ATOM  12983  CD2 PHE B 197      18.936  32.845  34.255  1.00 18.42     0.007 A
ATOM  12985  CE1 PHE B 197      16.336  33.442  33.756  1.00 19.78     0.001 A
ATOM  12987  CE2 PHE B 197      18.371  33.963  34.858  1.00 11.34     0.001 A
ATOM  12989  CZ  PHE B 197      17.046  34.264  34.575  1.00 17.07     0.000 A
ATOM  12991  N   THR B 198      18.168  32.130  29.528  1.00 10.81    -0.344 N
ATOM  12992  HN  THR B 198      17.236  31.721  29.460  1.00  0.00     0.163 HD
ATOM  12993  CA  THR B 198      18.604  33.162  28.573  1.00 11.25     0.205 C
ATOM  12995  C   THR B 198      17.613  34.307  28.524  1.00 12.04     0.243 C
ATOM  12996  O   THR B 198      17.706  35.113  27.580  1.00 12.87    -0.271 OA
ATOM  12997  CB  THR B 198      18.678  32.555  27.137  1.00 14.62     0.146 C
ATOM  12999  OG1 THR B 198      19.882  31.644  27.008  1.00 15.77    -0.393 OA
ATOM  13003  HG1 THR B 198      17.525  31.779  26.813  1.00 14.17     0.210 HD
ATOM  13004  N   ASP B 199      16.770  32.350  26.894  1.00  0.00    -0.345 N
ATOM  13005  HN  ASP B 199      16.749  34.479  29.506  1.00  8.43     0.163 HD
ATOM  13006  CA  ASP B 199      16.757  33.851  30.309  1.00  0.00     0.186 C
ATOM  13008  C   ASP B 199      15.792  35.558  29.442  1.00  6.60     0.241 C
ATOM  13009  O   ASP B 199      16.501  36.915  29.339  1.00  8.91    -0.271 OA
ATOM  13010  CB  ASP B 199      17.553  37.109  29.975  1.00 10.65     0.147 C
ATOM  13011  CG  ASP B 199      15.060  35.659  30.802  1.00 10.46     0.175 C
ATOM  13012  OD1 ASP B 199      14.100  34.517  31.100  1.00 12.67    -0.648 OA
ATOM  13015  OD2 ASP B 199      14.084  33.528  30.347  1.00 13.74    -0.648 OA
ATOM  13017  N   ASP B 200      13.381  34.664  32.096  1.00 12.26    -0.345 N
ATOM  13018  HN  ASP B 200      15.816  37.853  28.691  1.00  8.82     0.163 HD
ATOM  13019  CA  ASP B 200      15.005  37.616  28.119  1.00  6.00     0.186 C
ATOM  13021  C   ASP B 200      16.272  39.251  28.830  1.00 13.04     0.241 C
ATOM  13022  O   ASP B 200      15.546  39.683  30.109  1.00 12.08    -0.271 OA
ATOM  13023  CB  ASP B 200      14.424  40.150  30.027  1.00 10.48     0.147 C
ATOM  13026  CG  ASP B 200      15.802  40.075  27.621  1.00  9.69     0.175 C
ATOM  13027  OD1 ASP B 200      16.269  41.527  27.706  1.00 19.15    -0.648 OA
ATOM  13028  OD2 ASP B 200      16.423  42.117  28.792  1.00 12.23    -0.648 OA
ATOM  13029  N   THR B 201      16.420  42.133  26.643  1.00 21.51    -0.648 OA
ATOM  13030  HN  THR B 201      16.095  39.467  31.310  1.00  0.00     8.37     0.344 N
ATOM  13031  CA  THR B 201      17.027  39.054  31.358  1.00  0.00     0.163 HD
ATOM  13032  C   THR B 201      15.406  39.802  32.560  1.00 10.99     0.205 C
ATOM  13033  O   THR B 201      14.976  41.241  32.704  1.00  8.21     0.243 C
ATOM  13034  CB  THR B 201      13.868  41.550  33.186  1.00 10.06    -0.271 OA
ATOM  13035  CG2 THR B 201      16.360  39.377  33.720  1.00 11.61     0.146 C
ATOM  13037  OG1 THR B 201      15.804  39.716  35.091  1.00  8.78     0.042 C
ATOM  13041  N   ALA B 202      16.515  37.951  33.559  1.00 12.75    -0.393 OA
ATOM  13042  HG1 THR B 201      16.863  37.739  32.701  1.00  7.00     0.210 HD
ATOM  13043  CA  ALA B 202      15.786  42.207  32.236  1.00  8.55    -0.346 N
ATOM  13044  HN  ALA B 202      16.692  41.969  31.832  1.00  0.00     0.163 HD
ATOM  13045  CB  ALA B 202      15.356  43.603  32.312  1.00 10.66     0.172 C
ATOM  13047  C   ALA B 202      14.061  43.829  31.546  1.00 10.65     0.240 C
ATOM  13048  O   ALA B 202      13.158  44.517  31.995  1.00  9.78    -0.271 OA
ATOM  13049  CB  ALA B 202      16.510  44.451  31.743  1.00 10.77     0.042 C
ATOM  13053  N   MET B 203      13.962  43.316  30.307  1.00  8.01    -0.346 N
ATOM  13054  HN  MET B 203      14.748  42.793  29.922  1.00  0.00     0.163 HD
ATOM  13055  CA  MET B 203      12.761  43.488  29.500  1.00  7.55     0.177 C
ATOM  13057  C   MET B 203      11.584  42.780  30.148  1.00  9.81     0.241 C
ATOM  13058  O   MET B 203      10.464  43.294  30.163  1.00  9.76    -0.271 OA
ATOM  13059  CB  MET B 203      13.001  42.969  28.072  1.00 10.57     0.045 C
ATOM  13062  CG  MET B 203      11.813  43.077  27.128  1.00 21.09     0.076 C
ATOM  13065  SD  MET B 203      12.213  42.310  25.487  1.00 24.15    -0.173 SA
ATOM  13066  CE  MET B 203      13.553  43.381  25.016  1.00 18.51     0.089 C
ATOM  13070  N   ARG B 204      11.787  41.613  30.772  1.00 10.56    -0.346 N
ATOM  13071  HN  ARG B 204      12.718  41.197  30.762  1.00  0.00     0.163 HD
ATOM  13072  CA  ARG B 204      10.715  40.930  31.460  1.00  6.38     0.176 C
ATOM  13074  C   ARG B 204      10.153  41.784  32.606  1.00  5.47     0.241 C
ATOM  13075  O   ARG B 204       8.938  41.875  32.832  1.00  9.29    -0.271 OA
ATOM  13076  CB  ARG B 204      11.331  39.614  32.033  1.00  7.06     0.036 C
ATOM  13079  CG  ARG B 204      10.446  38.886  33.016  1.00 11.00     0.023 C
ATOM  13082  CD  ARG B 204      11.195  37.745  33.754  1.00  8.30     0.138 C
ATOM  13085  NE  ARG B 204      10.361  37.215  34.819  1.00  9.52    -0.227 N
ATOM  13086  HE  ARG B 204       9.360  37.401  34.758  1.00  0.00     0.177 HD
ATOM  13087  CZ  ARG B 204      10.777  36.517  35.856  1.00  9.64     0.665 C
ATOM  13088  NH1 ARG B 204      12.065  36.192  36.022  1.00  9.22    -0.235 N
ATOM  13089 1HH1 ARG B 204      12.756  36.480  35.329  1.00  0.00     0.174 HD
ATOM  13090 2HH1 ARG B 204      12.387  35.652  36.825  1.00  0.00     0.174 HD
ATOM  13091  NH2 ARG B 204       9.878  36.142  36.758  1.00 13.31    -0.235 N
ATOM  13092 1HH2 ARG B 204       8.897  36.390  36.632  1.00  0.00     0.174 HD
ATOM  13093 2HH2 ARG B 204      10.200  35.602  37.561  1.00  0.00     0.174 HD
ATOM  13094  N   PHE B 205      11.040  42.419  33.399  1.00  6.45    -0.346 N
ATOM  13095  HN  PHE B 205      12.040  42.325  33.221  1.00  0.00     0.163 HD
ATOM  13096  CA  PHE B 205      10.570  43.245  34.519  1.00  7.50     0.180 C
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ATOM  13098  C   PHE B 205       9.944  44.551  34.048  1.00  6.52      0.241 C
ATOM  13099  O   PHE B 205       8.987  45.038  34.668  1.00  9.98     -0.271 OA
ATOM  13100  CB  PHE B 205      11.716  43.422  35.530  1.00  5.67      0.073 C
ATOM  13103  CG  PHE B 205      11.736  42.266  36.513  1.00  8.29     -0.056 A
ATOM  13104  CD1 PHE B 205      12.169  41.011  36.140  1.00 12.22      0.007 A
ATOM  13106  CD2 PHE B 205      11.274  42.482  37.818  1.00  8.67      0.007 A
ATOM  13108  CE1 PHE B 205      12.184  39.959  37.062  1.00 14.62      0.001 A
ATOM  13110  CE2 PHE B 205      11.267  41.425  38.741  1.00 10.08      0.001 A
ATOM  13112  CZ  PHE B 205      11.720  40.182  38.365  1.00  9.01      0.000 A
ATOM  13114  N   GLU B 206      10.407  45.097  32.916  1.00 10.45     -0.346 N
ATOM  13115  HN  GLU B 206      11.224  44.720  32.435  1.00  0.00      0.163 HD
ATOM  13116  CA  GLU B 206       9.674  46.275  32.396  1.00 11.80      0.177 C
ATOM  13118  C   GLU B 206       8.280  45.874  31.980  1.00  8.85      0.241 C
ATOM  13119  O   GLU B 206       7.315  46.646  32.035  1.00  8.72     -0.271 OA
ATOM  13120  CB  GLU B 206      10.496  46.909  31.260  1.00 14.29      0.045 C
ATOM  13123  CG  GLU B 206      11.723  47.591  31.926  1.00 16.57      0.116 C
ATOM  13126  CD  GLU B 206      12.602  48.321  30.915  1.00 27.10      0.172 C
ATOM  13127  OE1 GLU B 206      12.627  47.936  29.737  1.00 25.39     -0.648 OA
ATOM  13128  OE2 GLU B 206      13.254  49.307  31.341  1.00 25.43     -0.648 OA
ATOM  13129  N   ALA B 207       8.061  44.642  31.497  1.00  8.60     -0.346 N
ATOM  13130  HN  ALA B 207       8.868  44.027  31.390  1.00  0.00      0.163 HD
ATOM  13131  CA  ALA B 207       6.770  44.121  31.117  1.00  7.88      0.172 C
ATOM  13133  C   ALA B 207       5.886  44.012  32.341  1.00 11.36      0.240 C
ATOM  13134  O   ALA B 207       4.640  44.089  32.190  1.00 10.23     -0.271 OA
ATOM  13135  CB  ALA B 207       6.920  42.715  30.480  1.00  6.60      0.042 C
ATOM  13139  N   TYR B 208       6.458  43.859  33.555  1.00  7.49     -0.346 N
ATOM  13140  HN  TYR B 208       7.468  43.745  33.634  1.00  0.00      0.163 HD
ATOM  13141  CA  TYR B 208       5.624  43.858  34.755  1.00  7.62      0.180 C
ATOM  13143  C   TYR B 208       5.362  45.264  35.284  1.00 12.93      0.241 C
ATOM  13144  O   TYR B 208       4.743  45.412  36.342  1.00 12.92     -0.271 OA
ATOM  13145  CB  TYR B 208       6.309  43.131  35.948  1.00  7.66      0.073 C
ATOM  13148  CG  TYR B 208       6.611  41.669  35.725  1.00  9.84     -0.056 A
ATOM  13149  CD1 TYR B 208       5.769  40.869  34.952  1.00  9.29      0.010 A
ATOM  13151  CD2 TYR B 208       7.741  41.092  36.311  1.00 11.97      0.010 A
ATOM  13153  CE1 TYR B 208       6.067  39.514  34.788  1.00 10.74      0.037 A
ATOM  13155  CE2 TYR B 208       8.042  39.752  36.147  1.00 10.38      0.037 A
ATOM  13157  CZ  TYR B 208       7.169  38.975  35.384  1.00 12.92      0.065 A
ATOM  13158  OH  TYR B 208       7.467  37.647  35.211  1.00 10.26     -0.361 OA
ATOM  13159  HH  TYR B 208       8.235  37.272  35.626  1.00  7.00      0.237 HD
ATOM  13160  N   GLY B 209       5.895  46.283  34.626  1.00 11.63     -0.351 N
ATOM  13161  HN  GLY B 209       6.461  46.099  33.797  1.00  0.00      0.163 HD
ATOM  13162  CA  GLY B 209       5.690  47.672  35.062  1.00 12.22      0.225 C
ATOM  13165  C   GLY B 209       6.670  48.052  36.184  1.00 14.01      0.236 C
ATOM  13166  O   GLY B 209       6.386  48.955  36.984  1.00 12.19     -0.272 OA
ATOM  13167  N   TRP B 210       7.784  47.361  36.331  1.00 10.86     -0.346 N
ATOM  13168  HN  TRP B 210       7.945  46.542  35.745  1.00  0.00      0.163 HD
ATOM  13169  CA  TRP B 210       8.795  47.749  37.318  1.00  8.59      0.181 C
ATOM  13171  C   TRP B 210       9.714  48.821  36.716  1.00 10.62      0.241 C
ATOM  13172  O   TRP B 210       9.872  48.957  35.500  1.00 10.15     -0.271 OA
ATOM  13173  CB  TRP B 210       9.718  46.580  37.698  1.00  8.23      0.075 C
ATOM  13176  CG  TRP B 210       9.037  45.574  38.610  1.00  8.95     -0.028 A
ATOM  13177  CD1 TRP B 210       7.791  45.030  38.524  1.00  9.85      0.096 A
ATOM  13179  CD2 TRP B 210       9.654  45.003  39.778  1.00  7.59     -0.002 A
ATOM  13180  CE2 TRP B 210       8.746  44.113  40.341  1.00  6.18      0.042 A
ATOM  13181  CE3 TRP B 210      10.889  45.234  40.397  1.00  8.33      0.014 A
ATOM  13183  NE1 TRP B 210       7.604  44.154  39.588  1.00  8.06     -0.365 N
ATOM  13184  HE1 TRP B 210       6.752  43.626  39.777  1.00  0.00      0.165 HD
ATOM  13185  CZ2 TRP B 210       9.025  43.418  41.532  1.00  8.16      0.030 A
ATOM  13187  CZ3 TRP B 210      11.205  44.510  41.554  1.00  6.52      0.001 A
ATOM  13189  CH2 TRP B 210      10.250  43.625  42.100  1.00 10.93      0.002 A
ATOM  13191  N   HIS B 211      10.349  49.572  37.595  1.00 10.45     -0.346 N
ATOM  13192  HN  HIS B 211      10.063  49.540  38.574  1.00  0.00      0.163 HD
ATOM  13193  CA  HIS B 211      11.473  50.466  37.315  1.00 13.17      0.182 C
ATOM  13195  C   HIS B 211      12.713  49.599  37.225  1.00 14.44      0.241 C
ATOM  13196  O   HIS B 211      13.005  48.913  38.221  1.00 12.91     -0.271 OA
ATOM  13197  CB  HIS B 211      11.556  51.549  38.286  1.00  9.99      0.093 C
ATOM  13200  CG  HIS B 211      12.857  52.278  38.204  1.00 11.25      0.028 A
ATOM  13201  CD2 HIS B 211      13.524  53.009  37.388  1.00 16.93      0.114 A
ATOM  13203  ND1 HIS B 211      13.628  52.333  39.489  1.00 13.44     -0.354 N
ATOM  13204  HD1 HIS B 211      13.407  51.875  40.373  1.00  0.00      0.166 HD
ATOM  13205  CE1 HIS B 211      14.698  53.075  39.255  1.00 11.07      0.180 A
ATOM  13207  NE2 HIS B 211      14.668  53.503  37.977  1.00 13.95     -0.360 N
ATOM  13208  HE2 HIS B 211      15.369  54.090  37.525  1.00  0.00      0.166 HD
ATOM  13209  N   VAL B 212      13.557  49.566  36.176  1.00  9.19     -0.346 N
ATOM  13210  HN  VAL B 212      13.382  50.187  35.386  1.00  0.00      0.163 HD
ATOM  13211  CA  VAL B 212      14.692  48.691  36.128  1.00 11.42      0.180 C
ATOM  13213  C   VAL B 212      15.981  49.460  35.834  1.00 14.23      0.241 C
ATOM  13214  O   VAL B 212      15.974  50.326  34.948  1.00 13.60     -0.271 OA
ATOM  13215  CB  VAL B 212      14.498  47.676  34.954  1.00 13.94      0.009 C
ATOM  13217  CG1 VAL B 212      15.739  46.783  34.863  1.00 14.93      0.012 C
ATOM  13221  CG2 VAL B 212      13.280  46.811  35.213  1.00 11.52      0.012 C
ATOM  13225  N   ILE B 213      16.995  49.240  36.644  1.00 12.36     -0.346 N
ATOM  13226  HN  ILE B 213      16.872  48.647  37.464  1.00  0.00      0.163 HD
ATOM  13227  CA  ILE B 213      18.307  49.849  36.368  1.00 12.00      0.180 C
ATOM  13229  C   ILE B 213      19.265  48.752  35.924  1.00 13.46      0.241 C
ATOM  13230  O   ILE B 213      19.608  47.849  36.692  1.00 11.85     -0.271 OA
ATOM  13231  CB  ILE B 213      18.869  50.582  37.619  1.00 14.77      0.013 C
ATOM  13233  CG1 ILE B 213      17.897  51.677  38.066  1.00 13.95      0.002 C
ATOM  13236  CG2 ILE B 213      20.245  51.152  37.243  1.00 12.75      0.012 C
ATOM  13240  CD1 ILE B 213      18.394  52.499  39.269  1.00 15.53      0.005 C
ATOM  13244  N   ARG B 214      19.739  48.822  34.679  1.00 11.84     -0.346 N
ATOM  13245  HN  ARG B 214      19.490  49.625  34.101  1.00  0.00      0.163 HD
ATOM  13246  CA  ARG B 214      20.596  47.796  34.120  1.00 16.32      0.176 C
ATOM  13248  C   ARG B 214      22.085  48.034  34.378  1.00 16.79      0.241 C
ATOM  13249  O   ARG B 214      22.512  49.172  34.538  1.00 16.88     -0.271 OA
ATOM  13250  CB  ARG B 214      20.429  47.866  32.576  1.00 11.52      0.036 C
ATOM  13253  CG  ARG B 214      19.038  47.462  32.074  1.00 16.46      0.023 C
ATOM  13256  CD  ARG B 214      18.903  47.820  30.586  1.00 23.62      0.138 C
ATOM  13259  NE  ARG B 214      17.757  47.247  29.889  1.00 24.60     -0.227 N
ATOM  13260  HE  ARG B 214      17.948  46.492  29.231  1.00  0.00      0.177 HD
ATOM  13261  CZ  ARG B 214      16.488  47.614  30.029  1.00 25.89      0.665 C
ATOM  13262  NH1 ARG B 214      16.200  48.575  30.896  1.00 18.84     -0.235 N
ATOM  13263 1HH1 ARG B 214      16.997  48.983  31.385  1.00  0.00      0.174 HD
ATOM  13264 2HH1 ARG B 214      15.226  48.857  31.003  1.00  0.00      0.174 HD
ATOM  13265  NH2 ARG B 214      15.432  47.073  29.381  1.00 24.55     -0.235 N
ATOM  13266 1HH2 ARG B 214      15.654  46.334  28.714  1.00  0.00      0.174 HD
ATOM  13267 2HH2 ARG B 214      14.458  47.355  29.488  1.00  0.00      0.174 HD
ATOM  13268  N   ASP B 215      22.867  46.979  34.304  1.00 11.64     -0.346 N
ATOM  13269  HN  ASP B 215      22.420  46.062  34.282  1.00  0.00      0.163 HD
ATOM  13270  CA  ASP B 215      24.311  47.019  34.251  1.00 22.24      0.186 C
ATOM  13272  C   ASP B 215      25.029  47.780  35.344  1.00 20.42      0.241 C
ATOM  13273  O   ASP B 215      25.907  48.600  35.057  1.00 14.70     -0.271 OA
ATOM  13274  CB  ASP B 215      24.682  47.709  32.914  1.00 28.78      0.147 C
ATOM  13277  CG  ASP B 215      24.204  46.846  31.751  1.00 40.57      0.175 C
ATOM  13278  OD1 ASP B 215      24.131  45.608  31.924  1.00 41.89     -0.648 OA
ATOM  13279  OD2 ASP B 215      23.878  47.442  30.712  1.00 43.41     -0.648 OA
ATOM  13280  N   ILE B 216      24.611  47.588  36.568  1.00 16.47     -0.346 N
ATOM  13281  HN  ILE B 216      23.825  46.962  36.743  1.00  0.00      0.163 HD
ATOM  13282  CA  ILE B 216      25.261  48.263  37.685  1.00 15.19      0.180 C
ATOM  13284  C   ILE B 216      26.513  47.435  37.978  1.00 16.96      0.241 C
ATOM  13285  O   ILE B 216      26.478  46.207  38.014  1.00 15.60     -0.271 OA
ATOM  13286  CB  ILE B 216      24.348  48.283  38.912  1.00 11.57      0.013 C
ATOM  13288  CG1 ILE B 216      23.080  49.119  38.591  1.00 10.89      0.002 C
ATOM  13291  CG2 ILE B 216      25.090  48.901  40.125  1.00 16.13      0.012 C
ATOM  13295  CD1 ILE B 216      21.963  48.769  39.597  1.00 16.72      0.005 C
ATOM  13299  N   ASP B 217      27.638  48.112  38.161  1.00 15.25     -0.345 N
ATOM  13300  HN  ASP B 217      27.637  49.126  38.049  1.00  0.00      0.163 HD
ATOM  13301  CA  ASP B 217      28.873  47.435  38.519  1.00 15.47      0.186 C
ATOM  13303  C   ASP B 217      28.702  47.128  40.014  1.00 15.60      0.225 C
ATOM  13304  O   ASP B 217      28.823  48.003  40.869  1.00 14.31     -0.271 OA
ATOM  13305  CB  ASP B 217      30.061  48.370  38.265  1.00 23.24      0.147 C
ATOM  13308  CG  ASP B 217      31.357  47.723  38.742  1.00 24.27      0.175 C
ATOM  13309  OD1 ASP B 217      31.373  46.696  39.448  1.00 16.22     -0.648 OA
ATOM  13310  OD2 ASP B 217      32.399  48.238  38.316  1.00 19.00     -0.648 OA
ATOM  13311  N   GLY B 218      28.499  45.863  40.333  1.00 14.97     -0.351 N
ATOM  13312  HN  GLY B 218      28.543  45.153  39.602  1.00  0.00      0.163 HD
ATOM  13313  CA  GLY B 218      28.213  45.453  41.706  1.00 21.37      0.225 C
ATOM  13316  C   GLY B 218      29.420  45.455  42.621  1.00 15.36      0.236 C
ATOM  13317  O   GLY B 218      29.339  45.062  43.783  1.00 15.15     -0.272 OA
ATOM  13318  N   HIS B 219      30.591  45.880  42.103  1.00 16.59     -0.346 N
ATOM  13319  HN  HIS B 219      30.632  46.160  41.123  1.00  0.00      0.163 HD
ATOM  13320  CA  HIS B 219      31.806  45.947  42.920  1.00 14.63      0.182 C
ATOM  13322  C   HIS B 219      32.298  47.377  42.984  1.00 17.03      0.241 C
ATOM  13323  O   HIS B 219      33.429  47.636  43.413  1.00 18.53     -0.271 OA
ATOM  13324  CB  HIS B 219      32.914  45.016  42.394  1.00 14.92      0.093 C
ATOM  13327  CG  HIS B 219      32.428  43.589  42.461  1.00 13.84      0.028 A
ATOM  13328  CD2 HIS B 219      32.264  42.696  41.460  1.00 16.87      0.114 A
ATOM  13330  ND1 HIS B 219      32.057  42.962  43.616  1.00 16.18     -0.354 N
ATOM  13331  HD1 HIS B 219      32.087  43.383  44.545  1.00  0.00      0.166 HD
ATOM  13332  CE1 HIS B 219      31.654  41.734  43.356  1.00 17.72      0.180 A
ATOM  13334  NE2 HIS B 219      31.783  41.547  42.029  1.00 19.56     -0.360 N
ATOM  13335  HE2 HIS B 219      31.558  40.687  41.528  1.00  0.00      0.166 HD
ATOM  13336  N   ASP B 220      31.429  48.311  42.620  1.00 12.22     -0.345 N
ATOM  13337  HN  ASP B 220      30.504  48.040  42.286  1.00  0.00      0.163 HD
ATOM  13338  CA  ASP B 220      31.789  49.731  42.694  1.00 13.78      0.186 C
ATOM  13340  C   ASP B 220      30.820  50.463  43.616  1.00 14.88      0.241 C
ATOM  13341  O   ASP B 220      29.687  50.724  43.177  1.00 16.03     -0.271 OA
ATOM  13342  CB  ASP B 220      31.732  50.340  41.273  1.00 15.20      0.147 C
ATOM  13345  CG  ASP B 220      32.148  51.809  41.362  1.00 31.71      0.175 C
ATOM  13346  OD1 ASP B 220      33.150  52.075  42.039  1.00 34.77     -0.648 OA
ATOM  13347  OD2 ASP B 220      31.485  52.725  40.844  1.00 32.41     -0.648 OA
ATOM  13348  N   ALA B 221      31.197  50.821  44.953  1.00 13.83     -0.346 N
ATOM  13349  HN  ALA B 221      32.151  50.631  45.136  1.00  0.00      0.163 HD
ATOM  13350  CA  ALA B 221      30.277  51.480  45.738  1.00 17.48      0.172 C
ATOM  13352  C   ALA B 221      29.632  52.718  45.162  1.00 20.35      0.240 C
ATOM  13353  O   ALA B 221      28.458  52.948  45.474  1.00 17.48     -0.271 OA
ATOM  13354  CB  ALA B 221      30.922  51.796  47.092  1.00 13.67      0.042 C
ATOM  13358  N   ALA B 222      30.328  53.585  44.408  1.00 19.08     -0.346 N
ATOM  13359  HN  ALA B 222      31.305  53.406  44.176  1.00  0.00      0.163 HD
ATOM  13360  CA  ALA B 222      29.655  54.793  43.926  1.00 19.75      0.172 C
ATOM  13362  C   ALA B 222      28.509  54.449  42.993  1.00 16.31      0.240 C
ATOM  13363  O   ALA B 222      27.488  55.128  42.948  1.00 19.51     -0.271 OA
ATOM  13364  CB  ALA B 222      30.634  55.733  43.179  1.00 18.49      0.042 C
ATOM  13368  N   SER B 223      28.736  53.460  42.125  1.00 14.78     -0.344 N
ATOM  13369  HN  SER B 223      29.628  52.964  42.125  1.00  0.00      0.163 HD
ATOM  13370  CA  SER B 223      27.673  53.095  41.163  1.00 18.34      0.200 C
ATOM  13372  C   SER B 223      26.428  52.541  41.852  1.00 18.88      0.243 C
ATOM  13373  O   SER B 223      25.270  52.852  41.517  1.00 14.62     -0.271 OA
ATOM  13374  CB  SER B 223      28.359  52.113  40.219  1.00 21.67      0.199 C
ATOM  13377  OG ASER B 223      27.463  51.385  39.416  0.50 23.19     -0.398 OA
ATOM  13378  HG ASER B 223      27.890  50.773  38.828  1.00  0.00      0.209 HD
ATOM  13379  N   ILE B 224      26.672  51.706  42.858  1.00 15.68     -0.346 N
ATOM  13380  HN  ILE B 224      27.637  51.482  43.100  1.00  0.00      0.163 HD
ATOM  13381  CA  ILE B 224      25.579  51.101  43.625  1.00 14.99      0.180 C
ATOM  13383  C   ILE B 224      24.799  52.183  44.361  1.00 14.73      0.241 C
ATOM  13384  O   ILE B 224      23.560  52.229  44.322  1.00 13.95     -0.271 OA
ATOM  13385  CB  ILE B 224      26.173  50.156  44.706  1.00 11.21      0.013 C
ATOM  13387  CG1 ILE B 224      26.937  49.033  43.955  1.00 15.71      0.002 C
ATOM  13390  CG2 ILE B 224      25.100  49.552  45.585  1.00 14.80      0.012 C
ATOM  13391  CD1 ILE B 224      27.778  48.159  44.867  1.00 13.69      0.005 C
ATOM  13398  N   LYS B 225      25.552  53.103  44.992  1.00 12.79     -0.346 N
ATOM  13399  HN  LYS B 225      26.570  53.057  44.955  1.00  0.00      0.163 HD
ATOM  13400  CA  LYS B 225      24.879  54.172  45.733  1.00 11.78      0.176 C
ATOM  13402  C   LYS B 225      23.987  55.020  44.851  1.00 14.13      0.241 C
ATOM  13403  O   LYS B 225      22.842  55.348  45.195  1.00 16.17     -0.271 OA
ATOM  13404  CB  LYS B 225      25.924  55.027  46.478  1.00 16.51      0.035 C
ATOM  13407  CG  LYS B 225      25.250  56.134  47.326  1.00 25.58      0.004 C
ATOM  13410  CD  LYS B 225      26.283  56.682  48.310  1.00 31.66      0.027 C
ATOM  13413  CE  LYS B 225      25.795  57.917  49.049  1.00 37.40     -0.229 C
ATOM  13416  NZ  LYS B 225      24.769  57.528  50.061  1.00 51.06     -0.079 N
ATOM  13417  HZ1 LYS B 225      24.441  58.357  50.557  1.00  0.00      0.274 HD
ATOM  13418  HZ2 LYS B 225      25.112  56.810  50.699  1.00  0.00      0.274 HD
ATOM  13419  HZ3 LYS B 225      24.001  57.001  49.645  1.00  0.00      0.274 HD
ATOM  13420  N   ARG B 226      24.459  55.436  43.672  1.00 14.01     -0.346 N
ATOM  13421  HN  ARG B 226      25.402  55.187  43.375  1.00  0.00      0.163 HD
ATOM  13422  CA  ARG B 226      23.605  56.252  42.817  1.00 17.37      0.176 C
ATOM  13424  C   ARG B 226      22.374  55.484  42.336  1.00 13.56      0.241 C
ATOM  13425  O   ARG B 226      21.313  56.093  42.186  1.00 12.62     -0.271 OA
ATOM  13426  CB  ARG B 226      24.397  56.619  41.529  1.00 21.06      0.036 C
ATOM  13429  CG  ARG B 226      25.495  57.631  41.839  1.00 53.95      0.023 C
ATOM  13432  CD  ARG B 226      26.429  57.731  40.644  1.00 71.55      0.138 C
ATOM  13435  NE  ARG B 226      27.692  58.388  40.950  1.00 87.99     -0.227 N
ATOM  13436  HE  ARG B 226      27.703  59.112  41.669  1.00  0.00      0.177 HD
ATOM  13437  CZ  ARG B 226      28.836  58.086  40.332  1.00 95.65      0.665 C
ATOM  13438  NH1 ARG B 226      28.855  57.139  39.401  1.00 97.33     -0.235 N
ATOM  13439 1HH1 ARG B 226      29.729  56.908  38.929  1.00  0.00      0.174 HD
ATOM  13440 2HH1 ARG B 226      27.996  56.645  39.158  1.00  0.00      0.174 HD
ATOM  13441  NH2 ARG B 226      29.953  58.729  40.648 1.00100.29     -0.235 N
ATOM  13442 1HH2 ARG B 226      30.827  58.498  40.176  1.00  0.00      0.174 HD
ATOM  13443 2HH2 ARG B 226      29.938  59.456  41.363  1.00  0.00      0.174 HD
ATOM  13444  N   ALA B 227      22.531  54.176  42.096  1.00 11.85     -0.346 N
ATOM  13445  HN  ALA B 227      23.441  53.729  42.204  1.00  0.00      0.163 HD
ATOM  13446  CA  ALA B 227      21.347  53.397  41.669  1.00 13.87      0.172 C
ATOM  13448  C   ALA B 227      20.311  53.347  42.788  1.00 12.53      0.240 C
ATOM  13449  O   ALA B 227      19.134  53.487  42.502  1.00 12.71     -0.271 OA
ATOM  13450  CB  ALA B 227      21.810  52.031  41.215  1.00 11.89      0.042 C
ATOM  13454  N   VAL B 228      20.715  53.166  44.043  1.00 12.14     -0.346 N
ATOM  13455  HN  VAL B 228      21.712  53.057  44.228  1.00  0.00      0.163 HD
ATOM  13456  CA  VAL B 228      19.780  53.118  45.164  1.00 11.01      0.180 C
ATOM  13458  C   VAL B 228      19.083  54.440  45.296  1.00 13.19      0.241 C
ATOM  13459  O   VAL B 228      17.850  54.516  45.468  1.00 11.75     -0.271 OA
ATOM  13460  CB  VAL B 228      20.431  52.672  46.491  1.00 13.07      0.009 C
ATOM  13462  CG1 VAL B 228      19.388  52.630  47.620  1.00 12.57      0.012 C
ATOM  13466  CG2 VAL B 228      21.073  51.307  46.314  1.00 17.41      0.012 C
ATOM  13470  N   GLU B 229      19.861  55.547  45.174  1.00 11.60     -0.346 N
ATOM  13471  HN  GLU B 229      20.874  55.480  45.075  1.00  0.00      0.163 HD
ATOM  13472  CA  GLU B 229      19.171  56.850  45.191  1.00 10.92      0.177 C
ATOM  13474  C   GLU B 229      18.136  56.995  44.074  1.00 11.86      0.241 C
ATOM  13475  O   GLU B 229      17.055  57.554  44.282  1.00 12.32     -0.271 OA
ATOM  13476  CB  GLU B 229      20.205  58.009  45.009  1.00 11.36      0.045 C
ATOM  13479  CG  GLU B 229      21.052  58.072  46.270  1.00 23.45      0.116 C
ATOM  13482  CD  GLU B 229      22.229  59.030  46.219  1.00 38.99      0.172 C
ATOM  13483  OE1 GLU B 229      22.674  59.419  45.118  1.00 36.88     -0.648 OA
ATOM  13484  OE2 GLU B 229      22.712  59.379  47.321  1.00 45.51     -0.648 OA
ATOM  13485  N   GLU B 230      18.415  56.584  42.840  1.00 12.22     -0.346 N
ATOM  13486  HN  GLU B 230      19.325  56.171  42.636  1.00  0.00      0.163 HD
ATOM  13487  CA  GLU B 230      17.426  56.721  41.780  1.00 15.64      0.177 C
ATOM  13489  C   GLU B 230      16.187  55.875  42.083  1.00 18.58      0.241 C
ATOM  13490  O   GLU B 230      15.057  56.307  41.837  1.00 14.98     -0.271 OA
ATOM  13491  CB  GLU B 230      18.038  56.263  40.446  1.00 18.58      0.045 C
ATOM  13494  CG  GLU B 230      16.970  55.915  39.408  1.00 32.57      0.116 C
ATOM  13497  CD  GLU B 230      17.429  55.681  37.980  1.00 42.85      0.172 C
ATOM  13498  OE1 GLU B 230      18.638  55.911  37.715  1.00 39.69     -0.648 OA
ATOM  13499  OE2 GLU B 230      16.615  55.274  37.092  1.00 23.45     -0.648 OA
ATOM  13500  N   ALA B 231      16.425  54.674  42.600  1.00 15.53     -0.346 N
ATOM  13501  HN  ALA B 231      17.380  54.380  42.806  1.00  0.00      0.163 HD
ATOM  13502  CA  ALA B 231      15.281  53.764  42.874  1.00 14.30      0.172 C
ATOM  13504  C   ALA B 231      14.395  54.326  43.960  1.00 12.83      0.240 C
ATOM  13505  O   ALA B 231      13.156  54.266  43.913  1.00 13.43     -0.271 OA
ATOM  13506  CB  ALA B 231      15.811  52.393  43.286  1.00 14.18      0.042 C
ATOM  13510  N   ARG B 232      14.985  54.960  44.995  1.00 14.14     -0.346 N
ATOM  13511  HN  ARG B 232      16.000  55.053  45.020  1.00  0.00      0.163 HD
ATOM  13512  CA  ARG B 232      14.184  55.509  46.071  1.00 11.24      0.176 C
ATOM  13514  C   ARG B 232      13.362  56.727  45.653  1.00 16.22      0.241 C
ATOM  13515  O   ARG B 232      12.339  57.016  46.276  1.00 19.27     -0.271 OA
ATOM  13516  CB  ARG B 232      15.009  55.891  47.347  1.00 11.24      0.036 C
ATOM  13519  CG  ARG B 232      15.596  54.656  48.023  1.00 13.09      0.023 C
ATOM  13522  CD  ARG B 232      16.700  54.994  49.036  1.00 22.28      0.138 C
ATOM  13525  NE  ARG B 232      16.338  56.151  49.885  1.00 31.59     -0.227 N
ATOM  13526  HE  ARG B 232      16.554  57.091  49.552  1.00  0.00      0.177 HD
ATOM  13527  CZ  ARG B 232      15.745  56.012  51.058  1.00 35.04      0.665 C
ATOM  13529  NH1 ARG B 232      15.478  54.795  51.499  1.00 38.57     -0.235 N
ATOM  13530 1HH1 ARG B 232      15.757  54.005  50.918  1.00  0.00      0.174 HD
ATOM  13531 2HH1 ARG B 232      15.020  54.688  52.404  1.00  0.00      0.174 HD
ATOM  13532  NH2 ARG B 232      15.384  57.033  51.809  1.00 38.69     -0.235 N
ATOM  13533 1HH2 ARG B 232      15.590  57.972  51.469  1.00  0.00      0.174 HD
ATOM  13534 2HH2 ARG B 232      14.926  56.926  52.714  1.00  0.00      0.174 HD
ATOM  13535  N   ALA B 233      13.752  57.430  44.621  1.00 16.36     -0.346 N
ATOM  13536  HN  ALA B 233      14.620  57.175  44.150  1.00  0.00      0.163 HD
ATOM  13537  CA  ALA B 233      12.989  58.561  44.125  1.00 19.01      0.172 C
ATOM  13538  C   ALA B 233      11.845  58.139  43.204  1.00 20.30      0.240 C
ATOM  13539  O   ALA B 233      11.051  59.005  42.835  1.00 17.98     -0.271 OA
ATOM  13540  CB  ALA B 233      13.928  59.458  43.301  1.00 20.39      0.042 C
ATOM  13544  N   ASP B 234      11.803  56.881  42.764  1.00 10.87     -0.346 N
ATOM  13545  HN  ASP B 234      12.545  56.226  43.011  1.00  0.00      0.163 HD
ATOM  13546  CA  ASP B 234      10.673  56.442  41.915  1.00 14.35      0.180 C
ATOM  13548  C   ASP B 234       9.616  55.914  42.868  1.00 15.75      0.241 C
ATOM  13549  O   ASP B 234       9.789  54.860  43.514  1.00 16.65     -0.271 OA
ATOM  13550  CB  ASP B 234      11.101  55.344  40.945  1.00 13.98      0.009 C
ATOM  13552  CG1 VAL B 234       9.865  54.802  40.202  1.00 19.92      0.012 C
ATOM  13556  CG2 VAL B 234      12.142  55.862  39.967  1.00 19.74      0.012 C
ATOM  13560  N   THR B 235       8.526  56.622  43.117  1.00 15.91     -0.344 N
ATOM  13561  HN  THR B 235       8.324  57.470  42.588  1.00  0.00      0.163 HD
ATOM  13562  CA  THR B 235       7.616  56.162  44.168  1.00 14.85      0.205 C
ATOM  13564  C   THR B 235       6.436  55.345  43.720  1.00 19.74      0.243 C
ATOM  13565  O   THR B 235       5.708  54.860  44.591  1.00 18.41     -0.271 OA
ATOM  13566  CB  THR B 235       7.099  57.448  44.900  1.00 27.59      0.146 C
ATOM  13568  CG2 THR B 235       8.228  58.348  45.335  1.00 26.77      0.042 C
ATOM  13572  OG1 THR B 235       6.316  58.192  43.956  1.00 20.69     -0.393 OA
ATOM  13573  HG1 THR B 235       5.605  57.625  43.682  1.00  0.00      0.210 HD
ATOM  13574  N   ASP B 236       6.208  55.178  42.432  1.00 16.96     -0.345 N
ATOM  13575  HN  ASP B 236       6.878  55.526  41.746  1.00  0.00      0.163 HD
ATOM  13576  CA  ASP B 236       4.984  54.487  41.983  1.00 18.37      0.186 C
ATOM  13578  C   ASP B 236       5.228  53.149  41.310  1.00 16.66      0.241 C
ATOM  13579  O   ASP B 236       4.307  52.590  40.721  1.00 17.43     -0.271 OA
ATOM  13580  CB  ASP B 236       4.280  55.460  41.030  1.00 26.06      0.147 C
ATOM  13583  CG  ASP B 236       5.093  55.784  39.800  1.00 31.87      0.175 C
ATOM  13584  OD1 ASP B 236       6.324  55.604  39.661  1.00 24.86     -0.648 OA
ATOM  13585  OD2 ASP B 236       4.450  56.298  38.856  1.00 42.43     -0.648 OA
ATOM  13586  N   LYS B 237       6.482  52.669  41.291  1.00 14.44     -0.346 N
ATOM  13587  HN  LYS B 237       7.232  53.229  41.695  1.00  0.00      0.163 HD
ATOM  13588  CA  LYS B 237       6.801  51.379  40.714  1.00 11.70      0.176 C
ATOM  13590  C   LYS B 237       7.887  50.722  41.583  1.00 12.60      0.243 C
ATOM  13591  O   LYS B 237       8.801  51.438  41.996  1.00  9.48     -0.271 OA
ATOM  13592  CB  LYS B 237       7.535  51.529  39.344  1.00 13.83      0.035 C
ATOM  13595  CG  LYS B 237       6.708  52.219  38.290  1.00 20.25      0.004 C
ATOM  13598  CD  LYS B 237       7.563  52.177  37.025  1.00 18.57      0.027 C
ATOM  13601  CE  LYS B 237       6.538  52.772  35.941  1.00 32.07      0.229 C
ATOM  13604  NZ  LYS B 237       7.257  52.619  34.631 1.00 51.14     -0.079 N
ATOM  13605  HZ1 LYS B 237       6.580  52.880  33.915  1.00  0.00      0.274 HD
ATOM  13606  HZ2 LYS B 237       7.663  51.694  34.493  1.00  0.00      0.274 HD
ATOM  13607  HZ3 LYS B 237       8.130  53.144  34.579  1.00  0.00      0.274 HD
ATOM  13608  N   PRO B 238       7.825  49.422  41.760  1.00  9.48     -0.337 N
ATOM  13609  CA  PRO B 238       8.901  48.690  42.413  1.00  9.94      0.179 C
ATOM  13611  C   PRO B 238      10.143  48.802  41.532  1.00  7.87      0.241 C
ATOM  13612  O   PRO B 238      10.009  48.927  40.305 1.00 10.58     -0.271 OA
ATOM  13613  CB  PRO B 238       8.378  47.268  42.535  1.00  8.46      0.037 C
ATOM  13616  CG  PRO B 238       7.215  47.151  41.592  1.00 12.45      0.022 C
ATOM  13619  CD  PRO B 238       6.741  48.517  41.214  1.00  8.07      0.127 C
ATOM  13622  N   SER B 239      11.332  48.690  42.096  1.00  9.74     -0.344 N
ATOM  13623  HN  SER B 239      11.391  48.535  43.102  1.00  0.00      0.163 HD
ATOM  13624  CA  SER B 239      12.567  48.782  41.317  1.00  8.92      0.200 C
ATOM  13626  C   SER B 239      13.399  47.497  41.397  1.00 11.34      0.243 C
ATOM  13627  O   SER B 239      13.513  46.913  42.492  1.00 11.38     -0.271 OA
ATOM  13628  CB  SER B 239      13.521  49.885  41.856  1.00 12.02      0.199 C
ATOM  13631  OG  SER B 239      12.937  51.162  41.754  1.00 10.45     -0.398 OA
ATOM  13632  HG  SER B 239      13.520  51.836  42.083  1.00  0.00      0.209 HD
ATOM  13633  N   LEU B 240      13.991  47.178  40.264  1.00  8.86     -0.346 N
ATOM  13634  HN  LEU B 240      13.782  47.721  39.426  1.00  0.00      0.163 HD
ATOM  13635  CA  LEU B 240      14.941  46.066  40.173  1.00  9.70      0.177 C
ATOM  13637  C   LEU B 240      16.303  46.616  39.740  1.00 12.95      0.241 C
ATOM  13638  O   LEU B 240      16.445  47.268  38.687  1.00 10.97     -0.271 OA
ATOM  13639  CB  LEU B 240      14.522  45.044  39.073  1.00  7.15      0.038 C
ATOM  13642  CG  LEU B 240      15.513  43.867  38.937  1.00 12.12     -0.020 C
ATOM  13644  CD1 LEU B 240      15.450  42.959  40.170  1.00 18.52      0.009 C
ATOM  13648  CD2 LEU B 240      15.169  43.063  37.686  1.00 17.33      0.009 C
ATOM  13652  N   LEU B 241      17.297  46.423  40.603  1.00  8.95     -0.346 N
ATOM  13653  HN  LEU B 241      17.077  45.953  41.481  1.00  0.00      0.163 HD
ATOM  13654  CA  LEU B 241      18.681  46.835  40.384  1.00  7.90      0.177 C
ATOM  13656  C   LEU B 241      19.483  45.623  39.932  1.00 11.13      0.241 C
ATOM  13657  O   LEU B 241      19.672  44.658  40.696  1.00 11.75     -0.271 OA
ATOM  13658  CB  LEU B 241      19.256  47.347  41.742  1.00  9.84      0.038 C
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ATOM  13661  CG  LEU B 241      19.000  48.838  41.998  1.00 22.31      -0.020 C
ATOM  13663  CD1 LEU B 241      17.531  49.211  41.877  1.00 20.12       0.009 C
ATOM  13667  CD2 LEU B 241      19.510  49.271  43.379  1.00 22.17       0.009 C
ATOM  13671  N   MET B 242      19.889  45.598  38.663  1.00 10.62      -0.346 N
ATOM  13672  HN  MET B 242      19.696  46.392  38.053  1.00  0.00       0.163 HD
ATOM  13673  CA  MET B 242      20.616  44.429  38.136  1.00  8.11       0.177 C
ATOM  13675  C   MET B 242      22.095  44.664  38.358  1.00 15.63       0.241 C
ATOM  13676  O   MET B 242      22.657  45.536  37.689  1.00 14.05      -0.271 OA
ATOM  13677  CB  MET B 242      20.292  44.347  36.620  1.00 11.78       0.045 C
ATOM  13680  CG  MET B 242      18.770  44.034  36.532  1.00 20.69       0.076 C
ATOM  13683  SD  MET B 242      18.323  43.806  34.800  1.00 23.38      -0.173 SA
ATOM  13684  CE  MET B 242      19.029  42.193  34.504  1.00 18.12       0.089 C
ATOM  13688  N   CYS B 243      22.650  43.937  39.350  1.00 11.37      -0.345 N
ATOM  13689  HN  CYS B 243      22.096  43.230  39.834  1.00  0.00       0.163 HD
ATOM  13690  CA  CYS B 243      24.025  44.157  39.728  1.00 10.47       0.186 C
ATOM  13692  C   CYS B 243      24.916  43.070  39.191  1.00 11.55       0.241 C
ATOM  13693  O   CYS B 243      24.772  41.880  39.525  1.00 14.41      -0.271 OA
ATOM  13694  CB  CYS B 243      24.151  44.117  41.283  1.00 12.10       0.121 C
ATOM  13697  SG  CYS B 243      23.095  45.404  42.028  1.00 17.73      -0.095 SA
ATOM  13698  N   LYS B 244      25.878  43.511  38.380  1.00 13.27      -0.346 N
ATOM  13699  HN  LYS B 244      25.954  44.508  38.180  1.00  0.00       0.163 HD
ATOM  13700  CA  LYS B 244      26.831  42.569  37.771  1.00 14.06       0.176 C
ATOM  13702  C   LYS B 244      27.935  42.281  38.799  1.00 14.34       0.241 C
ATOM  13703  O   LYS B 244      28.572  43.216  39.253  1.00 13.51      -0.271 OA
ATOM  13704  CB  LYS B 244      27.468  43.237  36.537  1.00 22.28       0.035 C
ATOM  13707  CG  LYS B 244      26.595  42.885  35.328  1.00 33.35       0.004 C
ATOM  13710  CD  LYS B 244      26.373  44.068  34.421  1.00 57.24       0.027 C
ATOM  13713  CE  LYS B 244      26.991  43.876  33.047  1.00 63.65       0.229 C
ATOM  13716  NZ  LYS B 244      27.156  45.193  32.361  1.00 71.97      -0.079 N
ATOM  13717  HZ1 LYS B 244      27.571  45.064  31.438  1.00  0.00       0.274 HD
ATOM  13718  HZ2 LYS B 244      27.689  45.853  32.928  1.00  0.00       0.274 HD
ATOM  13719  HZ3 LYS B 244      26.277  45.709  32.313  1.00  0.00       0.274 HD
ATOM  13720  N   THR B 245      27.964  41.037  39.283  1.00 13.65      -0.344 N
ATOM  13721  HN  THR B 245      27.307  40.339  38.935  1.00  0.00       0.163 HD
ATOM  13722  CA  THR B 245      28.938  40.674  40.313  1.00 14.16       0.205 C
ATOM  13724  C   THR B 245      29.752  39.461  39.854  1.00 19.08       0.243 C
ATOM  13725  O   THR B 245      29.410  38.746  38.906  1.00 15.35      -0.271 OA
ATOM  13726  CB  THR B 245      28.306  40.299  41.663  1.00 16.04       0.146 C
ATOM  13728  CG2 THR B 245      27.399  41.375  42.247  1.00 16.00       0.042 C
ATOM  13732  OG1 THR B 245      27.528  39.094  41.437  1.00 19.02      -0.393 OA
ATOM  13733  HG1 THR B 245      27.137  38.862  42.271  1.00  0.00       0.210 HD
ATOM  13734  N   ILE B 246      30.803  39.177  40.619  1.00 16.53      -0.346 N
ATOM  13735  HN  ILE B 246      31.027  39.774  41.416  1.00  0.00       0.163 HD
ATOM  13736  CA  ILE B 246      31.647  38.003  40.321  1.00 18.65       0.180 C
ATOM  13738  C   ILE B 246      31.441  37.068  41.521  1.00 14.59       0.241 C
ATOM  13739  O   ILE B 246      31.811  37.520  42.614  1.00 14.93      -0.271 OA
ATOM  13740  CB  ILE B 246      33.123  38.430  40.233  1.00 21.80       0.013 C
ATOM  13742  CG1 ILE B 246      33.363  39.309  38.981  1.00 21.20       0.002 C
ATOM  13745  CG2 ILE B 246      34.037  37.212  40.168  1.00 20.51       0.012 C
ATOM  13749  CD1 ILE B 246      34.758  39.932  39.047  1.00 25.95       0.005 C
ATOM  13753  N   ILE B 247      30.898  35.892  41.304  1.00 16.41      -0.346 N
ATOM  13754  HN  ILE B 247      30.631  35.604  40.362  1.00  0.00       0.163 HD
ATOM  13755  CA  ILE B 247      30.684  34.998  42.458  1.00 14.77       0.180 C
ATOM  13757  C   ILE B 247      32.040  34.634  43.036  1.00 15.45       0.241 C
ATOM  13758  O   ILE B 247      33.040  34.477  42.332  1.00 13.80      -0.271 OA
ATOM  13759  CB  ILE B 247      29.889  33.753  42.059  1.00 14.20       0.013 C
ATOM  13761  CG1 ILE B 247      29.376  33.009  43.311  1.00 18.15       0.002 C
ATOM  13764  CG2 ILE B 247      30.682  32.821  41.137  1.00 16.82       0.012 C
ATOM  13768  CD1 ILE B 247      28.410  31.884  42.940  1.00 22.18       0.005 C
ATOM  13772  N   GLY B 248      32.123  34.605  44.377  1.00 13.49      -0.351 N
ATOM  13773  HN  GLY B 248      31.306  34.808  44.952  1.00  0.00       0.163 HD
ATOM  13774  CA  GLY B 248      33.404  34.278  44.995  1.00 15.19       0.225 C
ATOM  13777  C   GLY B 248      34.442  35.378  44.820  1.00 12.40       0.236 C
ATOM  13778  O   GLY B 248      35.629  35.086  44.932  1.00 17.55      -0.272 OA
ATOM  13779  N   PHE B 249      34.027  36.634  44.642  1.00 18.30      -0.346 N
ATOM  13780  HN  PHE B 249      33.026  36.827  44.663  1.00  0.00       0.163 HD
ATOM  13781  CA  PHE B 249      34.950  37.740  44.419  1.00 16.16       0.180 C
ATOM  13783  C   PHE B 249      36.136  37.773  45.386  1.00 21.67       0.241 C
ATOM  13784  O   PHE B 249      35.923  37.785  46.606  1.00 18.58      -0.271 OA
ATOM  13785  CB  PHE B 249      34.188  39.057  44.495  1.00 13.87       0.073 C
ATOM  13788  CG  PHE B 249      35.039  40.290  44.295  1.00 24.99      -0.056 A
ATOM  13789  CD1 PHE B 249      35.807  40.810  45.325  1.00 24.30       0.007 A
ATOM  13791  CD2 PHE B 249      35.028  40.935  43.083  1.00 23.14       0.007 A
ATOM  13793  CE1 PHE B 249      36.590  41.927  45.147  1.00 28.65       0.001 A
ATOM  13795  CE2 PHE B 249      35.819  42.069  42.895  1.00 25.85       0.001 A
ATOM  13797  CZ  PHE B 249      36.599  42.568  43.914  1.00 25.68       0.000 A
ATOM  13799  N   GLY B 250      37.350  37.869  44.822  1.00 17.76      -0.351 N
ATOM  13800  HN  GLY B 250      37.439  37.941  43.808  1.00  0.00       0.163 HD
ATOM  13801  CA  GLY B 250      38.546  37.870  45.665  1.00 17.87       0.225 C
ATOM  13804  C   GLY B 250      39.334  36.567  45.584  1.00 23.39       0.236 C
ATOM  13805  O   GLY B 250      40.552  36.571  45.830  1.00 22.40      -0.272 OA
ATOM  13806  N   SER B 251      38.725  35.434  45.240  1.00 19.23      -0.344 N
ATOM  13807  HN  SER B 251      37.728  35.462  45.025  1.00  0.00       0.163 HD
ATOM  13808  CA  SER B 251      39.422  34.152  45.157  1.00 20.55       0.200 C
ATOM  13810  C   SER B 251      40.109  34.010  43.821  1.00 23.10       0.245 C
ATOM  13811  O   SER B 251      39.434  34.007  42.779  1.00 22.63      -0.271 OA
ATOM  13812  CB  SER B 251      38.441  32.985  45.377  1.00 16.49       0.199 C
ATOM  13815  OG  SER B 251      38.978  31.792  44.843  1.00 12.44      -0.398 OA
ATOM  13816  HG  SER B 251      38.373  31.072  44.979  1.00  0.00       0.209 HD
ATOM  13817  N   PRO B 252      41.438  33.897  43.801  1.00 24.47      -0.337 N
ATOM  13818  CA  PRO B 252      42.163  33.847  42.547  1.00 25.16       0.179 C
ATOM  13820  C   PRO B 252      41.746  32.657  41.708  1.00 25.36       0.241 C
ATOM  13821  O   PRO B 252      41.677  32.753  40.474  1.00 26.71      -0.271 OA
ATOM  13822  CB  PRO B 252      43.641  33.751  42.935  1.00 24.51       0.037 C
ATOM  13825  CG  PRO B 252      43.716  33.992  44.384  1.00 25.63       0.022 C
ATOM  13828  CD  PRO B 252      42.337  33.893  44.973  1.00 25.08       0.127 C
ATOM  13831  N   ASN B 253      41.509  31.493  42.316  1.00 22.29      -0.346 N
ATOM  13832  HN  ASN B 253      41.540  31.421  43.333  1.00  0.00       0.163 HD
ATOM  13833  CA  ASN B 253      41.206  30.332  41.501  1.00 23.70       0.185 C
ATOM  13835  C   ASN B 253      39.753  29.960  41.334  1.00 26.84       0.247 C
ATOM  13836  O   ASN B 253      39.469  29.179  40.415  1.00 27.12      -0.271 OA
ATOM  13837  CB  ASN B 253      41.923  29.108  42.123  1.00 26.27       0.137 C
ATOM  13840  CG  ASN B 253      43.427  29.373  42.008  1.00 37.20       0.217 C
ATOM  13841  ND2 ASN B 253      44.096  29.601  43.120  1.00 42.50      -0.370 N
ATOM  13842 1HD2 ASN B 253      45.098  29.777  43.052  1.00  0.00       0.159 HD
ATOM  13843 2HD2 ASN B 253      43.693  29.583  44.066  1.00  0.00       0.159 HD
ATOM  13844  OD1 ASN B 253      43.911  29.394  40.884  1.00 29.70      -0.274 OA
ATOM  13845  N   LYS B 254      38.893  30.412  42.245  1.00 19.70      -0.346 N
ATOM  13846  HN  LYS B 254      39.203  31.065  42.965  1.00  0.00       0.163 HD
ATOM  13847  CA  LYS B 254      37.507  29.968  42.206  1.00 22.36       0.176 C
ATOM  13849  C   LYS B 254      36.491  31.081  41.975  1.00 20.19       0.241 C
ATOM  13850  O   LYS B 254      35.340  30.706  41.712  1.00 21.92      -0.271 OA
ATOM  13851  CB  LYS B 254      37.186  29.230  43.516  1.00 23.53       0.035 C
ATOM  13854  CG  LYS B 254      38.037  28.003  43.732  1.00 24.81       0.004 C
ATOM  13857  CD  LYS B 254      37.464  27.015  44.747  1.00 30.16       0.027 C
ATOM  13860  CE  LYS B 254      38.548  26.023  45.173  1.00 32.49       0.229 C
ATOM  13863  NZ  LYS B 254      38.135  25.231  46.370  1.00 51.71      -0.079 N
ATOM  13864  HZ1 LYS B 254      38.858  24.570  46.654  1.00  0.00       0.274 HD
ATOM  13865  HZ2 LYS B 254      37.242  24.762  46.215  1.00  0.00       0.274 HD
ATOM  13866  HZ3 LYS B 254      37.864  25.839  47.143  1.00  0.00       0.274 HD
ATOM  13867  N   ALA B 255      36.940  32.333  41.991  1.00 14.33      -0.346 N
ATOM  13868  HN  ALA B 255      37.910  32.556  42.213  1.00  0.00       0.163 HD
ATOM  13869  CA  ALA B 255      35.951  33.382  41.669  1.00 20.24       0.172 C
ATOM  13871  C   ALA B 255      35.419  33.167  40.252  1.00 23.45       0.240 C
ATOM  13872  O   ALA B 255      36.177  32.794  39.342  1.00 22.23      -0.271 OA
ATOM  13873  CB  ALA B 255      36.603  34.752  41.723  1.00 19.24       0.042 C
ATOM  13877  N   GLY B 256      34.125  33.383  40.049  1.00 21.37      -0.351 N
ATOM  13878  HN  GLY B 256      33.525  33.623  40.838  1.00  0.00       0.163 HD
ATOM  13879  CA  GLY B 256      33.551  33.281  38.711  1.00 26.36       0.225 C
ATOM  13882  C   GLY B 256      33.300  31.859  38.258  1.00 26.01       0.236 C
ATOM  13883  O   GLY B 256      33.032  31.623  37.088  1.00 27.10      -0.272 OA
ATOM  13884  N   THR B 257      33.415  30.880  39.147  1.00 23.45      -0.344 N
ATOM  13885  HN  THR B 257      33.671  31.102  40.109  1.00  0.00       0.163 HD
ATOM  13886  CA  THR B 257      33.180  29.493  38.767  1.00 25.18       0.205 C
ATOM  13888  C   THR B 257      32.087  28.948  39.688  1.00 26.91       0.243 C
ATOM  13889  O   THR B 257      31.928  29.386  40.833  1.00 22.54      -0.271 OA
ATOM  13890  CB  THR B 257      34.413  28.595  38.975  1.00 27.61       0.146 C
ATOM  13892  CG2 THR B 257      35.684  29.193  38.416  1.00 34.38       0.042 C
ATOM  13896  OG1 THR B 257      34.574  28.406  40.402  1.00 31.93      -0.393 OA
ATOM  13897  HG1 THR B 257      35.335  27.852  40.530  1.00  0.00       0.210 HD
ATOM  13898  N   HIS B 258      31.510  27.817  39.252  1.00 21.50      -0.346 N
ATOM  13899  HN  HIS B 258      31.794  27.383  38.374  1.00  0.00       0.163 HD
ATOM  13900  CA  HIS B 258      30.455  27.228  40.086  1.00 27.56       0.182 C
ATOM  13902  C   HIS B 258      31.088  26.500  41.264  1.00 27.04       0.241 C
ATOM  13903  O   HIS B 258      30.348  26.168  42.203  1.00 20.06      -0.271 OA
ATOM  13904  CB  HIS B 258      29.511  26.375  39.243  1.00 29.03       0.093 C
ATOM  13907  CG  HIS B 258      30.247  25.187  38.689  1.00 48.40       0.028 A
ATOM  13908  CD2 HIS B 258      30.254  23.891  39.076  1.00 55.00       0.114 A
ATOM  13910  ND1 HIS B 258      31.103  25.273  37.615  1.00 54.90      -0.354 N
ATOM  13911  HD1 HIS B 258      31.312  26.126  37.097  1.00  0.00       0.166 HD
ATOM  13912  CE1 HIS B 258      31.611  24.085  37.358  1.00 56.13       0.180 A
ATOM  13914  NE2 HIS B 258      31.115  23.228  38.231  1.00 58.22      -0.360 N
ATOM  13915  HE2 HIS B 258      31.335  22.233  38.273  1.00  0.00       0.166 HD
ATOM  13916  N   ASP B 259      32.405  26.313  41.300  1.00 22.21      -0.345 N
ATOM  13917  HN  ASP B 259      32.964  26.605  40.498  1.00  0.00       0.163 HD
ATOM  13918  CA  ASP B 259      33.078  25.709  42.436  1.00 29.21       0.186 C
ATOM  13920  C   ASP B 259      33.015  26.590  43.689  1.00 27.82       0.241 C
ATOM  13921  O   ASP B 259      33.189  26.073  44.784  1.00 30.49      -0.271 OA
ATOM  13922  CB  ASP B 259      34.579  25.532  42.141  1.00 37.29       0.147 C
ATOM  13925  CG  ASP B 259      34.734  24.612  40.939  1.00 53.72       0.175 C
ATOM  13926  OD1 ASP B 259      34.698  25.135  39.806  1.00 61.58      -0.648 OA
ATOM  13927  OD2 ASP B 259      34.870  23.398  41.163  1.00 55.40      -0.648 OA
ATOM  13928  N   SER B 260      32.796  27.890  43.567  1.00 22.56      -0.344 N
ATOM  13929  HN  SER B 260      32.713  28.308  42.640  1.00  0.00       0.163 HD
ATOM  13930  CA  SER B 260      32.673  28.725  44.754  1.00 20.37       0.200 C
ATOM  13932  C   SER B 260      31.219  28.776  45.210  1.00 19.94       0.243 C
ATOM  13933  O   SER B 260      30.966  29.374  46.260  1.00 21.40      -0.271 OA
ATOM  13934  CB  SER B 260      33.168  30.148  44.480  1.00 22.86       0.199 C
ATOM  13937  OG  SER B 260      32.374  30.708  43.434  1.00 23.70      -0.398 OA
ATOM  13938  HG  SER B 260      32.681  31.591  43.264  1.00  0.00       0.209 HD
ATOM  13939  N   HIS B 261      30.273  28.128  44.520  1.00 20.29      -0.346 N
ATOM  13940  HN  HIS B 261      30.504  27.571  43.697  1.00  0.00       0.163 HD
ATOM  13941  CA  HIS B 261      28.891  28.251  44.994  1.00 20.38       0.182 C
ATOM  13943  C   HIS B 261      28.609  27.675  46.378  1.00 21.21       0.241 C
ATOM  13944  O   HIS B 261      27.957  28.298  47.211  1.00 22.25      -0.271 OA
ATOM  13945  CB  HIS B 261      27.924  27.591  43.964  1.00 21.29       0.093 C
ATOM  13948  CG  HIS B 261      26.568  27.325  44.544  1.00 22.09       0.028 A
ATOM  13949  CD2 HIS B 261      26.045  26.207  45.116  1.00 21.12       0.114 A
ATOM  13951  ND1 HIS B 261      25.587  28.306  44.640  1.00 22.45      -0.354 N
ATOM  13952  HD1 HIS B 261      25.681  29.266  44.308  1.00  0.00       0.166 HD
ATOM  13953  CE1 HIS B 261      24.524  27.810  45.222  1.00 23.18       0.180 A
ATOM  13955  NE2 HIS B 261      24.769  26.536  45.544  1.00 20.35      -0.360 N
ATOM  13956  HE2 HIS B 261      24.123  25.910  46.025  1.00  0.00       0.166 HD
ATOM  13957  N   GLY B 262      28.847  26.377  46.554  1.00 17.70      -0.351 N
ATOM  13958  HN  GLY B 262      29.401  25.896  45.846  1.00  0.00       0.163 HD
ATOM  13959  CA  GLY B 262      28.379  25.609  47.669  1.00 19.67       0.225 C
ATOM  13962  C   GLY B 262      29.344  24.687  48.378  1.00 20.68       0.236 C
ATOM  13963  O   GLY B 262      28.882  23.719  48.986  1.00 20.81      -0.272 OA
ATOM  13964  N   ALA B 263      30.652  24.981  48.374  1.00 21.56      -0.347 N
ATOM  13965  HN  ALA B 263      31.003  25.741  47.791  1.00  0.00       0.163 HD
ATOM  13966  CA  ALA B 263      31.582  24.203  49.215  1.00 21.54       0.172 C
ATOM  13968  C   ALA B 263      32.676  25.134  49.754  1.00 18.36       0.243 C
ATOM  13969  O   ALA B 263      33.004  26.161  49.170  1.00 17.96      -0.271 OA
ATOM  13970  CB  ALA B 263      32.195  23.086  48.388  1.00 19.38       0.042 C
ATOM  13974  N   PRO B 264      33.305  24.762  50.865  1.00 20.11      -0.337 N
ATOM  13975  CA  PRO B 264      34.401  25.543  51.408  1.00 17.36       0.179 C
ATOM  13977  C   PRO B 264      35.486  25.781  50.357  1.00 20.13       0.241 C
ATOM  13978  O   PRO B 264      35.789  24.955  49.481  1.00 17.09      -0.271 OA
ATOM  13979  CB  PRO B 264      34.942  24.674  52.560  1.00 19.82       0.037 C
ATOM  13982  CG  PRO B 264      33.812  23.769  52.912  1.00 21.29       0.022 C
ATOM  13985  CD  PRO B 264      32.999  23.522  51.652  1.00 18.17       0.127 C
ATOM  13988  N   LEU B 265      36.080  26.980  50.361  1.00 20.58      -0.346 N
ATOM  13989  HN  LEU B 265      35.787  27.691  51.031  1.00  0.00       0.163 HD
ATOM  13990  CA  LEU B 265      37.146  27.272  49.409  1.00 14.03       0.177 C
ATOM  13992  C   LEU B 265      38.415  26.445  49.595  1.00 16.42       0.240 C
ATOM  13993  O   LEU B 265      39.181  26.230  48.627  1.00 17.62      -0.271 OA
ATOM  13994  CB  LEU B 265      37.567  28.731  49.566  1.00 13.78       0.038 C
ATOM  13997  CG  LEU B 265      36.498  29.775  49.188  1.00 22.30      -0.020 C
ATOM  13999  CD1 LEU B 265      37.121  31.148  49.384  1.00 23.72       0.009 C
ATOM  14003  CD2 LEU B 265      35.995  29.612  47.765  1.00 22.13       0.009 C
ATOM  14007  N   GLY B 266      38.702  26.072  50.844  1.00 16.00      -0.351 N
ATOM  14008  HN  GLY B 266      38.063  26.290  51.609  1.00  0.00       0.163 HD
ATOM  14009  CA  GLY B 266      39.973  25.331  51.105  1.00 17.88       0.225 C
ATOM  14012  C   GLY B 266      40.942  26.317  51.784  1.00 15.85       0.236 C
ATOM  14013  O   GLY B 266      40.972  27.475  51.395  1.00 17.48      -0.272 OA
ATOM  14014  N   ASP B 267      41.732  25.854  52.770  1.00 16.86      -0.346 N
ATOM  14015  HN  ASP B 267      41.689  24.866  53.020  1.00  0.00       0.163 HD
ATOM  14016  CA  ASP B 267      42.646  26.730  53.489  1.00 14.10       0.186 C
ATOM  14018  CB  ASP B 267      43.677  27.424  52.587  1.00 17.17       0.241 C
ATOM  14019  O   ASP B 267      44.028  28.604  52.754  1.00 15.49      -0.271 OA
ATOM  14020  CB  ASP B 267      43.424  25.965  54.559  1.00 12.15       0.147 C
ATOM  14023  CG  ASP B 267      42.560  25.512  55.712  1.00 20.24       0.175 C
ATOM  14024  OD2 ASP B 267      41.633  26.231  56.149  1.00 18.43      -0.648 OA
ATOM  14025  OD2 ASP B 267      42.741  24.392  56.208  1.00 14.85      -0.648 OA
ATOM  14026  N   ALA B 268      44.233  26.669  51.644  1.00 15.81      -0.346 N
ATOM  14027  HN  ALA B 268      43.962  25.691  51.544  1.00  0.00       0.163 HD
ATOM  14028  CA  ALA B 268      45.239  27.252  50.749  1.00 17.80       0.172 C
ATOM  14030  C   ALA B 268      44.632  28.356  49.885  1.00 16.82       0.240 C
ATOM  14031  O   ALA B 268      45.217  29.415  49.633  1.00 18.77      -0.271 OA
ATOM  14032  CB  ALA B 268      45.870  26.150  49.911  1.00 16.11       0.042 C
ATOM  14036  N   GLU B 269      43.419  28.125  49.380  1.00 17.83      -0.346 N
ATOM  14037  HN  GLU B 269      42.935  27.246  49.560  1.00  0.00       0.163 HD
ATOM  14038  CA  GLU B 269      42.787  29.197  48.539  1.00 16.86       0.177 C
ATOM  14040  C   GLU B 269      42.409  30.385  49.393  1.00 15.32       0.241 C
ATOM  14041  O   GLU B 269      42.511  31.554  49.007  1.00 15.22      -0.271 OA
ATOM  14042  CB  GLU B 269      41.584  28.573  47.830  1.00 20.73       0.045 C
ATOM  14045  CG  GLU B 269      40.863  29.516  46.895  1.00 21.96       0.116 C
ATOM  14048  CD  GLU B 269      41.690  29.866  45.669  1.00 22.10       0.172 C
ATOM  14051  OE1 GLU B 269      42.664  29.144  45.322  1.00 22.29      -0.648 OA
ATOM  14050  OE2 GLU B 269      41.364  30.877  45.040  1.00 23.18      -0.648 OA
ATOM  14051  N   ILE B 270      42.007  30.159  50.643  1.00 14.90      -0.346 N
ATOM  14052  HN  ILE B 270      41.905  29.199  50.973  1.00  0.00       0.163 HD
ATOM  14053  CA  ILE B 270      41.709  31.270  51.551  1.00 16.61       0.180 C
ATOM  14055  C   ILE B 270      42.947  32.132  51.813  1.00 20.80       0.241 C
ATOM  14056  O   ILE B 270      42.861  33.375  51.861  1.00 14.73      -0.271 OA
ATOM  14057  CB  ILE B 270      41.130  30.742  52.873  1.00 17.72       0.013 C
ATOM  14059  CG1 ILE B 270      39.637  30.380  52.620  1.00 17.90       0.002 C
ATOM  14062  CG2 ILE B 270      41.180  31.864  53.912  1.00 19.62       0.012 C
ATOM  14066  CD1 ILE B 270      39.053  29.569  53.795  1.00 15.65       0.005 C
ATOM  14070  N   ALA B 271      44.116  31.510  51.974  1.00 17.22      -0.346 N
ATOM  14071  HN  ALA B 271      44.146  30.490  51.968  1.00  0.00       0.163 HD
ATOM  14072  CA  ALA B 271      45.364  32.270  52.160  1.00 21.15       0.172 C
ATOM  14074  C   ALA B 271      45.619  33.148  50.936  1.00 19.56       0.240 C
ATOM  14075  O   ALA B 271      45.873  34.337  51.070  1.00 20.41      -0.271 OA
ATOM  14076  CB  ALA B 271      46.530  31.293  52.406  1.00 18.41       0.042 C
ATOM  14080  N   LEU B 272      45.442  32.608  49.724  1.00 16.81      -0.346 N
ATOM  14081  HN  LEU B 272      45.198  31.620  49.647  1.00  0.00       0.163 HD
ATOM  14082  CA  LEU B 272      45.591  33.406  48.507  1.00 14.74       0.177 C
ATOM  14084  C   LEU B 272      44.538  34.503  48.397  1.00 18.37       0.241 C
ATOM  14085  O   LEU B 272      44.845  35.626  47.977  1.00 20.17      -0.271 OA
ATOM  14086  CB  LEU B 272      45.495  32.478  47.292  1.00 24.15       0.038 C
ATOM  14089  CG  LEU B 272      46.593  31.403  47.205  1.00 29.12      -0.020 C
ATOM  14091  CD1 LEU B 272      46.416  30.494  45.997  1.00 24.91       0.009 C
ATOM  14095  CD2 LEU B 272      47.960  32.072  47.167  1.00 30.98       0.009 C
ATOM  14099  N   THR B 273      43.298  34.213  48.781  1.00 12.56      -0.344 N
ATOM  14100  HN  THR B 273      43.087  33.273  49.117  1.00  0.00       0.163 HD
ATOM  14101  CA  THR B 273      42.210  35.230  48.732  1.00 16.91       0.205 C
ATOM  14103  C   THR B 273      42.510  36.385  49.677  1.00 15.65       0.243 C
ATOM  14104  O   THR B 273      42.323  37.561  49.359  1.00 17.05      -0.271 OA
ATOM  14105  CB  THR B 273      40.881  34.566  49.159  1.00 15.18       0.146 C
ATOM  14107  CG2 THR B 273      39.663  35.489  49.188  1.00 16.82       0.042 C
ATOM  14111  OG1 THR B 273      40.623  33.462  48.252  1.00 19.63      -0.393 OA
ATOM  14112  HG1 THR B 273      39.806  33.054  48.514  1.00  0.00       0.210 HD
ATOM  14113  N   ARG B 274      42.983  36.080  50.906  1.00 17.57      -0.346 N
ATOM  14114  HN  ARG B 274      43.081  35.103  51.183  1.00  0.00       0.163 HD
ATOM  14115  CA  ARG B 274      43.354  37.140  51.839  1.00 17.07       0.176 C
ATOM  14117  C   ARG B 274      44.399  38.082  51.232  1.00 20.20       0.241 C
ATOM  14118  O   ARG B 274      44.392  39.300  51.416  1.00 21.43      -0.271 OA
ATOM  14119  CB  ARG B 274      43.976  36.540  53.118  1.00 18.34       0.036 C
ATOM  14122  CG  ARG B 274      42.953  36.273  54.213  1.00 22.15       0.023 C
ATOM  14125  CD  ARG B 274      43.638  35.644  55.472  1.00 19.78       0.138 C
ATOM  14128  NE  ARG B 274      42.741  35.927  56.598  1.00 21.67      -0.227 N
ATOM  14129  HE  ARG B 274      43.019  36.675  57.233  1.00  0.00       0.177 HD
ATOM  14131  CZ  ARG B 274      41.601  35.301  56.869  1.00 25.71       0.665 C
ATOM  14131  NH1 ARG B 274      41.207  34.259  56.140  1.00 20.68      -0.235 N
ATOM  14132 1HH1 ARG B 274      41.769  33.938  55.352  1.00  0.00       0.174 HD
ATOM  14133 2HH1 ARG B 274      40.332  33.778  56.348  1.00  0.00       0.174 HD
ATOM  14134  NH2 ARG B 274      40.870  35.718  57.894  1.00 18.75      -0.235 N
ATOM  14135 1HH2 ARG B 274      41.172  36.516  58.453  1.00  0.00       0.174 HD
ATOM  14136 2HH2 ARG B 274      39.995  35.237  58.102  1.00  0.00       0.174 HD
ATOM  14137  N   GLU B 275      45.379  37.501  50.545  1.00 22.19      -0.346 N
ATOM  14138  HN  GLU B 275      45.395  36.485  50.458  1.00  0.00       0.163 HD
ATOM  14139  CA  GLU B 275      46.432  38.291  49.913  1.00 24.25       0.177 C
ATOM  14141  C   GLU B 275      45.904  39.105  48.747  1.00 25.49       0.241 C
ATOM  14142  O   GLU B 275      46.362  40.222  48.529  1.00 22.58      -0.271 OA
ATOM  14143  CB  GLU B 275      47.498  37.337  49.363  1.00 29.82       0.045 C
ATOM  14146  CG  GLU B 275      48.487  36.877  50.427  1.00 52.50       0.116 C
ATOM  14149  CD  GLU B 275      49.535  36.001  49.748  1.00 59.47       0.172 C
ATOM  14150  OE1 GLU B 275      50.064  36.408  48.689  1.00 62.51      -0.648 OA
ATOM  14151  OE2 GLU B 275      49.781  34.908  50.293  1.00 72.94      -0.648 OA
ATOM  14152  N   GLN B 276      45.002  38.514  47.954  1.00 22.09      -0.346 N
ATOM  14153  HN  GLN B 276      44.703  37.555  48.133  1.00  0.00       0.163 HD
ATOM  14154  CA  GLN B 276      44.451  39.267  46.824  1.00 25.06       0.177 C
ATOM  14156  C   GLN B 276      43.583  40.400  47.336  1.00 26.29       0.241 C
ATOM  14157  O   GLN B 276      43.558  41.512  46.789  1.00 25.90      -0.271 OA
ATOM  14158  CB  GLN B 276      43.637  38.277  45.989  1.00 25.88       0.044 C
ATOM  14161  CG  GLN B 276      42.848  39.011  44.905  1.00 40.78       0.105 C
ATOM  14164  CD  GLN B 276      42.801  38.174  43.638  1.00 49.25       0.215 C
ATOM  14165  OE1 GLN B 276      41.596  38.108  43.087  1.00 49.30      -0.346 N
ATOM  14166 1HE2 GLN B 276      41.564  37.546  42.236  1.00  0.00       0.159 HD
ATOM  14167 2HE2 GLN B 276      40.758  38.565  43.446  1.00  0.00       0.159 HD
ATOM  14168  OE1 GLN B 276      43.813  37.622  43.205  1.00 56.34      -0.274 OA
ATOM  14169  N   LEU B 277      42.790  40.168  48.399  1.00 23.17      -0.346 N
ATOM  14170  HN  LEU B 277      42.771  39.241  48.824  1.00  0.00       0.163 HD
ATOM  14171  CA  LEU B 277      41.964  41.224  48.944  1.00 21.35       0.177 C
ATOM  14173  C   LEU B 277      42.787  42.223  49.749  1.00 25.08       0.240 C
ATOM  14174  O   LEU B 277      42.208  43.247  50.082  1.00 27.29      -0.271 OA
ATOM  14175  CB  LEU B 277      40.871  40.718  49.921  1.00 18.62       0.038 C
ATOM  14178  CG  LEU B 277      39.802  39.868  49.177  1.00 22.08      -0.020 C
ATOM  14180  CD1 LEU B 277      38.883  39.236  50.216  1.00 22.62       0.009 C
ATOM  14184  CD2 LEU B 277      39.076  40.692  48.134  1.00 24.05       0.009 C
ATOM  14188  N   GLY B 278      43.987  41.847  50.192  1.00 23.07      -0.351 N
ATOM  14189  HN  GLY B 278      44.392  40.957  49.902  1.00  0.00       0.163 HD
ATOM  14190  CA  GLY B 278      44.713  42.736  51.103  1.00 21.88       0.225 C
ATOM  14193  C   GLY B 278      44.087  42.623  52.492  1.00 24.33       0.236 C
ATOM  14194  O   GLY B 278      44.207  43.598  53.234  1.00 26.46      -0.272 OA
ATOM  14195  N   TRP B 279      43.506  41.488  52.881  1.00 21.18      -0.346 N
ATOM  14196  HN  TRP B 279      43.488  40.687  52.249  1.00  0.00       0.163 HD
ATOM  14197  CA  TRP B 279      42.893  41.380  54.206  1.00 22.54       0.181 C
ATOM  14199  C   TRP B 279      43.918  40.753  55.137  1.00 28.09       0.241 C
ATOM  14200  O   TRP B 279      44.253  39.584  54.941  1.00 22.57      -0.271 OA
ATOM  14201  CB  TRP B 279      41.618  40.534  54.180  1.00 23.70       0.075 C
ATOM  14204  CG  TRP B 279      40.932  40.482  55.520  1.00 19.46      -0.028 A
ATOM  14205  CD1 TRP B 279      40.992  39.449  56.401  1.00 13.51       0.096 A
ATOM  14207  CD2 TRP B 279      40.108  41.483  56.136  1.00 15.40      -0.002 A
ATOM  14208  CE2 TRP B 279      39.685  40.975  57.371  1.00 19.76       0.042 A
ATOM  14209  CE3 TRP B 279      39.657  42.734  55.736  1.00 20.87       0.014 A
ATOM  14211  NE1 TRP B 279      40.242  41.342  57.530  1.00 18.49      -0.365 N
ATOM  14212  HE1 TRP B 279      40.160  39.141  58.348  1.00  0.00       0.165 HD
ATOM  14213  CZ2 TRP B 279      38.853  41.681  58.248  1.00 19.64       0.030 A
ATOM  14215  CZ3 TRP B 279      38.821  43.440  56.582  1.00 18.98       0.001 A
ATOM  14217  CH2 TRP B 279      38.425  42.918  57.813  1.00 20.42       0.002 A
ATOM  14219  N   LYS B 280      44.437  41.525  56.091  1.00 28.58      -0.346 N
ATOM  14220  HN  LYS B 280      44.075  42.466  56.243  1.00  0.00       0.163 HD
ATOM  14221  CA  LYS B 280      45.526  41.016  56.916  1.00 34.58       0.176 C
ATOM  14223  C   LYS B 280      45.207  40.337  58.222  1.00 34.82       0.241 C
ATOM  14224  O   LYS B 280      46.133  39.795  58.850  1.00 36.45      -0.271 OA
ATOM  14225  CB  LYS B 280      46.459  42.229  57.202  1.00 50.66       0.035 C
ATOM  14228  CG  LYS B 280      47.139  42.699  55.921  1.00 65.25       0.004 C
ATOM  14231  CD  LYS B 280      47.803  41.569  55.154  1.00 76.19       0.027 C
ATOM  14234  CE  LYS B 280      47.343  41.421  53.723  1.00 78.13       0.229 C
ATOM  14237  NZ  LYS B 280      47.205  40.015  53.259  1.00 74.37      -0.079 N
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ATOM  14238  HZ1 LYS B 280      46.894  39.915  52.293  1.00  0.00      0.274 HD
ATOM  14239  HZ2 LYS B 280      46.590  39.494  53.885  1.00  0.00      0.274 HD
ATOM  14240  HZ3 LYS B 280      48.077  39.506  53.405  1.00  0.00      0.274 HD
ATOM  14241  N   TYR B 281      43.954  40.279  58.628  1.00 25.25     -0.346 N
ATOM  14242  HN  TYR B 281      43.228  40.643  58.011  1.00  0.00      0.163 HD
ATOM  14243  CA  TYR B 281      43.554  39.724  59.908  1.00 21.51      0.180 C
ATOM  14245  C   TYR B 281      43.271  38.236  59.914  1.00 24.46      0.241 C
ATOM  14246  O   TYR B 281      42.797  37.678  58.930  1.00 23.16     -0.271 OA
ATOM  14247  CB  TYR B 281      42.310  40.510  60.406  1.00 23.59      0.073 C
ATOM  14250  CG  TYR B 281      42.694  41.989  60.375  1.00 27.28     -0.056 A
ATOM  14251  CD1 TYR B 281      43.527  42.501  61.379  1.00 30.29      0.010 A
ATOM  14253  CD2 TYR B 281      42.280  42.817  59.351  1.00 28.09      0.010 A
ATOM  14255  CE1 TYR B 281      43.901  43.835  61.355  1.00 34.65      0.037 A
ATOM  14257  CE2 TYR B 281      42.646  44.150  59.308  1.00 34.25      0.037 A
ATOM  14259  CZ  TYR B 281      43.460  44.652  60.336  1.00 39.11      0.065 A
ATOM  14260  OH  TYR B 281      43.834  45.979  60.303  1.00 41.08     -0.361 OA
ATOM  14261  HH  TYR B 281      44.392  46.323  60.991  1.00  0.00      0.217 HD
ATOM  14262  N   ALA B 282      43.609  37.606  61.031  1.00 18.17     -0.346 N
ATOM  14263  HN  ALA B 282      44.002  38.153  61.797  1.00  0.00      0.163 HD
ATOM  14264  CA  ALA B 282      43.446  36.168  61.216  1.00 23.31      0.172 C
ATOM  14266  C   ALA B 282      41.958  35.828  61.259  1.00 19.80      0.243 C
ATOM  14267  O   ALA B 282      41.106  36.717  61.397  1.00 19.24     -0.271 OA
ATOM  14268  CB  ALA B 282      44.104  35.805  62.547  1.00 19.71      0.042 C
ATOM  14272  N   PRO B 283      41.630  34.546  61.173  1.00 26.35     -0.337 N
ATOM  14273  CA  PRO B 283      40.227  34.135  61.173  1.00 21.92      0.179 C
ATOM  14275  C   PRO B 283      39.482  34.658  62.368  1.00 21.87      0.241 C
ATOM  14276  O   PRO B 283      39.923  34.488  63.514  1.00 16.48     -0.271 OA
ATOM  14277  CB  PRO B 283      40.303  32.600  61.182  1.00 23.75      0.037 C
ATOM  14280  CG  PRO B 283      41.595  32.311  60.475  1.00 26.99      0.022 C
ATOM  14283  CD  PRO B 283      42.540  33.398  60.973  1.00 24.58      0.127 C
ATOM  14286  N   PHE B 284      38.273  35.223  62.188  1.00 15.97     -0.346 N
ATOM  14287  HN  PHE B 284      37.944  35.342  61.230  1.00  0.00      0.163 HD
ATOM  14288  CA  PHE B 284      37.411  35.671  63.251  1.00 21.26      0.180 C
ATOM  14290  C   PHE B 284      37.997  36.829  64.051  1.00 21.02      0.241 C
ATOM  14291  O   PHE B 284      37.578  37.025  65.187  1.00 24.72     -0.271 OA
ATOM  14292  CB  PHE B 284      36.963  34.562  64.238  1.00 18.32      0.073 C
ATOM  14295  CG  PHE B 284      36.371  33.392  63.448  1.00 19.44     -0.056 A
ATOM  14296  CD1 PHE B 284      35.172  33.507  62.801  1.00 21.71      0.007 A
ATOM  14298  CD2 PHE B 284      37.089  32.213  63.323  1.00 22.37      0.007 A
ATOM  14300  CE1 PHE B 284      34.656  32.452  62.046  1.00 17.37      0.001 A
ATOM  14302  CE2 PHE B 284      36.601  31.148  62.571  1.00 24.79      0.001 A
ATOM  14304  CZ  PHE B 284      35.373  31.275  61.935  1.00 22.18      0.000 A
ATOM  14306  N   GLU B 285      38.920  37.562  63.471  1.00 23.35     -0.346 N
ATOM  14307  HN  GLU B 285      39.230  37.305  62.534  1.00  0.00      0.163 HD
ATOM  14308  CA  GLU B 285      39.517  38.721  64.107  1.00 21.20      0.177 C
ATOM  14310  C   GLU B 285      39.096  39.985  63.366  1.00 17.81      0.241 C
ATOM  14311  O   GLU B 285      39.356  40.083  62.160  1.00 20.12     -0.271 OA
ATOM  14312  CB  GLU B 285      41.047  38.595  64.074  1.00 25.33      0.045 C
ATOM  14315  CG  GLU B 285      41.487  37.750  65.268  1.00 48.80      0.116 C
ATOM  14318  CD  GLU B 285      42.944  37.983  65.625  1.00 59.84      0.172 C
ATOM  14319  OE1 GLU B 285      43.439  39.109  65.386  1.00 74.19     -0.648 OA
ATOM  14320  OE2 GLU B 285      43.570  37.037  66.141  1.00 64.55     -0.648 OA
ATOM  14321  N   ILE B 286      38.393  40.873  64.056  1.00 16.86     -0.346 N
ATOM  14322  HN  ILE B 286      38.154  40.712  65.034  1.00  0.00      0.163 HD
ATOM  14323  CA  ILE B 286      37.966  42.109  63.356  1.00 18.27      0.180 C
ATOM  14325  C   ILE B 286      38.535  43.260  64.182  1.00 18.51      0.243 C
ATOM  14326  O   ILE B 286      38.255  43.269  65.380  1.00 19.21     -0.271 OA
ATOM  14327  CB  ILE B 286      36.425  42.214  63.349  1.00 16.98      0.013 C
ATOM  14329  CG1 ILE B 286      35.727  41.089  62.573  1.00 14.19      0.002 C
ATOM  14332  CG2 ILE B 286      36.018  43.583  62.803  1.00 17.10      0.012 C
ATOM  14336  CD1 ILE B 286      36.087  41.004  61.096  1.00 19.91      0.005 C
ATOM  14340  N   PRO B 287      39.343  44.133  63.618  1.00 21.84     -0.337 N
ATOM  14341  CA  PRO B 287      39.917  45.215  64.421  1.00 21.50      0.179 C
ATOM  14343  C   PRO B 287      38.869  46.187  64.916  1.00 25.55      0.241 C
ATOM  14344  O   PRO B 287      37.854  46.537  64.279  1.00 17.06     -0.271 OA
ATOM  14345  CB  PRO B 287      40.896  45.891  63.466  1.00 23.29      0.037 C
ATOM  14348  CG  PRO B 287      40.540  45.459  62.096  1.00 26.67      0.022 C
ATOM  14351  CD  PRO B 287      39.727  44.176  62.205  1.00 19.56      0.127 C
ATOM  14354  N   SER B 288      39.158  46.817  66.064  1.00 22.67     -0.344 N
ATOM  14355  HN  SER B 288      40.017  46.566  66.553  1.00  0.00      0.163 HD
ATOM  14356  CA  SER B 288      38.311  47.833  66.641  1.00 24.77      0.200 C
ATOM  14358  C   SER B 288      37.842  48.909  65.684  1.00 20.12      0.243 C
ATOM  14359  O   SER B 288      36.694  49.355  65.711  1.00 21.60     -0.271 OA
ATOM  14360  CB  SER B 288      39.114  48.549  67.767  1.00 30.43      0.199 C
ATOM  14363  OG  SER B 288      38.306  48.354  68.924  1.00 45.06     -0.398 OA
ATOM  14364  HG  SER B 288      38.796  48.791  69.611  1.00  0.00      0.209 HD
ATOM  14365  N   GLU B 289      38.739  49.428  64.870  1.00 23.43     -0.346 N
ATOM  14366  HN  GLU B 289      39.693  49.072  64.928  1.00  0.00      0.163 HD
ATOM  14367  CA  GLU B 289      38.465  50.474  63.892  1.00 27.00      0.177 C
ATOM  14369  C   GLU B 289      37.407  50.096  62.857  1.00 27.38      0.241 C
ATOM  14370  O   GLU B 289      36.670  50.946  62.347  1.00 23.75     -0.271 OA
ATOM  14371  CB  GLU B 289      39.805  50.818  63.247  1.00 37.22      0.045 C
ATOM  14374  CG  GLU B 289      39.798  51.998  62.299  1.00 61.71      0.116 C
ATOM  14377  CD  GLU B 289      41.048  52.046  61.433  1.00 77.54      0.172 C
ATOM  14378  OE1 GLU B 289      41.953  51.202  61.638  1.00 84.94     -0.648 OA
ATOM  14379  OE2 GLU B 289      41.123  52.926  60.543  1.00 81.85     -0.648 OA
ATOM  14380  N   ILE B 290      37.334  48.830  62.476  1.00 23.40     -0.346 N
ATOM  14381  HN  ILE B 290      38.007  48.168  62.862  1.00  0.00      0.163 HD
ATOM  14382  CA  ILE B 290      36.337  48.335  61.531  1.00 20.77      0.180 C
ATOM  14384  C   ILE B 290      34.990  48.213  62.245  1.00 17.24      0.241 C
ATOM  14385  O   ILE B 290      33.987  48.668  61.681  1.00 17.67     -0.271 OA
ATOM  14386  CB  ILE B 290      36.785  46.988  60.931  1.00 19.67      0.013 C
ATOM  14388  CG1 ILE B 290      38.010  47.268  60.069  1.00 23.59      0.002 C
ATOM  14391  CG2 ILE B 290      35.625  46.338  60.170  1.00 17.48      0.012 C
ATOM  14395  CD1AILE B 290      37.789  48.154  58.876  0.50 22.46      0.005 C
ATOM  14399  N   TYR B 291      34.950  47.660  63.445  1.00 14.27     -0.346 N
ATOM  14400  HN  TYR B 291      35.783  47.237  63.853  1.00  0.00      0.163 HD
ATOM  14401  CA  TYR B 291      33.679  47.670  64.175  1.00 18.04      0.180 C
ATOM  14403  C   TYR B 291      33.123  49.076  64.339  1.00 21.91      0.241 C
ATOM  14404  O   TYR B 291      31.907  49.245  64.277  1.00 18.09     -0.271 OA
ATOM  14405  CB  TYR B 291      33.784  47.114  65.598  1.00 16.53      0.073 C
ATOM  14408  CG  TYR B 291      33.788  45.600  65.675  1.00 16.73     -0.056 A
ATOM  14409  CD1 TYR B 291      32.708  44.856  65.212  1.00 14.86      0.010 A
ATOM  14411  CD2 TYR B 291      34.880  44.899  66.164  1.00 16.76      0.010 A
ATOM  14413  CE1 TYR B 291      32.667  43.480  65.299  1.00 14.83      0.037 A
ATOM  14415  CE2 TYR B 291      34.864  43.518  66.253  1.00 18.68      0.037 A
ATOM  14417  CZ  TYR B 291      33.740  42.811  65.854  1.00 19.81      0.065 A
ATOM  14418  OH  TYR B 291      33.750  41.439  65.901  1.00 16.63     -0.361 OA
ATOM  14419  HH  TYR B 291      34.488  40.979  66.283  1.00  0.00      0.217 HD
ATOM  14420  N   ALA B 292      33.958  50.075  64.669  1.00 20.02     -0.346 N
ATOM  14421  HN  ALA B 292      34.952  49.875  64.777  1.00  0.00      0.163 HD
ATOM  14422  CA  ALA B 292      33.486  51.428  64.876  1.00 21.90      0.172 C
ATOM  14424  C   ALA B 292      32.800  52.004  63.650  1.00 17.21      0.240 C
ATOM  14425  O   ALA B 292      31.826  52.746  63.838  1.00 19.11     -0.271 OA
ATOM  14426  CB  ALA B 292      34.614  52.384  65.297  1.00 27.44      0.042 C
ATOM  14430  N   GLN B 293      33.230  51.659  62.440  1.00 15.45     -0.346 N
ATOM  14431  HN  GLN B 293      34.022  51.021  62.360  1.00  0.00      0.163 HD
ATOM  14432  CA  GLN B 293      32.608  52.162  61.233  1.00 15.06      0.177 C
ATOM  14434  C   GLN B 293      31.373  51.334  60.863  1.00 16.71      0.241 C
ATOM  14435  O   GLN B 293      30.506  51.848  60.157  1.00 15.55     -0.271 OA
ATOM  14436  CB  GLN B 293      33.628  52.114  60.084  1.00 11.51      0.044 C
ATOM  14439  CG  GLN B 293      34.758  53.156  60.375  1.00 22.13      0.105 C
ATOM  14442  CD  GLN B 293      35.878  52.964  59.368  1.00 33.80      0.215 C
ATOM  14443  NE2 GLN B 293      36.852  52.117  59.688  1.00 32.26     -0.370 N
ATOM  14444 1HE2 GLN B 293      36.887  51.626  60.591  1.00  0.00      0.159 HD
ATOM  14445 2HE2 GLN B 293      37.604  51.988  59.012  1.00  0.00      0.159 HD
ATOM  14446  OE1 GLN B 293      35.836  53.554  58.294  1.00 31.74     -0.274 OA
ATOM  14447  N   TRP B 294      31.322  50.071  61.275  1.00 14.35     -0.346 N
ATOM  14448  HN  TRP B 294      32.092  49.676  61.814  1.00  0.00      0.163 HD
ATOM  14449  CA  TRP B 294      30.148  49.253  60.948  1.00 15.92      0.181 C
ATOM  14451  C   TRP B 294      29.008  49.375  61.952  1.00 14.27      0.241 C
ATOM  14452  O   TRP B 294      27.798  49.187  61.665  1.00 15.06     -0.271 OA
ATOM  14453  CB  TRP B 294      30.610  47.786  60.902  1.00 11.35      0.075 C
ATOM  14456  CG  TRP B 294      30.917  47.262  59.529  1.00 11.62     -0.028 A
ATOM  14457  CD1 TRP B 294      32.131  46.894  59.041  1.00 14.18      0.096 A
ATOM  14459  CD2 TRP B 294      29.958  46.993  58.493  1.00 12.77     -0.002 A
ATOM  14460  CE2 TRP B 294      30.661  46.510  57.375  1.00 15.67      0.042 A
ATOM  14461  CE3 TRP B 294      28.573  47.166  58.403  1.00 11.71      0.014 A
ATOM  14463  NE1 TRP B 294      31.976  46.453  57.723  1.00 15.40     -0.365 N
ATOM  14464  HE1 TRP B 294      32.732  46.137  57.116  1.00  0.00      0.165 HD
ATOM  14465  CZ2 TRP B 294      30.027  46.137  56.175  1.00 13.73      0.030 A
ATOM  14467  CZ3 TRP B 294      27.932  46.775  57.234  1.00 10.70      0.001 A
ATOM  14469  CH2 TRP B 294      28.652  46.286  56.137  1.00 11.32      0.002 A
ATOM  14471  N   ASP B 295      29.319  49.614  63.239  1.00 14.16     -0.345 N
ATOM  14472  HN  ASP B 295      30.284  49.830  63.491  1.00  0.00      0.163 HD
ATOM  14473  CA  ASP B 295      28.287  49.569  64.294  1.00 12.04      0.186 C
ATOM  14475  C   ASP B 295      27.159  50.543  64.048  1.00 16.52      0.241 C
ATOM  14476  O   ASP B 295      27.402  51.713  63.665  1.00 15.90     -0.271 OA
ATOM  14477  CB  ASP B 295      28.943  49.865  65.672  1.00 18.63      0.147 C
ATOM  14480  CG  ASP B 295      28.011  49.496  66.801  1.00 13.58      0.175 C
ATOM  14481  OD1 ASP B 295      27.969  48.316  67.197  1.00 15.61     -0.648 OA
ATOM  14482  OD2 ASP B 295      27.231  50.360  67.259  1.00 15.32     -0.648 OA
ATOM  14483  N   ALA B 296      25.914  50.123  64.315  1.00 11.33     -0.348 N
ATOM  14484  HN  ALA B 296      25.757  49.185  64.683  1.00  0.00      0.163 HD
ATOM  14485  CA  ALA B 296      24.781  51.019  64.075  1.00 13.55      0.172 C
ATOM  14487  C   ALA B 296      23.956  51.262  65.347  1.00 12.28      0.240 C
ATOM  14488  O   ALA B 296      22.820  51.720  65.252  1.00 16.90     -0.271 OA
ATOM  14489  CB  ALA B 296      23.823  50.374  63.049  1.00 14.37      0.042 C
ATOM  14493  N   LYS B 297      24.545  50.997  66.506  1.00 10.78     -0.346 N
ATOM  14494  HN  LYS B 297      25.523  50.709  66.530  1.00  0.00      0.163 HD
ATOM  14495  CA  LYS B 297      23.781  51.120  67.752  1.00 14.09      0.176 C
ATOM  14497  C   LYS B 297      23.458  52.596  68.005  1.00 14.42      0.241 C
ATOM  14498  O   LYS B 297      22.375  52.870  68.508  1.00 15.66     -0.271 OA
ATOM  14499  CB  LYS B 297      24.533  50.533  68.942  1.00 12.88      0.035 C
ATOM  14502  CG  LYS B 297      24.740  49.013  68.952  1.00 14.75      0.004 C
ATOM  14505  CD  LYS B 297      25.468  48.681  70.289  1.00 18.30      0.027 C
ATOM  14508  CE  LYS B 297      26.168  47.343  70.245  1.00 17.40      0.229 C
ATOM  14511  NZ  LYS B 297      27.532  47.388  69.658  1.00 12.61     -0.079 N
ATOM  14512  HZ1 LYS B 297      28.005  46.484  69.634  1.00  0.00      0.274 HD
ATOM  14513  HZ2 LYS B 297      28.106  48.080  70.140  1.00  0.00      0.274 HD
ATOM  14514  HZ3 LYS B 297      27.507  47.803  68.727  1.00  0.00      0.274 HD
ATOM  14515  N   GLU B 298      24.421  53.482  67.748  1.00 17.14     -0.346 N
ATOM  14516  HN  GLU B 298      25.315  53.200  67.345  1.00  0.00      0.163 HD
ATOM  14517  CA  GLU B 298      24.129  54.884  68.074  1.00 21.00      0.177 C
ATOM  14519  C   GLU B 298      23.085  55.462  67.145  1.00 17.88      0.241 C
ATOM  14520  O   GLU B 298      22.146  56.083  67.629  1.00 19.68     -0.271 OA
ATOM  14521  CB  GLU B 298      25.425  55.708  68.104  1.00 23.70      0.045 C
ATOM  14524  CG  GLU B 298      26.234  55.293  69.360  1.00 40.41      0.116 C
ATOM  14527  CD  GLU B 298      27.515  56.113  69.482  1.00 44.16      0.172 C
ATOM  14528  OE1 GLU B 298      27.428  57.355  69.464  1.00 49.96     -0.648 OA
ATOM  14529  OE2 GLU B 298      28.603  55.509  69.575  1.00 39.02     -0.648 OA
ATOM  14530  N   ALA B 299      23.246  55.296  65.845  1.00 12.90     -0.346 N
ATOM  14531  HN  ALA B 299      24.073  54.802  65.508  1.00  0.00      0.163 HD
ATOM  14532  CA  ALA B 299      22.276  55.798  64.874  1.00 15.35      0.172 C
ATOM  14534  C   ALA B 299      20.927  55.120  65.016  1.00 16.47      0.240 C
ATOM  14535  O   ALA B 299      19.857  55.764  64.924  1.00 17.93     -0.271 OA
ATOM  14536  CB  ALA B 299      22.867  55.566  63.468  1.00 18.33      0.042 C
ATOM  14540  N   GLY B 300      20.956  53.823  65.327  1.00 11.80     -0.351 N
ATOM  14541  HN  GLY B 300      21.856  53.361  65.453  1.00  0.00      0.163 HD
ATOM  14542  CA  GLY B 300      19.717  53.043  65.492  1.00 11.77      0.225 C
ATOM  14545  C   GLY B 300      18.869  53.582  66.633  1.00 16.46      0.236 C
ATOM  14546  O   GLY B 300      17.651  53.757  66.545  1.00 15.14     -0.272 OA
ATOM  14547  N   GLN B 301      19.547  53.882  67.749  1.00 14.26     -0.346 N
ATOM  14548  HN  GLN B 301      20.558  53.755  67.794  1.00  0.00      0.163 HD
ATOM  14549  CA  GLN B 301      18.801  54.399  68.911  1.00 14.61      0.177 C
ATOM  14551  C   GLN B 301      18.274  55.794  68.600  1.00 12.22      0.241 C
ATOM  14552  O   GLN B 301      17.139  56.127  68.981  1.00 17.60     -0.271 OA
ATOM  14553  CB  GLN B 301      19.698  54.387  70.156  1.00 16.88      0.042 C
ATOM  14556  CG  GLN B 301      19.116  55.190  71.335  1.00 24.60      0.105 C
ATOM  14559  CD  GLN B 301      20.016  55.115  72.564  1.00 34.98      0.215 C
ATOM  14560  NE2 GLN B 301      19.738  54.232  73.522  1.00 34.18     -0.370 N
ATOM  14561 1HE2 GLN B 301      20.340  54.182  74.344  1.00  0.00      0.159 HD
ATOM  14562 2HE2 GLN B 301      18.938  53.602  73.467  1.00  0.00      0.159 HD
ATOM  14563  OE1 GLN B 301      20.984  55.877  72.631  1.00 44.89     -0.274 OA
ATOM  14564  N   ALA B 302      19.059  56.625  67.913  1.00 15.63     -0.346 N
ATOM  14565  HN  ALA B 302      19.997  56.336  67.634  1.00  0.00      0.163 HD
ATOM  14566  CA  ALA B 302      18.561  57.952  67.565  1.00 17.58      0.172 C
ATOM  14568  C   ALA B 302      17.322  57.877  66.663  1.00 20.59      0.240 C
ATOM  14569  O   ALA B 302      16.364  58.641  66.864  1.00 16.99     -0.271 OA
ATOM  14570  CB  ALA B 302      19.642  58.803  66.898  1.00 20.10      0.042 C
ATOM  14574  N   LYS B 303      17.333  57.042  65.628  1.00 14.06     -0.346 N
ATOM  14575  HN  LYS B 303      18.152  56.456  65.463  1.00  0.00      0.163 HD
ATOM  14576  CA  LYS B 303      16.196  56.952  64.729  1.00 14.76      0.176 C
ATOM  14578  C   LYS B 303      14.985  56.406  65.440  1.00 11.32      0.241 C
ATOM  14579  O   LYS B 303      13.877  56.870  65.177  1.00 11.71     -0.271 OA
ATOM  14580  CB  LYS B 303      16.513  56.101  63.482  1.00 14.89      0.035 C
ATOM  14583  CG  LYS B 303      17.672  56.762  62.694  1.00 20.34      0.004 C
ATOM  14586  CD  LYS B 303      18.086  55.822  61.566  1.00 31.43      0.027 C
ATOM  14589  CE  LYS B 303      19.422  56.121  60.906  1.00 35.67      0.229 C
ATOM  14592  NZ  LYS B 303      19.826  55.056  59.930  1.00 36.42     -0.079 N
ATOM  14593  HZ1 LYS B 303      20.723  55.257  59.487  1.00  0.00      0.274 HD
ATOM  14594  HZ2 LYS B 303      19.098  54.900  59.233  1.00  0.00      0.274 HD
ATOM  14595  HZ3 LYS B 303      19.830  54.136  60.370  1.00  0.00      0.274 HD
ATOM  14596  N   GLU B 304      15.084  55.351  66.233  1.00  9.09     -0.346 N
ATOM  14597  HN  GLU B 304      15.991  54.908  66.377  1.00  0.00      0.163 HD
ATOM  14598  CA  GLU B 304      13.902  54.820  66.901  1.00  8.43      0.177 C
ATOM  14600  C   GLU B 304      13.404  55.819  67.949  1.00 12.36      0.241 C
ATOM  14601  O   GLU B 304      12.196  55.984  68.165  1.00  9.98     -0.271 OA
ATOM  14602  CB  GLU B 304      14.254  53.485  67.621  1.00  8.55      0.045 C
ATOM  14605  CG  GLU B 304      13.000  52.874  68.208  1.00 11.94      0.116 C
ATOM  14608  CD  GLU B 304      13.212  51.524  68.875  1.00 18.74      0.172 C
ATOM  14609  OE1 GLU B 304      14.270  50.901  68.714  1.00 27.02     -0.648 OA
ATOM  14610  OE2 GLU B 304      12.259  51.084  69.514  1.00 16.61     -0.648 OA
ATOM  14611  N   SER B 305      14.328  56.505  68.642  1.00 14.52     -0.344 N
ATOM  14612  HN  SER B 305      15.317  56.308  68.488  1.00  0.00      0.163 HD
ATOM  14613  CA  SER B 305      13.943  57.532  69.615  1.00 14.34      0.200 C
ATOM  14615  C   SER B 305      13.073  58.617  69.015  1.00 13.77      0.243 C
ATOM  14616  O   SER B 305      12.068  59.052  69.594  1.00 14.36     -0.271 OA
ATOM  14617  CB  SER B 305      15.193  58.268  70.219  1.00 15.70      0.199 C
ATOM  14620  OG  SER B 305      15.539  57.487  71.349  1.00 39.67     -0.398 OA
ATOM  14621  HG  SER B 305      16.295  57.932  71.714  1.00  0.00      0.209 HD
ATOM  14622  N   ALA B 306      13.476  59.079  67.832  1.00 15.97     -0.346 N
ATOM  14623  HN  ALA B 306      14.347  58.720  67.441  1.00  0.00      0.163 HD
ATOM  14624  CA  ALA B 306      12.731  60.073  67.070  1.00 15.66      0.172 C
ATOM  14626  C   ALA B 306      11.366  59.538  66.676  1.00 15.23      0.240 C
ATOM  14627  O   ALA B 306      10.362  60.261  66.772  1.00 17.14     -0.271 OA
ATOM  14628  CB  ALA B 306      13.534  60.467  65.824  1.00 11.76      0.042 C
ATOM  14632  N   TRP B 307      11.262  58.255  66.292  1.00 11.37     -0.346 N
ATOM  14633  HN  TRP B 307      12.099  57.673  66.245  1.00  0.00      0.163 HD
ATOM  14634  CA  TRP B 307       9.959  57.681  65.939  1.00 14.64      0.181 C
ATOM  14636  C   TRP B 307       9.096  57.565  67.176  1.00 13.00      0.241 C
ATOM  14637  O   TRP B 307       7.879  57.783  67.129  1.00 10.31     -0.271 OA
ATOM  14638  CB  TRP B 307      10.120  56.274  65.306  1.00 13.41      0.075 C
ATOM  14641  CG  TRP B 307       8.813  55.710  64.800  1.00 16.06     -0.028 A
ATOM  14642  CD1 TRP B 307       8.200  55.908  63.584  1.00 10.56      0.096 A
ATOM  14644  CD2 TRP B 307       7.998  54.795  65.521  1.00 10.68     -0.002 A
ATOM  14645  CE2 TRP B 307       6.887  54.484  64.714  1.00  9.78      0.042 A
ATOM  14646  CE3 TRP B 307       8.096  54.204  66.800  1.00 13.59      0.014 A
ATOM  14648  NE1 TRP B 307       7.040  55.158  63.556  1.00 11.56     -0.365 N
ATOM  14649  HE1 TRP B 307       6.391  55.120  62.770  1.00  0.00      0.165 HD
ATOM  14650  CZ2 TRP B 307       5.880  53.626  65.172  1.00 14.58      0.030 A
ATOM  14652  CZ3 TRP B 307       7.110  53.345  67.233  1.00 10.27      0.001 A
ATOM  14654  CH2 TRP B 307       5.993  53.064  66.401  1.00 16.51      0.002 A
ATOM  14656  N   ASN B 308       9.683  57.220  68.327  1.00 12.20     -0.346 N
ATOM  14657  HN  ASN B 308      10.684  57.025  68.364  1.00  0.00      0.163 HD
ATOM  14658  CA  ASN B 308       8.862  57.128  69.529  1.00 12.04      0.185 C
ATOM  14660  C   ASN B 308       8.301  58.508  69.893  1.00  8.65      0.241 C
ATOM  14661  O   ASN B 308       7.211  58.556  70.444  1.00 11.22     -0.271 OA
ATOM  14662  CB  ASN B 308       9.635  56.600  70.737  1.00 12.86      0.137 C
ATOM  14665  CG  ASN B 308       9.936  55.116  70.657  1.00 19.41      0.217 C
ATOM  14666  ND2 ASN B 308      10.997  54.747  71.370  1.00 14.43     -0.370 N
ATOM  14667 1HD2 ASN B 308      11.199  53.749  71.316  1.00  0.00      0.159 HD
ATOM  14668 2HD2 ASN B 308      11.546  55.403  71.926  1.00  0.00      0.159 HD
ATOM  14669  OD1 ASN B 308       9.273  54.324  69.986  1.00 14.43     -0.274 OA
ATOM  14670  N   GLU B 309       9.087  59.548  69.668  1.00 12.82     -0.346 N
ATOM  14671  HN  GLU B 309      10.040  59.438  69.321  1.00  0.00      0.163 HD
ATOM  14672  CA  GLU B 309       8.507  60.876  69.948  1.00 16.23      0.177 C
ATOM  14674  C   GLU B 309       7.345  61.171  68.994  1.00 19.38      0.241 C
ATOM  14675  O   GLU B 309       6.339  61.777  69.356  1.00 13.33     -0.271 OA
ATOM  14676  CB  GLU B 309       9.540  61.970  69.769  1.00 17.86      0.045 C
ATOM  14679  CG  GLU B 309      10.668  62.036  70.773  1.00 31.24      0.116 C
ATOM  14682  CD  GLU B 309      11.393  63.381  70.593  1.00 44.03      0.172 C
ATOM  14683  OE1 GLU B 309      12.226  63.485  69.670  1.00 44.11     -0.648 OA
ATOM  14684  OE2 GLU B 309      11.089  64.313  71.364  1.00 49.87     -0.648 OA
ATOM  14685  N   LYS B 310       7.492  60.811  67.716  1.00 13.73     -0.346 N
ATOM  14686  HN  LYS B 310       8.369  60.395  67.403  1.00  0.00      0.163 HD
ATOM  14687  CA  LYS B 310       6.398  61.011  66.764  1.00 12.73      0.176 C
ATOM  14689  C   LYS B 310       5.206  60.147  67.117  1.00 14.88      0.241 C
ATOM  14690  O   LYS B 310       4.073  60.611  67.002  1.00 13.34     -0.271 OA
ATOM  14691  CB  LYS B 310       6.916  60.699  65.343  1.00 15.87      0.035 C
ATOM  14694  CG  LYS B 310       5.831  60.385  64.344  1.00 32.23      0.004 C
ATOM  14697  CD  LYS B 310       6.176  60.719  62.911  1.00 42.86      0.027 C
ATOM  14700  CE  LYS B 310       7.601  60.408  62.497  1.00 49.33      0.229 C
ATOM  14703  NZ  LYS B 310       7.666  60.367  61.004  1.00 56.01     -0.079 N
ATOM  14704  HZ1 LYS B 310       8.625  60.158  60.725  1.00  0.00      0.274 HD
ATOM  14705  HZ2 LYS B 310       7.312  61.221  60.574  1.00  0.00      0.274 HD
ATOM  14706  HZ3 LYS B 310       6.991  59.717  60.601  1.00  0.00      0.274 HD
ATOM  14707  N   PHE B 311       5.392  58.901  67.576  1.00  9.12     -0.346 N
ATOM  14708  HN  PHE B 311       6.335  58.528  67.681  1.00  0.00      0.163 HD
ATOM  14709  CA  PHE B 311       4.230  58.079  67.926  1.00 11.38      0.180 C
ATOM  14711  C   PHE B 311       3.523  58.649  69.143  1.00 13.93      0.241 C
ATOM  14712  O   PHE B 311       2.302  58.558  69.316  1.00 10.51     -0.271 OA
ATOM  14713  CB  PHE B 311       4.700  56.622  68.228  1.00 12.71      0.073 C
ATOM  14716  CG  PHE B 311       3.524  55.688  68.454  1.00 18.31     -0.056 A
ATOM  14718  CD1 PHE B 311       2.815  55.190  67.366  1.00 15.23      0.007 A
ATOM  14719  CD2 PHE B 311       3.128  55.337  69.727  1.00 21.11      0.007 A
ATOM  14721  CE1 PHE B 311       1.724  54.350  67.590  1.00 16.89      0.001 A
ATOM  14723  CE2 PHE B 311       2.040  54.507  69.957  1.00 19.82      0.001 A
ATOM  14725  CZ  PHE B 311       1.345  54.003  68.864  1.00 17.84      0.000 A
ATOM  14727  N   ALA B 312       4.305  59.208  70.087  1.00 12.34     -0.346 N
ATOM  14728  HN  ALA B 312       5.319  59.229  69.979  1.00  0.00      0.163 HD
ATOM  14729  CA  ALA B 312       3.663  59.786  71.275  1.00 13.32      0.172 C
ATOM  14731  C   ALA B 312       2.793  60.988  70.896  1.00 11.59      0.240 C
ATOM  14732  O   ALA B 312       1.777  61.161  71.539  1.00 11.76     -0.271 OA
ATOM  14733  CB  ALA B 312       4.712  60.205  72.308  1.00 19.19      0.042 C
ATOM  14737  N   ALA B 313       3.171  61.815  69.933  1.00 11.83     -0.346 N
ATOM  14738  HN  ALA B 313       4.083  61.661  69.502  1.00  0.00      0.163 HD
ATOM  14739  CA  ALA B 313       2.366  62.932  69.449  1.00 13.21      0.172 C
ATOM  14741  C   ALA B 313       1.111  62.422  68.740  1.00 14.65      0.240 C
ATOM  14742  O   ALA B 313      -0.023  62.871  68.950  1.00 13.68     -0.271 OA
ATOM  14743  CB  ALA B 313       3.163  63.816  68.463  1.00 12.68      0.042 C
ATOM  14747  N   TYR B 314       1.249  61.315  67.995  1.00 13.70     -0.346 N
ATOM  14748  HN  TYR B 314       2.172  60.886  67.921  1.00  0.00      0.163 HD
ATOM  14749  CA  TYR B 314       0.134  60.701  67.288  1.00 12.38      0.180 C
ATOM  14751  C   TYR B 314      -0.877  60.194  68.308  1.00 13.60      0.241 C
ATOM  14752  O   TYR B 314      -2.090  60.356  68.148  1.00 13.64     -0.271 OA
ATOM  14753  CB  TYR B 314       0.654  59.504  66.455  1.00 12.22      0.073 C
ATOM  14756  CG  TYR B 314      -0.365  58.678  65.696  1.00 14.42     -0.056 A
ATOM  14758  CD1 TYR B 314      -1.043  57.603  66.229  1.00 16.99      0.010 A
ATOM  14759  CD2 TYR B 314      -0.630  58.978  64.367  1.00 13.48      0.010 A
ATOM  14761  CE1 TYR B 314      -1.996  56.901  65.525  1.00 12.49      0.037 A
ATOM  14763  CE2 TYR B 314      -1.556  58.294  63.620  1.00 10.36      0.037 A
ATOM  14765  CZ  TYR B 314      -2.212  57.217  64.197  1.00 13.47      0.065 A
ATOM  14767  OH  TYR B 314      -3.095  56.521  63.418  1.00 15.65     -0.361 OA
ATOM  14767  HH  TYR B 314      -3.544  55.783  63.813  1.00  0.00      0.217 HD
ATOM  14768  N   ALA B 315      -0.409  59.570  69.389  1.00 14.52     -0.346 N
ATOM  14769  HN  ALA B 315       0.598  59.476  69.522  1.00  0.00      0.163 HD
ATOM  14770  CA  ALA B 315      -1.328  59.019  70.387  1.00 13.17      0.172 C
ATOM  14772  C   ALA B 315      -2.056  60.121  71.160  1.00 14.49      0.240 C
ATOM  14773  O   ALA B 315      -3.113  59.862  71.723  1.00 13.74     -0.271 OA
ATOM  14774  CB  ALA B 315      -0.550  58.136  71.366  1.00 11.50      0.042 C
ATOM  14778  N   LYS B 316      -1.494  61.310  71.238  1.00 13.15     -0.346 N
ATOM  14779  HN  LYS B 316      -0.579  61.468  70.816  1.00  0.00      0.163 HD
ATOM  14780  CA  LYS B 316      -2.188  62.421  71.938  1.00 14.66      0.176 C
ATOM  14782  C   LYS B 316      -3.315  62.968  71.075  1.00 15.62      0.241 C
ATOM  14783  O   LYS B 316      -4.391  63.258  71.594  1.00 16.75     -0.271 OA
ATOM  14784  CB  LYS B 316      -1.128  63.483  72.237  1.00 20.73      0.035 C
ATOM  14787  CG  LYS B 316      -1.521  64.708  73.022  1.00 35.17      0.004 C
ATOM  14790  CD  LYS B 316      -0.302  65.638  73.067  1.00 42.59      0.027 C
ATOM  14793  CE  LYS B 316      -0.136  66.333  74.396  1.00 55.79      0.229 C
ATOM  14796  NZ  LYS B 316       0.296  65.401  75.474  1.00 55.41     -0.079 N
ATOM  14797  HZ1 LYS B 316       0.408  65.871  76.372  1.00  0.00      0.274 HD
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ATOM  14798  HZ2 LYS B 316       1.146  64.903  75.211  1.00  0.00     0.274 HD
ATOM  14799  HZ3 LYS B 316      -0.340  64.608  75.551  1.00  0.00     0.274 HD
ATOM  14800  N   ALA B 317      -3.172  63.036  69.754  1.00 12.02    -0.346 N
ATOM  14801  HN  ALA B 317      -2.279  62.774  69.336  1.00  0.00     0.163 HD
ATOM  14802  CA  ALA B 317      -4.269  63.480  68.883  1.00 11.61     0.172 C
ATOM  14804  C   ALA B 317      -5.211  62.376  68.483  1.00 13.28     0.240 C
ATOM  14805  O   ALA B 317      -6.411  62.567  68.304  1.00 13.32    -0.271 OA
ATOM  14806  CB  ALA B 317      -3.610  64.070  67.627  1.00 12.47     0.042 C
ATOM  14810  N   TYR B 318      -4.746  61.126  68.351  1.00  7.56    -0.346 N
ATOM  14811  HN  TYR B 318      -3.774  60.948  68.603  1.00  0.00     0.163 HD
ATOM  14812  CA  TYR B 318      -5.556  59.990  67.862  1.00  8.29     0.181 C
ATOM  14814  C   TYR B 318      -5.450  58.809  68.788  1.00 13.42     0.243 C
ATOM  14815  O   TYR B 318      -4.825  57.780  68.421  1.00 14.01    -0.271 OA
ATOM  14816  CB  TYR B 318      -4.894  59.583  66.479  1.00  9.02     0.073 C
ATOM  14819  CG  TYR B 318      -4.894  60.742  65.483  1.00 15.44    -0.056 A
ATOM  14820  CD1 TYR B 318      -6.047  61.239  64.891  1.00 20.17     0.010 A
ATOM  14822  CD2 TYR B 318      -3.698  61.342  65.143  1.00 21.27     0.010 A
ATOM  14824  CE1 TYR B 318      -6.003  62.323  63.990  1.00 17.15     0.037 A
ATOM  14826  CE2 TYR B 318      -3.643  62.406  64.234  1.00 17.68     0.037 A
ATOM  14828  CZ  TYR B 318      -4.809  62.894  63.694  1.00 17.86     0.065 A
ATOM  14829  OH  TYR B 318      -4.689  63.981  62.812  1.00 20.35    -0.361 OA
ATOM  14830  HH  TYR B 318      -5.495  64.318  62.439  1.00  0.00     0.217 HD
ATOM  14831  N   PRO B 319      -5.882  58.903  70.037  1.00 15.58    -0.337 N
ATOM  14832  CA  PRO B 319      -5.699  57.846  71.017  1.00 16.12     0.179 C
ATOM  14834  C   PRO B 319      -6.282  56.496  70.645  1.00 16.79     0.241 C
ATOM  14835  O   PRO B 319      -5.646  55.472  70.952  1.00 15.00    -0.271 OA
ATOM  14836  CB  PRO B 319      -6.322  58.367  72.328  1.00 18.55     0.037 C
ATOM  14839  CG  PRO B 319      -7.081  59.609  71.948  1.00 19.63     0.022 C
ATOM  14842  CD  PRO B 319      -6.608  60.070  70.596  1.00 17.77     0.127 C
ATOM  14845  N   GLN B 320      -7.453  56.479  69.995  1.00 15.72    -0.346 N
ATOM  14846  HN  GLN B 320      -7.924  57.348  69.743  1.00  0.00     0.163 HD
ATOM  14847  CA  GLN B 320      -8.042  55.176  69.654  1.00 16.85     0.177 C
ATOM  14849  C   GLN B 320      -7.224  54.461  68.555  1.00 18.34     0.241 C
ATOM  14850  O   GLN B 320      -7.010  53.247  68.633  1.00 15.57    -0.271 OA
ATOM  14851  CB  GLN B 320      -9.477  55.325  69.203  1.00 22.32     0.044 C
ATOM  14854  CG  GLN B 320     -10.506  55.992  70.070  1.00 54.74     0.105 C
ATOM  14857  CD  GLN B 320     -10.345  55.737  71.557  1.00 73.74     0.215 C
ATOM  14858  NE2 GLN B 320     -10.471  56.788  72.369  1.00 77.59    -0.370 N
ATOM  14859 1HE2 GLN B 320     -10.363  56.617  73.369  1.00  0.00     0.159 HD
ATOM  14860 2HE2 GLN B 320     -10.670  57.726  72.021  1.00  0.00     0.159 HD
ATOM  14861  OE1 GLN B 320     -10.104  54.601  71.978  1.00 83.41    -0.274 OA
ATOM  14862  N   GLU B 321      -6.783  55.225  67.563  1.00 12.91    -0.346 N
ATOM  14863  HN  GLU B 321      -7.044  56.211  67.553  1.00  0.00     0.163 HD
ATOM  14864  CA  GLU B 321      -5.941  54.716  66.486  1.00 11.77     0.177 C
ATOM  14866  C   GLU B 321      -4.629  54.230  67.046  1.00 13.44     0.241 C
ATOM  14867  O   GLU B 321      -4.157  53.156  66.652  1.00 11.85    -0.271 OA
ATOM  14868  CB  GLU B 321      -5.718  55.813  65.398  1.00 13.76     0.045 C
ATOM  14871  CG  GLU B 321      -7.036  56.055  64.654  1.00 22.52     0.116 C
ATOM  14874  CD  GLU B 321      -7.922  57.128  65.233  1.00 27.01     0.172 C
ATOM  14875  OE1 GLU B 321      -7.799  57.565  66.404  1.00 23.95    -0.648 OA
ATOM  14876  OE2 GLU B 321      -8.814  57.588  64.491  1.00 49.48    -0.648 OA
ATOM  14877  N   ALA B 322      -3.970  54.955  67.949  1.00 10.12    -0.346 N
ATOM  14878  HN  ALA B 322      -4.356  55.854  68.235  1.00  0.00     0.163 HD
ATOM  14879  CA  ALA B 322      -2.724  54.510  68.538  1.00 12.69     0.172 C
ATOM  14881  C   ALA B 322      -2.886  53.163  69.269  1.00 15.45     0.240 C
ATOM  14882  O   ALA B 322      -1.999  52.302  69.159  1.00 13.25    -0.271 OA
ATOM  14883  CB  ALA B 322      -2.140  55.537  69.507  1.00 13.92     0.042 C
ATOM  14887  N   ALA B 323      -3.966  53.000  70.011  1.00 14.53    -0.346 N
ATOM  14888  HN  ALA B 323      -4.654  53.750  70.082  1.00  0.00     0.163 HD
ATOM  14889  CA  ALA B 323      -4.179  51.727  70.741  1.00 14.94     0.172 C
ATOM  14891  C   ALA B 323      -4.435  50.588  69.754  1.00 13.40     0.240 C
ATOM  14892  O   ALA B 323      -3.970  49.465  69.989  1.00 13.47    -0.271 OA
ATOM  14893  CB  ALA B 323      -5.349  51.835  71.725  1.00 14.37     0.042 C
ATOM  14897  N   GLU B 324      -5.141  50.841  68.646  1.00 10.58    -0.346 N
ATOM  14898  HN  GLU B 324      -5.532  51.771  68.497  1.00  0.00     0.163 HD
ATOM  14899  CA  GLU B 324      -5.356  49.793  67.646  1.00 12.25     0.177 C
ATOM  14901  C   GLU B 324      -4.048  49.453  66.961  1.00 15.51     0.241 C
ATOM  14902  O   GLU B 324      -3.805  48.303  66.639  1.00 12.82    -0.271 OA
ATOM  14903  CB  GLU B 324      -6.429  50.201  66.631  1.00 13.08     0.045 C
ATOM  14906  CG  GLU B 324      -7.826  49.981  67.229  1.00 19.10     0.116 C
ATOM  14909  CD  GLU B 324      -8.083  48.477  67.259  1.00 18.23     0.172 C
ATOM  14910  OE1 GLU B 324      -8.195  47.953  66.120  1.00 18.17    -0.648 OA
ATOM  14911  OE2 GLU B 324      -8.071  47.882  68.359  1.00 20.35    -0.648 OA
ATOM  14912  N   PHE B 325      -3.222  50.470  66.635  1.00  9.97    -0.346 N
ATOM  14913  HN  PHE B 325      -3.489  51.433  66.838  1.00  0.00     0.163 HD
ATOM  14914  CA  PHE B 325      -1.947  50.184  65.992  1.00 12.43     0.180 C
ATOM  14916  C   PHE B 325      -1.125  49.246  66.859  1.00 14.58     0.241 C
ATOM  14917  O   PHE B 325      -0.573  48.266  66.360  1.00 11.24    -0.271 OA
ATOM  14918  CB  PHE B 325      -1.175  51.492  65.764  1.00 13.77     0.073 C
ATOM  14921  CG  PHE B 325       0.164  51.332  65.103  1.00 15.66    -0.056 A
ATOM  14922  CD1 PHE B 325       0.258  51.275  63.731  1.00 13.78     0.007 A
ATOM  14924  CD2 PHE B 325       1.316  51.269  65.874  1.00 15.59     0.007 A
ATOM  14926  CE1 PHE B 325       1.516  51.156  63.121  1.00 13.96     0.001 A
ATOM  14928  CE2 PHE B 325       2.560  51.139  65.282  1.00 15.13     0.001 A
ATOM  14930  CZ  PHE B 325       2.654  51.097  63.907  1.00 12.39     0.000 A
ATOM  14932  N   THR B 326      -0.996  49.592  68.143  1.00 12.00    -0.344 N
ATOM  14933  HN  THR B 326      -1.442  50.434  68.506  1.00  0.00     0.163 HD
ATOM  14934  CA  THR B 326      -0.181  48.713  69.033  1.00 14.15     0.205 C
ATOM  14936  C   THR B 326      -0.792  47.334  69.187  1.00 14.38     0.243 C
ATOM  14937  O   THR B 326      -0.063  46.310  69.128  1.00 16.09    -0.271 OA
ATOM  14938  CB  THR B 326      -0.206  49.487  70.399  1.00 18.96     0.146 C
ATOM  14940  CG2 THR B 326       0.314  48.651  71.530  1.00 29.33     0.042 C
ATOM  14944  OG1 THR B 326       0.631  50.654  70.179  1.00 28.45    -0.393 OA
ATOM  14945  HG1 THR B 326       0.616  51.122  71.005  1.00  0.00     0.210 HD
ATOM  14946  N   ARG B 327      -2.110  47.227  69.306  1.00 11.34    -0.346 N
ATOM  14947  HN  ARG B 327      -2.703  48.057  69.295  1.00  0.00     0.163 HD
ATOM  14948  CA  ARG B 327      -2.707  45.865  69.456  1.00 11.23     0.176 C
ATOM  14950  C   ARG B 327      -2.448  45.016  68.215  1.00 13.27     0.241 C
ATOM  14951  O   ARG B 327      -2.082  43.816  68.290  1.00 12.48    -0.271 OA
ATOM  14952  CB  ARG B 327      -4.213  46.031  69.685  1.00 10.67     0.036 C
ATOM  14955  CG  ARG B 327      -5.012  44.725  69.866  1.00 12.02     0.023 C
ATOM  14958  CD  ARG B 327      -6.489  44.998  69.713  1.00 14.44     0.138 C
ATOM  14961  NE  ARG B 327      -7.043  45.377  68.407  1.00 12.85    -0.227 N
ATOM  14962  HE  ARG B 327      -7.302  46.357  68.289  1.00  0.00     0.177 HD
ATOM  14963  CZ  ARG B 327      -7.243  44.584  67.366  1.00 15.66     0.665 C
ATOM  14964  NH1 ARG B 327      -6.878  43.283  67.369  1.00 11.16    -0.235 N
ATOM  14965 1HH1 ARG B 327      -7.032  42.672  66.567  1.00  0.00     0.174 HD
ATOM  14966 2HH1 ARG B 327      -6.451  42.892  68.209  1.00  0.00     0.174 HD
ATOM  14967  NH2 ARG B 327      -7.804  45.098  66.263  1.00 13.44    -0.235 N
ATOM  14968 1HH2 ARG B 327      -7.958  44.487  65.461  1.00  0.00     0.174 HD
ATOM  14969 2HH2 ARG B 327      -8.080  46.080  66.261  1.00  0.00     0.174 HD
ATOM  14970  N   ARG B 328      -2.668  45.645  67.036  1.00 10.62    -0.346 N
ATOM  14971  HN  ARG B 328      -2.970  46.619  67.022  1.00  0.00     0.163 HD
ATOM  14972  CA  ARG B 328      -2.469  44.913  65.777  1.00 13.49     0.176 C
ATOM  14974  C   ARG B 328      -1.025  44.578  65.524  1.00 15.61     0.241 C
ATOM  14975  O   ARG B 328      -0.770  43.479  65.010  1.00 16.30    -0.271 OA
ATOM  14976  CB  ARG B 328      -3.053  45.739  64.589  1.00  9.91     0.036 C
ATOM  14979  CG  ARG B 328      -4.574  45.762  64.680  1.00  7.30     0.023 C
ATOM  14982  CD  ARG B 328      -5.312  46.617  63.666  1.00 10.42     0.138 C
ATOM  14985  NE  ARG B 328      -4.780  46.341  62.292  1.00  5.99    -0.227 N
ATOM  14986  HE  ARG B 328      -4.067  45.619  62.183  1.00  0.00     0.177 HD
ATOM  14987  CZ  ARG B 328      -5.189  46.986  61.220  1.00 10.78     0.665 C
ATOM  14988  NH1 ARG B 328      -6.217  47.871  61.265  1.00 12.90    -0.235 N
ATOM  14989 1HH1 ARG B 328      -6.534  48.371  60.434  1.00  0.00     0.174 HD
ATOM  14990 2HH1 ARG B 328      -6.632  48.110  62.166  1.00  0.00     0.174 HD
ATOM  14991  NH2 ARG B 328      -4.643  46.672  60.034  1.00  9.78    -0.235 N
ATOM  14992 1HH2 ARG B 328      -4.960  47.172  59.203  1.00  0.00     0.174 HD
ATOM  14993 2HH2 ARG B 328      -3.870  46.007  60.000  1.00  0.00     0.174 HD
ATOM  14994  N   MET B 329      -0.053  45.453  65.843  1.00 14.00    -0.346 N
ATOM  14995  HN  MET B 329      -0.299  46.348  66.265  1.00  0.00     0.163 HD
ATOM  14996  CA  MET B 329       1.356  45.134  65.591  1.00 16.02     0.177 C
ATOM  14998  C   MET B 329       1.795  43.970  66.486  1.00 22.21     0.241 C
ATOM  14999  O   MET B 329       2.626  43.167  66.058  1.00 21.35    -0.271 OA
ATOM  15000  CB  MET B 329       2.294  46.319  65.911  1.00 16.50     0.045 C
ATOM  15003  CG  MET B 329       2.303  47.373  64.812  1.00 18.04     0.076 C
ATOM  15006  SD  MET B 329       2.596  46.731  63.146  1.00 19.91    -0.173 SA
ATOM  15007  CE  MET B 329       4.244  46.075  63.289  1.00 14.41     0.089 C
ATOM  15011  N   LYS B 330       1.229  43.852  67.680  1.00 16.19    -0.346 N
ATOM  15012  HN  LYS B 330       0.572  44.574  67.978  1.00  0.00     0.163 HD
ATOM  15013  CA  LYS B 330       1.497  42.746  68.587  1.00 23.76     0.176 C
ATOM  15015  C   LYS B 330       0.764  41.451  68.207  1.00 21.37     0.240 C
ATOM  15016  O   LYS B 330       1.090  40.361  68.718  1.00 23.40    -0.271 OA
ATOM  15017  CB  LYS B 330       0.998  43.086  69.997  1.00 24.45     0.035 C
ATOM  15020  CG  LYS B 330       1.931  43.984  70.809  1.00 37.04     0.004 C
ATOM  15023  CD  LYS B 330       1.108  44.758  71.823  1.00 44.93     0.027 C
ATOM  15026  CE  LYS B 330       1.606  44.658  73.248  1.00 57.87     0.229 C
ATOM  15029  NZ  LYS B 330       0.956  45.680  74.124  1.00 66.23    -0.079 N
ATOM  15030  HZ1 LYS B 330       1.292  45.613  75.085  1.00  0.00     0.274 HD
ATOM  15031  HZ2 LYS B 330      -0.061  45.620  74.078  1.00  0.00     0.274 HD
ATOM  15032  HZ3 LYS B 330       1.075  46.622  73.751  1.00  0.00     0.274 HD
ATOM  15033  N   GLY B 331      -0.279  41.541  67.412  1.00 15.49    -0.351 N
ATOM  15034  HN  GLY B 331      -0.525  42.461  67.045  1.00  0.00     0.163 HD
ATOM  15035  CA  GLY B 331      -1.108  40.402  67.022  1.00 18.65     0.225 C
ATOM  15038  C   GLY B 331      -2.066  40.004  68.141  1.00 22.34     0.236 C
ATOM  15039  O   GLY B 331      -2.575  38.875  68.168  1.00 18.40    -0.272 OA
ATOM  15040  N   GLU B 332      -2.430  40.917  69.044  1.00 18.93    -0.346 N
ATOM  15041  HN  GLU B 332      -2.028  41.852  68.982  1.00  0.00     0.163 HD
ATOM  15042  CA  GLU B 332      -3.368  40.638  70.104  1.00 19.27     0.177 C
ATOM  15044  C   GLU B 332      -4.815  40.669  69.616  1.00 20.25     0.241 C
ATOM  15045  O   GLU B 332      -5.115  41.404  68.700  1.00 16.62    -0.271 OA
ATOM  15046  CB  GLU B 332      -3.274  41.637  71.262  1.00 22.42     0.045 C
ATOM  15049  CG  GLU B 332      -1.997  41.716  72.045  1.00 42.76     0.116 C
ATOM  15052  CD  GLU B 332      -2.100  42.780  73.142  1.00 52.62     0.172 C
ATOM  15053  OE1 GLU B 332      -2.919  43.717  72.996  1.00 48.49    -0.648 OA
ATOM  15054  OE2 GLU B 332      -1.356  42.645  74.141  1.00 61.84    -0.648 OA
ATOM  15055  N   MET B 333      -5.701  39.856  70.211  1.00 13.15    -0.346 N
ATOM  15056  HN  MET B 333      -5.401  39.251  70.975  1.00  0.00     0.163 HD
ATOM  15057  CA  MET B 333      -7.096  39.833  69.769  1.00 17.33     0.177 C
ATOM  15059  C   MET B 333      -7.847  40.968  70.468  1.00 17.21     0.243 C
ATOM  15060  O   MET B 333      -7.427  41.335  71.560  1.00 19.61    -0.271 OA
ATOM  15061  CB  MET B 333      -7.751  38.516  70.212  1.00 19.78     0.045 C
ATOM  15064  CG  MET B 333      -7.215  37.252  69.517  1.00 28.85     0.076 C
ATOM  15067  SD  MET B 333      -7.193  37.441  67.720  1.00 36.81    -0.173 SA
ATOM  15068  CE  MET B 333      -8.926  37.325  67.394  1.00 26.16     0.089 C
ATOM  15072  N   PRO B 334      -8.909  41.474  69.918  1.00 16.58    -0.337 N
ATOM  15073  CA  PRO B 334      -9.727  42.487  70.589  1.00 19.61     0.179 C
ATOM  15075  C   PRO B 334     -10.290  41.813  71.836  1.00 22.50     0.241 C
ATOM  15076  O   PRO B 334     -10.590  40.595  71.896  1.00 20.61    -0.271 OA
ATOM  15077  CB  PRO B 334     -10.804  42.882  69.611  1.00 17.67     0.037 C
ATOM  15080  CG  PRO B 334     -10.316  42.345  68.297  1.00 18.86     0.022 C
ATOM  15083  CD  PRO B 334      -9.500  41.120  68.605  1.00 16.64     0.127 C
ATOM  15086  N   SER B 335     -10.427  42.625  72.901  1.00 18.97    -0.344 N
ATOM  15087  HN  SER B 335     -10.266  43.630  72.829  1.00  0.00     0.163 HD
ATOM  15088  CA  SER B 335     -10.819  42.001  74.172  1.00 23.16     0.200 C
ATOM  15090  C   SER B 335     -12.229  41.448  74.214  1.00 22.47     0.243 C
ATOM  15091  O   SER B 335     -12.506  40.510  74.986  1.00 29.90    -0.271 OA
ATOM  15092  CB  SER B 335     -10.533  42.991  75.321  1.00 29.78     0.199 C
ATOM  15095  OG  SER B 335     -11.614  43.918  75.333  1.00 34.77    -0.398 OA
ATOM  15096  HG  SER B 335     -11.438  44.527  76.040  1.00  0.00     0.209 HD
ATOM  15097  N   ASP B 336     -13.165  41.916  73.415  1.00 25.15    -0.345 N
ATOM  15098  HN  ASP B 336     -12.921  42.684  72.790  1.00  0.00     0.163 HD
ATOM  15099  CA  ASP B 336     -14.519  41.407  73.369  1.00 29.93     0.186 C
ATOM  15101  C   ASP B 336     -14.702  40.307  72.303  1.00 29.19     0.241 C
ATOM  15102  O   ASP B 336     -15.833  39.857  72.178  1.00 26.72    -0.271 OA
ATOM  15103  CB  ASP B 336     -15.485  42.543  73.017  1.00 37.08     0.147 C
ATOM  15106  CG  ASP B 336     -15.105  43.269  71.745  1.00 50.66     0.175 C
ATOM  15107  OD1 ASP B 336     -13.911  43.304  71.377  1.00 55.61    -0.648 OA
ATOM  15108  OD2 ASP B 336     -16.020  43.839  71.100  1.00 59.70    -0.648 OA
ATOM  15109  N   PHE B 337     -13.662  39.908  71.572  1.00 27.00    -0.346 N
ATOM  15110  HN  PHE B 337     -12.728  40.260  71.784  1.00  0.00     0.163 HD
ATOM  15111  CA  PHE B 337     -13.849  38.979  70.479  1.00 21.71     0.180 C
ATOM  15113  C   PHE B 337     -14.411  37.633  70.904  1.00 21.86     0.241 C
ATOM  15114  O   PHE B 337     -15.338  37.132  70.264  1.00 20.59    -0.271 OA
ATOM  15115  CB  PHE B 337     -12.537  38.766  69.685  1.00 17.38     0.073 C
ATOM  15118  CG  PHE B 337     -12.767  37.712  68.626  1.00 18.58    -0.056 A
ATOM  15119  CD1 PHE B 337     -13.446  38.018  67.479  1.00 18.34     0.007 A
ATOM  15121  CD2 PHE B 337     -12.303  36.421  68.820  1.00 18.58     0.007 A
ATOM  15123  CE1 PHE B 337     -13.689  37.043  66.511  1.00 21.87     0.001 A
ATOM  15125  CE2 PHE B 337     -12.505  35.450  67.859  1.00 19.97     0.001 A
ATOM  15127  CZ  PHE B 337     -13.214  35.774  66.703  1.00 16.07     0.000 A
ATOM  15129  N   ASP B 338     -13.812  37.009  71.918  1.00 16.27    -0.345 N
ATOM  15130  HN  ASP B 338     -13.065  37.482  72.426  1.00  0.00     0.163 HD
ATOM  15131  CA  ASP B 338     -14.205  35.663  72.314  1.00 24.11     0.186 C
ATOM  15133  C   ASP B 338     -15.679  35.557  72.677  1.00 23.65     0.241 C
ATOM  15134  O   ASP B 338     -16.358  34.596  72.324  1.00 23.52    -0.271 OA
ATOM  15135  CB  ASP B 338     -13.288  35.185  73.443  1.00 26.91     0.147 C
ATOM  15138  CG  ASP B 338     -13.667  33.888  74.110  1.00 32.13     0.175 C
ATOM  15139  OD1 ASP B 338     -13.455  32.783  73.563  1.00 30.75    -0.648 OA
ATOM  15140  OD2 ASP B 338     -14.216  33.920  75.243  1.00 34.57    -0.648 OA
ATOM  15141  N   ALA B 339     -16.186  36.534  73.400  1.00 22.89    -0.346 N
ATOM  15142  HN  ALA B 339     -15.546  37.279  73.677  1.00  0.00     0.163 HD
ATOM  15143  CA  ALA B 339     -17.555  36.659  73.841  1.00 21.87     0.172 C
ATOM  15145  C   ALA B 339     -18.499  36.802  72.665  1.00 23.39     0.240 C
ATOM  15146  O   ALA B 339     -19.554  36.170  72.608  1.00 23.87    -0.271 OA
ATOM  15147  CB  ALA B 339     -17.767  37.892  74.742  1.00 22.83     0.042 C
ATOM  15151  N   LYS B 340     -18.125  37.688  71.730  1.00 17.09    -0.346 N
ATOM  15152  HN  LYS B 340     -17.256  38.215  71.815  1.00  0.00     0.163 HD
ATOM  15153  CA  LYS B 340     -19.013  37.867  70.588  1.00 17.89     0.176 C
ATOM  15155  C   LYS B 340     -18.980  36.659  69.657  1.00 18.15     0.241 C
ATOM  15156  O   LYS B 340     -20.003  36.387  69.039  1.00 21.33    -0.271 OA
ATOM  15157  CB  LYS B 340     -18.639  39.163  69.865  1.00 25.53     0.035 C
ATOM  15160  CG  LYS B 340     -19.230  40.371  70.602  1.00 35.63     0.004 C
ATOM  15163  CD  LYS B 340     -18.282  41.555  70.462  1.00 47.45     0.027 C
ATOM  15166  CE  LYS B 340     -18.898  42.779  71.142  1.00 58.93     0.229 C
ATOM  15169  NZ  LYS B 340     -20.051  43.306  70.366  1.00 63.81    -0.079 N
ATOM  15170  HZ1 LYS B 340     -20.462  44.122  70.819  1.00  0.00     0.274 HD
ATOM  15171  HZ2 LYS B 340     -20.749  42.582  70.195  1.00  0.00     0.274 HD
ATOM  15172  HZ3 LYS B 340     -19.792  43.506  69.400  1.00  0.00     0.274 HD
ATOM  15173  N   ALA B 341     -17.797  36.023  69.562  1.00 15.21    -0.346 N
ATOM  15174  HN  ALA B 341     -16.968  36.327  70.073  1.00  0.00     0.163 HD
ATOM  15175  CA  ALA B 341     -17.791  34.850  68.660  1.00 19.02     0.172 C
ATOM  15177  C   ALA B 341     -18.595  33.737  69.305  1.00 16.77     0.240 C
ATOM  15178  O   ALA B 341     -19.280  32.985  68.600  1.00 17.93    -0.271 OA
ATOM  15179  CB  ALA B 341     -16.355  34.445  68.378  1.00 15.63     0.042 C
ATOM  15183  N   LYS B 342     -18.553  33.598  70.633  1.00 16.86    -0.346 N
ATOM  15184  HN  LYS B 342     -18.000  34.238  71.203  1.00  0.00     0.163 HD
ATOM  15185  CA  LYS B 342     -19.314  32.511  71.260  1.00 21.00     0.176 C
ATOM  15187  C   LYS B 342     -20.809  32.736  71.118  1.00 19.83     0.241 C
ATOM  15188  O   LYS B 342     -21.545  31.765  70.960  1.00 19.17    -0.271 OA
ATOM  15189  CB  LYS B 342     -18.960  32.335  72.740  1.00 25.51     0.035 C
ATOM  15192  CG  LYS B 342     -17.505  31.969  72.955  1.00 36.33     0.004 C
ATOM  15195  CD  LYS B 342     -17.259  31.408  74.349  1.00 46.74     0.027 C
ATOM  15198  CE  LYS B 342     -15.840  30.878  74.482  1.00 53.27     0.229 C
ATOM  15201  NZ  LYS B 342     -15.762  29.407  74.261  1.00 65.34    -0.079 N
ATOM  15202  HZ1 LYS B 342     -14.810  29.051  74.350  1.00  0.00     0.274 HD
ATOM  15203  HZ2 LYS B 342     -16.169  29.148  73.362  1.00  0.00     0.274 HD
ATOM  15204  HZ3 LYS B 342     -16.401  28.907  74.880  1.00  0.00     0.274 HD
ATOM  15205  N   GLU B 343     -21.264  33.975  71.198  1.00 19.89    -0.346 N
ATOM  15206  HN  GLU B 343     -20.608  34.732  71.390  1.00  0.00     0.163 HD
ATOM  15207  CA  GLU B 343     -22.681  34.290  71.019  1.00 21.43     0.177 C
ATOM  15209  C   GLU B 343     -23.176  33.945  69.619  1.00 19.43     0.241 C
ATOM  15210  O   GLU B 343     -24.298  33.495  69.395  1.00 20.46    -0.271 OA
ATOM  15211  CB  GLU B 343     -22.854  35.788  71.264  1.00 27.19     0.045 C
ATOM  15214  CG  GLU B 343     -24.250  36.343  71.228  1.00 52.31     0.116 C
ATOM  15217  CD  GLU B 343     -24.351  37.849  71.387  1.00 58.92     0.172 C
ATOM  15218  OE1 GLU B 343     -23.388  38.548  71.772  1.00 57.91    -0.648 OA
ATOM  15219  OE2 GLU B 343     -25.465  38.352  71.111  1.00 67.16    -0.648 OA
ATOM  15220  N   PHE B 344     -22.375  34.238  68.608  1.00 17.06    -0.346 N
ATOM  15221  HN  PHE B 344     -21.501  34.724  68.810  1.00  0.00     0.163 HD
ATOM  15222  CA  PHE B 344     -22.675  33.902  67.217  1.00 15.83     0.180 C
ATOM  15224  C   PHE B 344     -22.756  32.386  67.046  1.00 15.14     0.241 C
ATOM  15225  O   PHE B 344     -23.680  31.902  66.367  1.00 16.17    -0.271 OA
ATOM  15226  CB  PHE B 344     -21.644  34.531  66.289  1.00 13.25     0.073 C
ATOM  15229  CG  PHE B 344     -21.710  34.094  64.853  1.00 17.66    -0.056 A
ATOM  15230  CD1 PHE B 344     -22.748  34.484  64.035  1.00 19.51     0.007 A
ATOM  15232  CD2 PHE B 344     -20.681  33.305  64.340  1.00 19.55     0.007 A
ATOM  15234  CE1 PHE B 344     -22.785  34.065  62.706  1.00 22.43     0.001 A
ATOM  15236  CE2 PHE B 344     -20.731  32.878  63.012  1.00 17.02     0.001 A
ATOM  15238  CZ  PHE B 344     -21.782  33.267  62.206  1.00 20.36     0.000 A
ATOM  15240  N   ILE B 345     -21.805  31.665  67.618  1.00 12.46    -0.346 N
ATOM  15241  HN  ILE B 345     -21.061  32.119  68.147  1.00  0.00     0.163 HD
ATOM  15242  CA  ILE B 345     -21.836  30.177  67.478  1.00 13.05     0.180 C
ATOM  15244  C   ILE B 345     -23.087  29.596  68.110  1.00 17.20     0.241 C
ATOM  15245  O   ILE B 345     -23.736  28.648  67.694  1.00 14.65    -0.271 OA
ATOM  15246  CB  ILE B 345     -20.579  29.568  68.114  1.00 16.00     0.013 C
ATOM  15248  CG1 ILE B 345     -19.347  29.846  67.201  1.00 17.69     0.002 C
ATOM  15251  CG2 ILE B 345     -20.659  28.042  68.262  1.00 16.53     0.012 C
ATOM  15255  CD1 ILE B 345     -18.043  29.674  67.992  1.00 19.47     0.005 C
ATOM  15259  N   ALA B 346     -23.477  30.156  69.283  1.00 16.34    -0.346 N
ATOM  15260  HN  ALA B 346     -22.962  30.952  69.659  1.00  0.00     0.163 HD
ATOM  15261  CA  ALA B 346     -24.639  29.624  70.020  1.00 22.33     0.172 C
ATOM  15263  C   ALA B 346     -25.915  29.854  69.214  1.00 16.88     0.240 C
ATOM  15264  O   ALA B 346     -26.819  29.015  69.161  1.00 17.10    -0.271 OA
ATOM  15265  CB  ALA B 346     -24.787  30.263  71.401  1.00 16.39     0.042 C
ATOM  15269  N   LYS B 347     -25.942  30.991  68.525  1.00 17.01    -0.346 N
ATOM  15270  HN  LYS B 347     -25.139  31.620  68.561  1.00  0.00     0.163 HD
ATOM  15271  CA  LYS B 347     -27.102  31.353  67.718  1.00 17.80     0.176 C
ATOM  15273  C   LYS B 347     -27.276  30.404  66.554  1.00 17.85     0.241 C
ATOM  15274  O   LYS B 347     -28.403  30.047  66.124  1.00 17.08    -0.271 OA
ATOM  15275  CB  LYS B 347     -26.915  32.792  67.250  1.00 27.91     0.035 C
ATOM  15278  CG  LYS B 347     -28.033  33.394  66.436  1.00 46.73     0.004 C
ATOM  15281  CD  LYS B 347     -27.477  34.277  65.325  1.00 65.80     0.027 C
ATOM  15284  CE  LYS B 347     -27.374  35.732  65.723  1.00 66.80     0.229 C
ATOM  15287  NZ  LYS B 347     -25.999  36.282  65.557  1.00 76.42    -0.079 N
ATOM  15288  HZ1 LYS B 347     -25.930  37.264  65.825  1.00  0.00     0.274 HD
ATOM  15289  HZ2 LYS B 347     -25.661  36.139  64.605  1.00  0.00     0.274 HD
ATOM  15290  HZ3 LYS B 347     -25.316  35.716  66.062  1.00  0.00     0.274 HD
ATOM  15291  N   LEU B 348     -26.157  30.035  65.913  1.00 14.19    -0.346 N
ATOM  15292  HN  LEU B 348     -25.249  30.399  66.202  1.00  0.00     0.163 HD
ATOM  15293  CA  LEU B 348     -26.261  29.100  64.790  1.00 11.03     0.177 C
ATOM  15295  C   LEU B 348     -26.745  27.751  65.305  1.00 11.44     0.241 C
ATOM  15296  O   LEU B 348     -27.511  27.078  64.600  1.00 14.96    -0.271 OA
ATOM  15297  CB  LEU B 348     -24.910  28.857  64.082  1.00 13.60     0.038 C
ATOM  15300  CG  LEU B 348     -24.266  30.096  63.448  1.00 15.98    -0.020 C
ATOM  15302  CD1 LEU B 348     -22.933  29.709  62.814  1.00 17.58     0.009 C
ATOM  15306  CD2 LEU B 348     -25.225  30.741  62.443  1.00 12.21     0.009 C
ATOM  15310  N   GLN B 349     -26.330  27.323  66.514  1.00 11.53    -0.346 N
ATOM  15311  HN  GLN B 349     -25.725  27.897  67.101  1.00  0.00     0.163 HD
ATOM  15312  CA  GLN B 349     -26.784  25.995  66.952  1.00 13.64     0.177 C
ATOM  15314  C   GLN B 349     -28.304  26.045  67.138  1.00 19.39     0.241 C
ATOM  15315  O   GLN B 349     -29.032  25.111  66.817  1.00 14.26    -0.271 OA
ATOM  15316  CB  GLN B 349     -26.087  25.510  68.216  1.00 10.40     0.044 C
ATOM  15319  CG  GLN B 349     -26.478  24.099  68.674  1.00 11.94     0.105 C
ATOM  15322  CD  GLN B 349     -26.052  23.020  67.693  1.00 12.78     0.215 C
ATOM  15323  NE2 GLN B 349     -27.012  22.267  67.134  1.00 14.97    -0.370 N
ATOM  15324 1HE2 GLN B 349     -28.000  22.403  67.347  1.00  0.00     0.159 HD
ATOM  15325 2HE2 GLN B 349     -26.726  21.543  66.475  1.00  0.00     0.159 HD
ATOM  15326  OE1 GLN B 349     -24.844  22.854  67.433  1.00 15.31    -0.274 OA
ATOM  15327  N   ALA B 350     -28.816  27.179  67.619  1.00 17.26    -0.346 N
ATOM  15328  HN  ALA B 350     -28.194  27.959  67.830  1.00  0.00     0.163 HD
ATOM  15329  CA  ALA B 350     -30.245  27.324  67.848  1.00 21.52     0.172 C
ATOM  15331  C   ALA B 350     -31.059  27.551  66.583  1.00 21.16     0.240 C
ATOM  15332  O   ALA B 350     -32.298  27.465  66.631  1.00 22.65    -0.271 OA
ATOM  15333  CB  ALA B 350     -30.459  28.484  68.829  1.00 20.95     0.042 C
ATOM  15337  N   ASN B 351     -30.500  27.904  65.443  1.00 18.32    -0.346 N
ATOM  15338  HN  ASN B 351     -29.483  27.977  65.422  1.00  0.00     0.163 HD
ATOM  15339  CA  ASN B 351     -31.228  28.201  64.197  1.00 17.09     0.185 C
ATOM  15341  C   ASN B 351     -30.639  27.359  63.071  1.00 16.38     0.243 C
ATOM  15342  O   ASN B 351     -29.825  27.873  62.299  1.00 17.18    -0.271 OA
ATOM  15343  CB  ASN B 351     -30.985  29.692  63.872  1.00 16.96     0.137 C
ATOM  15346  CG  ASN B 351     -31.827  30.530  64.842  1.00 30.02     0.217 C
ATOM  15347  ND2 ASN B 351     -31.159  31.051  65.855  1.00 29.92    -0.370 N
ATOM  15348 1HD2 ASN B 351     -30.152  30.977  65.999  1.00  0.00     0.159 HD
ATOM  15349 2HD2 ASN B 351     -31.719  31.608  66.500  1.00  0.00     0.159 HD
ATOM  15350  OD1 ASN B 351     -33.044  30.620  64.668  1.00 30.52    -0.274 OA
ATOM  15351  N   PRO B 352     -30.964  26.085  62.978  1.00 17.83    -0.337 N
ATOM  15352  CA  PRO B 352     -30.366  25.199  62.005  1.00 17.67     0.179 A
ATOM  15354  C   PRO B 352     -30.591  25.608  60.573  1.00 20.37     0.241 C
ATOM  15355  O   PRO B 352     -31.644  26.136  60.199  1.00 15.79    -0.271 OA
ATOM  15356  CB  PRO B 352     -30.961  23.821  62.281  1.00 20.72     0.037 A
ATOM  15359  CG  PRO B 352     -31.912  23.962  63.419  1.00 23.91     0.022 A
ATOM  15362  CD  PRO B 352     -31.966  25.396  63.816  1.00 19.88     0.127 A
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ATOM  15365  N   ALA B 353      -29.577  25.400  59.747  1.00 15.47     -0.346 N
ATOM  15366  HN  ALA B 353      -28.704  25.028  60.122  1.00  0.00      0.163 HD
ATOM  15367  CA  ALA B 353      -29.666  25.687  58.309  1.00 13.43      0.172 C
ATOM  15369  C   ALA B 353      -28.871  24.611  57.576  1.00 16.43      0.240 C
ATOM  15370  O   ALA B 353      -27.781  24.273  58.038  1.00 16.98     -0.271 OA
ATOM  15371  CB  ALA B 353      -29.043  27.050  58.063  1.00 12.18      0.042 C
ATOM  15375  N   LYS B 354      -29.358  24.028  56.499  1.00 14.11     -0.346 N
ATOM  15376  HN  LYS B 354      -30.293  24.295  56.191  1.00  0.00      0.163 HD
ATOM  15377  CA  LYS B 354      -28.646  23.031  55.725  1.00 13.67      0.176 C
ATOM  15379  C   LYS B 354      -27.937  23.774  54.590  1.00 13.62      0.241 C
ATOM  15380  O   LYS B 354      -28.604  23.985  53.567  1.00 12.57     -0.271 OA
ATOM  15381  CB  LYS B 354      -29.628  22.025  55.106  1.00 15.44      0.035 C
ATOM  15384  CG  LYS B 354      -28.874  20.826  54.486  1.00 16.23      0.004 C
ATOM  15387  CD  LYS B 354      -29.954  19.852  53.972  1.00 25.94      0.027 C
ATOM  15390  CE  LYS B 354      -29.335  18.755  53.128  1.00 41.05      0.229 C
ATOM  15393  NZ  LYS B 354      -30.343  18.185  52.180  1.00 45.81     -0.079 N
ATOM  15394  HZ1 LYS B 354      -29.927  17.447  51.612  1.00  0.00      0.274 HD
ATOM  15395  HZ2 LYS B 354      -30.772  18.909  51.604  1.00  0.00      0.274 HD
ATOM  15396  HZ3 LYS B 354      -31.179  17.862  52.667  1.00  0.00      0.274 HD
ATOM  15397  N   ILE B 355      -26.697  24.221  54.810  1.00  8.45     -0.346 N
ATOM  15398  HN  ILE B 355      -26.225  24.002  55.687  1.00  0.00      0.163 HD
ATOM  15399  CA  ILE B 355      -26.017  25.022  53.796  1.00  8.82      0.180 C
ATOM  15401  C   ILE B 355      -24.581  24.470  53.613  1.00  8.71      0.241 C
ATOM  15402  O   ILE B 355      -24.165  23.647  54.433  1.00 10.65     -0.271 OA
ATOM  15403  CB  ILE B 355      -25.894  26.512  54.145  1.00 13.71      0.013 C
ATOM  15405  CG1 ILE B 355      -25.168  26.683  55.508  1.00 14.08      0.002 C
ATOM  15408  CG2 ILE B 355      -27.269  27.205  54.203  1.00 14.94      0.012 C
ATOM  15412  CD1 ILE B 355      -24.907  28.135  55.906  1.00 12.10      0.005 C
ATOM  15416  N   ALA B 356      -23.935  24.866  52.511  1.00  9.21     -0.346 N
ATOM  15417  HN  ALA B 356      -24.362  25.517  51.852  1.00  0.00      0.163 HD
ATOM  15418  CA  ALA B 356      -22.573  24.322  52.285  1.00 10.70      0.172 C
ATOM  15420  C   ALA B 356      -21.662  24.903  53.339  1.00  9.42      0.240 C
ATOM  15421  O   ALA B 356      -21.835  26.091  53.707  1.00 12.77     -0.271 OA
ATOM  15422  CB  ALA B 356      -22.103  24.768  50.904  1.00  9.57      0.042 C
ATOM  15426  N   SER B 357      -20.579  24.218  53.720  1.00  9.12     -0.344 N
ATOM  15427  HN  SER B 357      -20.391  23.280  53.366  1.00  0.00      0.163 HD
ATOM  15428  CA  SER B 357      -19.668  24.877  54.673  1.00  6.31      0.200 C
ATOM  15430  C   SER B 357      -18.887  25.989  54.010  1.00  7.61      0.243 C
ATOM  15431  O   SER B 357      -18.407  26.878  54.715  1.00  9.80     -0.271 OA
ATOM  15432  CB  SER B 357      -18.774  23.874  55.406  1.00  9.18      0.199 C
ATOM  15435  OG  SER B 357      -18.110  23.018  54.454  1.00  7.80     -0.398 OA
ATOM  15436  HG  SER B 357      -17.555  22.395  54.909  1.00  0.00      0.209 HD
ATOM  15437  N   ARG B 358      -18.830  26.076  52.687  1.00  9.00     -0.346 N
ATOM  15438  HN  ARG B 358      -19.204  25.335  52.094  1.00  0.00      0.163 HD
ATOM  15439  CA  ARG B 358      -18.211  27.274  52.106  1.00 10.50      0.176 C
ATOM  15441  C   ARG B 358      -19.101  28.479  52.394  1.00 12.34      0.241 C
ATOM  15442  O   ARG B 358      -18.606  29.602  52.568  1.00  9.92     -0.271 OA
ATOM  15443  CB  ARG B 358      -17.985  27.151  50.597  1.00  8.98      0.036 C
ATOM  15446  CG  ARG B 358      -19.265  27.037  49.787  1.00 12.43      0.023 C
ATOM  15449  CD  ARG B 358      -18.858  27.120  48.292  1.00 15.01      0.138 C
ATOM  15452  NE  ARG B 358      -19.994  26.822  47.446  1.00 21.44     -0.227 N
ATOM  15453  HE  ARG B 358      -20.779  26.364  47.908  1.00  0.00      0.177 HD
ATOM  15454  CZ  ARG B 358      -20.152  27.062  46.159  1.00 26.59      0.665 C
ATOM  15455  NH1 ARG B 358      -19.204  27.634  45.424  1.00 18.58     -0.235 N
ATOM  15456 1HH1 ARG B 358      -18.319  27.926  45.840  1.00  0.00      0.174 HD
ATOM  15457 2HH1 ARG B 358      -19.326  27.820  44.429  1.00  0.00      0.174 HD
ATOM  15458  NH2 ARG B 358      -21.311  26.680  45.614  1.00 22.80     -0.235 N
ATOM  15459 1HH2 ARG B 358      -22.039  26.241  46.178  1.00  0.00      0.174 HD
ATOM  15460 2HH2 ARG B 358      -21.433  26.866  44.619  1.00  0.00      0.174 HD
ATOM  15461  N   LYS B 359      -20.435  28.253  52.449  1.00  9.73     -0.346 N
ATOM  15462  HN  LYS B 359      -20.819  27.321  52.294  1.00  0.00      0.163 HD
ATOM  15463  CA  LYS B 359      -21.315  29.403  52.742  1.00 10.41      0.176 C
ATOM  15465  C   LYS B 359      -21.251  29.693  54.238  1.00 13.00      0.241 C
ATOM  15466  O   LYS B 359      -21.267  30.869  54.621  1.00  9.78     -0.271 OA
ATOM  15467  CB  LYS B 359      -22.745  29.115  52.292  1.00  8.48      0.035 C
ATOM  15470  CG  LYS B 359      -23.784  30.189  52.528  1.00 15.50      0.004 C
ATOM  15473  CD  LYS B 359      -23.359  31.506  51.873  1.00 20.12      0.027 C
ATOM  15476  CE  LYS B 359      -24.439  32.546  52.114  1.00 31.31      0.229 C
ATOM  15479  NZ  LYS B 359      -23.947  33.876  52.512  1.00 29.09     -0.079 N
ATOM  15480  HZ1 LYS B 359      -24.672  34.575  52.674  1.00  0.00      0.274 HD
ATOM  15481  HZ2 LYS B 359      -23.273  34.221  51.828  1.00  0.00      0.274 HD
ATOM  15482  HZ3 LYS B 359      -23.345  33.798  53.332  1.00  0.00      0.274 HD
ATOM  15483  N   ALA B 360      -21.163  28.639  55.076  1.00  9.64     -0.346 N
ATOM  15484  HN  ALA B 360      -21.186  27.686  54.714  1.00  0.00      0.163 HD
ATOM  15485  CA  ALA B 360      -21.035  28.884  56.504  1.00 10.77      0.172 C
ATOM  15487  C   ALA B 360      -19.777  29.685  56.795  1.00 10.23      0.240 C
ATOM  15488  O   ALA B 360      -19.685  30.473  57.762  1.00 10.03     -0.271 OA
ATOM  15489  CB  ALA B 360      -21.016  27.518  57.245  1.00  8.36      0.042 C
ATOM  15493  N   SER B 361      -18.740  29.418  55.989  1.00  9.56     -0.344 N
ATOM  15494  HN  SER B 361      -18.827  28.695  55.275  1.00  0.00      0.163 HD
ATOM  15495  CA  SER B 361      -17.474  30.163  56.128  1.00  9.04      0.200 C
ATOM  15497  C   SER B 361      -17.650  31.631  55.770  1.00 10.42      0.243 C
ATOM  15498  O   SER B 361      -17.248  32.499  56.582  1.00 11.29     -0.271 OA
ATOM  15499  CB  SER B 361      -16.406  29.467  55.254  1.00 13.02      0.199 C
ATOM  15502  OG  SER B 361      -15.265  30.335  55.150  1.00 11.24     -0.398 OA
ATOM  15503  HG  SER B 361      -14.609  29.907  54.613  1.00  0.00      0.209 HD
ATOM  15504  N   GLN B 362      -18.324  31.895  54.639  1.00  9.16     -0.346 N
ATOM  15505  HN  GLN B 362      -18.625  31.155  54.005  1.00  0.00      0.163 HD
ATOM  15506  CA  GLN B 362      -18.606  33.328  54.365  1.00 10.07      0.177 C
ATOM  15508  C   GLN B 362      -19.439  33.956  55.487  1.00 11.79      0.241 C
ATOM  15509  O   GLN B 362      -19.173  35.118  55.814  1.00 10.64     -0.271 OA
ATOM  15510  CB  GLN B 362      -19.421  33.425  53.058  1.00 11.08      0.044 C
ATOM  15513  CG  GLN B 362      -19.545  34.909  52.619  1.00 15.00      0.105 C
ATOM  15516  CD  GLN B 362      -20.261  35.038  51.284  1.00 22.93      0.215 C
ATOM  15517  NE2 GLN B 362      -19.736  35.816  50.333  1.00 21.54     -0.370 N
ATOM  15518 1HE2 GLN B 362      -18.891  36.364  50.493  1.00  0.00      0.159 HD
ATOM  15519 2HE2 GLN B 362      -20.216  35.903  49.437  1.00  0.00      0.159 HD
ATOM  15520  OE1 GLN B 362      -21.279  34.378  51.091  1.00 20.79     -0.274 OA
ATOM  15521  N   ASN B 363      -20.427  33.257  56.084  1.00 10.92     -0.346 N
ATOM  15522  HN  ASN B 363      -20.632  32.306  55.777  1.00  0.00      0.163 HD
ATOM  15523  CA  ASN B 363      -21.206  33.854  57.168  1.00 11.81      0.185 C
ATOM  15525  C   ASN B 363      -20.347  34.169  58.377  1.00 15.42      0.241 C
ATOM  15526  O   ASN B 363      -20.614  35.118  59.114  1.00 12.99     -0.271 OA
ATOM  15527  CB  ASN B 363      -22.370  32.951  57.631  1.00  8.61      0.137 C
ATOM  15530  CG  ASN B 363      -23.434  32.774  56.559  1.00 17.57      0.217 C
ATOM  15531  ND2 ASN B 363      -24.212  31.710  56.642  1.00 14.84     -0.370 N
ATOM  15532 1HD2 ASN B 363      -24.926  31.591  55.923  1.00  0.00      0.159 HD
ATOM  15533 2HD2 ASN B 363      -24.153  31.029  57.399  1.00  0.00      0.159 HD
ATOM  15534  OD1 ASN B 363      -23.506  33.599  55.643  1.00 14.10     -0.274 OA
ATOM  15535  N   ALA B 364      -19.338  33.360  58.716  1.00 11.19     -0.346 N
ATOM  15536  HN  ALA B 364      -19.201  32.498  58.188  1.00  0.00      0.163 HD
ATOM  15537  CA  ALA B 364      -18.425  33.663  59.813  1.00 14.05      0.172 C
ATOM  15539  C   ALA B 364      -17.511  34.835  59.505  1.00 12.75      0.240 C
ATOM  15540  O   ALA B 364      -17.216  35.681  60.387  1.00 13.70     -0.271 OA
ATOM  15541  CB  ALA B 364      -17.608  32.377  60.177  1.00 12.11      0.042 C
ATOM  15545  N   ILE B 365      -17.037  34.987  58.244  1.00 11.14     -0.346 N
ATOM  15546  HN  ILE B 365      -17.247  34.273  57.547  1.00  0.00      0.163 HD
ATOM  15547  CA  ILE B 365      -16.241  36.135  57.858  1.00 10.10      0.180 C
ATOM  15549  C   ILE B 365      -17.103  37.405  58.046  1.00 14.73      0.241 C
ATOM  15550  O   ILE B 365      -16.645  38.440  58.553  1.00 13.13     -0.271 OA
ATOM  15551  CB  ILE B 365      -15.735  36.071  56.399  1.00  8.28      0.013 C
ATOM  15553  CG1 ILE B 365      -14.712  34.911  56.207  1.00  8.03      0.002 C
ATOM  15556  CG2 ILE B 365      -15.051  37.378  56.019  1.00 13.97      0.012 C
ATOM  15560  CD1 ILE B 365      -14.452  34.589  54.754  1.00 14.30      0.005 C
ATOM  15564  N   GLU B 366      -18.361  37.341  57.614  1.00 15.27     -0.346 N
ATOM  15565  HN  GLU B 366      -18.692  36.495  57.150  1.00  0.00      0.163 HD
ATOM  15566  CA  GLU B 366      -19.276  38.472  57.797  1.00 14.32      0.177 C
ATOM  15568  C   GLU B 366      -19.484  38.813  59.271  1.00 14.16      0.241 C
ATOM  15569  O   GLU B 366      -19.565  40.015  59.566  1.00 16.91     -0.271 OA
ATOM  15570  CB  GLU B 366      -20.628  38.150  57.163  1.00 13.45      0.045 C
ATOM  15573  CG  GLU B 366      -21.669  39.250  57.303  1.00 15.94      0.116 C
ATOM  15576  CD  GLU B 366      -21.375  40.352  56.282  1.00 23.25      0.172 C
ATOM  15577  OE1 GLU B 366      -20.966  40.129  55.129  1.00 18.64     -0.648 OA
ATOM  15578  OE2 GLU B 366      -21.553  41.531  56.607  1.00 21.56     -0.648 OA
ATOM  15579  N   ALA B 367      -19.628  37.832  60.130  1.00 11.25     -0.346 N
ATOM  15580  HN  ALA B 367      -19.612  36.869  59.795  1.00  0.00      0.163 HD
ATOM  15581  CA  ALA B 367      -19.811  38.092  61.561  1.00 17.28      0.172 C
ATOM  15583  C   ALA B 367      -18.541  38.585  62.222  1.00 15.83      0.240 C
ATOM  15584  O   ALA B 367      -18.583  39.437  63.129  1.00 13.70     -0.271 OA
ATOM  15585  CB  ALA B 367      -20.233  36.807  62.300  1.00 13.01      0.042 C
ATOM  15589  N   PHE B 368      -17.379  38.041  61.824  1.00 11.20     -0.346 N
ATOM  15590  HN  PHE B 368      -17.354  37.349  61.075  1.00  0.00      0.163 HD
ATOM  15591  CA  PHE B 368      -16.139  38.473  62.500  1.00 11.38      0.180 C
ATOM  15593  C   PHE B 368      -15.511  39.725  61.932  1.00 14.73      0.241 C
ATOM  15594  O   PHE B 368      -14.727  40.413  62.597  1.00 13.43     -0.271 OA
ATOM  15595  CB  PHE B 368      -15.070  37.357  62.435  1.00 15.10      0.073 C
ATOM  15598  CG  PHE B 368      -15.457  36.097  63.156  1.00 20.45     -0.056 A
ATOM  15599  CD1 PHE B 368      -16.547  35.995  63.954  1.00 19.98      0.007 A
ATOM  15601  CD2 PHE B 368      -14.642  34.961  63.006  1.00 27.66      0.007 A
ATOM  15603  CE1 PHE B 368      -16.916  34.820  64.605  1.00 23.26      0.001 A
ATOM  15605  CE2 PHE B 368      -14.983  33.791  63.672  1.00 21.09      0.001 A
ATOM  15607  CZ  PHE B 368      -16.108  33.717  64.444  1.00 26.21      0.000 A
ATOM  15609  N   GLY B 369      -15.837  40.057  60.696  1.00 11.86     -0.351 N
ATOM  15610  HN  GLY B 369      -16.531  39.477  60.225  1.00  0.00      0.163 HD
ATOM  15611  CA  GLY B 369      -15.292  41.178  59.951  1.00 15.02      0.225 C
ATOM  15614  C   GLY B 369      -15.327  42.506  60.678  1.00 19.31      0.238 C
ATOM  15615  O   GLY B 369      -14.330  43.229  60.747  1.00 16.44     -0.272 OA
ATOM  15616  N   PRO B 370      -16.472  42.909  61.210  1.00 18.67     -0.337 N
ATOM  15617  CA  PRO B 370      -16.556  44.157  61.975  1.00 17.79      0.179 C
ATOM  15619  C   PRO B 370      -15.739  44.100  63.252  1.00 20.58      0.241 C
ATOM  15620  O   PRO B 370      -15.434  45.154  63.813  1.00 18.54     -0.271 OA
ATOM  15621  CB  PRO B 370      -18.049  44.303  62.298  1.00 17.47      0.037 C
ATOM  15624  CG  PRO B 370      -18.774  43.298  61.492  1.00 20.62      0.022 C
ATOM  15627  CD  PRO B 370      -17.781  42.206  61.166  1.00 18.70      0.127 C
ATOM  15630  N   LEU B 371      -15.414  42.933  63.826  1.00 14.67     -0.346 N
ATOM  15631  HN  LEU B 371      -15.731  42.068  63.389  1.00  0.00      0.163 HD
ATOM  15632  CA  LEU B 371      -14.631  42.851  65.042  1.00 14.97      0.177 C
ATOM  15634  C   LEU B 371      -13.135  42.792  64.811  1.00 16.88      0.241 C
ATOM  15635  O   LEU B 371      -12.335  43.036  65.727  1.00 17.05     -0.271 OA
ATOM  15636  CB  LEU B 371      -14.952  41.523  65.771  1.00 15.62      0.038 C
ATOM  15639  CG  LEU B 371      -16.451  41.299  66.011  1.00 30.06     -0.020 C
ATOM  15641  CD1 LEU B 371      -16.688  39.929  66.618  1.00 26.70      0.009 C
ATOM  15645  CD2 LEU B 371      -16.970  42.409  66.924  1.00 32.24      0.009 C
ATOM  15649  N   LEU B 372      -12.723  42.437  63.601  1.00 16.57     -0.346 N
ATOM  15650  HN  LEU B 372      -13.406  42.288  62.859  1.00  0.00      0.163 HD
ATOM  15651  CA  LEU B 372      -11.287  42.255  63.318  1.00 12.58      0.177 C
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ATOM  15653  C   LEU B 372      -10.872  43.134  62.159  1.00 12.75      0.243 C
ATOM  15654  O   LEU B 372      -10.677  42.663  61.042  1.00 12.44     -0.271 OA
ATOM  15655  CB  LEU B 372      -11.041  40.763  62.936  1.00 11.55      0.038 C
ATOM  15658  CG  LEU B 372      -11.338  39.714  63.999  1.00 17.00     -0.020 C
ATOM  15660  CD1 LEU B 372      -11.151  38.305  63.404  1.00 20.73      0.009 C
ATOM  15664  CD2 LEU B 372      -10.451  39.875  65.236  1.00 18.99      0.009 C
ATOM  15668  N   PRO B 373      -10.607  44.424  62.361  1.00 14.23     -0.337 N
ATOM  15669  CA  PRO B 373      -10.147  45.321  61.321  1.00 15.59      0.179 C
ATOM  15671  C   PRO B 373       -8.821  44.914  60.692  1.00 15.26      0.241 C
ATOM  15672  O   PRO B 373       -8.441  45.419  59.631  1.00 13.67     -0.271 OA
ATOM  15673  CB  PRO B 373      -10.063  46.687  62.021  1.00 14.67      0.037 C
ATOM  15676  CG  PRO B 373       -9.936  46.375  63.482  1.00 16.28      0.022 C
ATOM  15679  CD  PRO B 373      -10.706  45.099  63.699  1.00 15.66      0.127 C
ATOM  15682  N   GLU B 374       -8.016  44.078  61.342  1.00 10.14     -0.346 N
ATOM  15683  HN  GLU B 374       -8.332  43.762  62.259  1.00  0.00      0.163 HD
ATOM  15684  CA  GLU B 374       -6.744  43.571  60.888  1.00 13.56      0.177 C
ATOM  15686  C   GLU B 374       -6.887  42.527  59.786  1.00  9.49      0.241 C
ATOM  15687  O   GLU B 374       -5.903  42.194  59.104  1.00  9.32     -0.271 OA
ATOM  15688  CB  GLU B 374       -5.926  42.988  62.063  1.00 12.07      0.045 C
ATOM  15691  CG  GLU B 374       -6.547  41.804  62.793  1.00 13.02      0.116 C
ATOM  15694  CD  GLU B 374       -7.257  42.257  64.063  1.00 20.20      0.172 C
ATOM  15695  OE1 GLU B 374       -8.085  43.200  64.029  1.00 11.21     -0.648 OA
ATOM  15696  OE2 GLU B 374       -7.014  41.684  65.137  1.00 16.87     -0.648 OA
ATOM  15697  N   PHE B 375       -8.115  42.072  59.445  1.00 10.95     -0.346 N
ATOM  15698  HN  PHE B 375       -8.944  42.359  59.965  1.00  0.00      0.163 HD
ATOM  15699  CA  PHE B 375       -8.221  41.150  58.301  1.00  9.60      0.180 C
ATOM  15701  C   PHE B 375       -7.626  41.751  57.033  1.00  9.40      0.241 C
ATOM  15702  O   PHE B 375       -7.831  42.919  56.638  1.00  8.92     -0.271 OA
ATOM  15703  CB  PHE B 375       -9.709  40.862  57.966  1.00  9.87      0.073 C
ATOM  15706  CG  PHE B 375      -10.368  39.667  58.599  1.00 13.34     -0.056 A
ATOM  15707  CD1 PHE B 375       -9.687  38.567  59.021  1.00 13.31      0.007 A
ATOM  15709  CD2 PHE B 375      -11.766  39.630  58.655  1.00 18.63      0.007 A
ATOM  15711  CE1 PHE B 375      -10.310  37.444  59.556  1.00 18.62      0.001 A
ATOM  15713  CE2 PHE B 375      -12.412  38.523  59.188  1.00 18.57      0.001 A
ATOM  15715  CZ  PHE B 375      -11.688  37.444  59.657  1.00 19.51      0.000 A
ATOM  15717  N   LEU B 376       -6.837  40.917  56.309  1.00  9.33     -0.346 N
ATOM  15718  HN  LEU B 376       -6.574  40.020  56.716  1.00  0.00      0.163 HD
ATOM  15719  CA  LEU B 376       -6.345  41.249  54.965  1.00  7.18      0.177 C
ATOM  15721  C   LEU B 376       -6.548  39.950  54.140  1.00 11.30      0.240 C
ATOM  15722  O   LEU B 376       -5.684  39.083  54.242  1.00 12.28     -0.271 OA
ATOM  15723  CB  LEU B 376       -4.904  41.724  54.966  1.00 10.82      0.038 C
ATOM  15726  CG  LEU B 376       -4.351  42.221  53.621  1.00 13.68     -0.020 C
ATOM  15728  CD1 LEU B 376       -5.317  43.156  52.886  1.00 14.59      0.009 C
ATOM  15732  CD2 LEU B 376       -3.084  43.024  53.876  1.00  9.00      0.009 C
ATOM  15736  N   GLY B 377       -7.695  39.782  53.472  1.00  6.29     -0.351 N
ATOM  15737  HN  GLY B 377       -8.342  40.565  53.375  1.00  0.00      0.163 HD
ATOM  15738  CA  GLY B 377       -8.033  38.480  52.875  1.00  7.45      0.225 C
ATOM  15741  C   GLY B 377       -7.976  38.472  51.350  1.00 10.27      0.235 C
ATOM  15742  O   GLY B 377       -7.681  39.500  50.764  1.00 13.24     -0.272 OA
ATOM  15743  N   GLY B 378       -8.132  37.295  50.741  1.00  7.56     -0.351 N
ATOM  15744  HN  GLY B 378       -8.261  36.424  51.256  1.00  0.00      0.163 HD
ATOM  15745  CA  GLY B 378       -8.103  37.349  49.245  1.00  8.21      0.225 C
ATOM  15748  C   GLY B 378       -8.346  35.908  48.776  1.00 10.34      0.236 C
ATOM  15749  O   GLY B 378       -8.330  34.956  49.563  1.00 11.91     -0.272 OA
ATOM  15750  N   SER B 379       -8.450  35.779  47.480  1.00  8.48     -0.344 N
ATOM  15751  HN  SER B 379       -8.340  36.600  46.885  1.00  0.00      0.163 HD
ATOM  15752  CA  SER B 379       -8.723  34.471  46.864  1.00  8.21      0.200 C
ATOM  15754  C   SER B 379       -7.947  34.483  45.545  1.00  8.46      0.243 C
ATOM  15755  O   SER B 379       -7.770  35.566  44.996  1.00  9.18     -0.271 OA
ATOM  15756  CB  SER B 379      -10.219  34.330  46.513  1.00  9.23      0.199 C
ATOM  15759  OG  SER B 379      -10.347  33.126  45.707  1.00 13.44     -0.398 OA
ATOM  15760  HG  SER B 379      -11.268  33.039  45.491  1.00  0.00      0.209 HD
ATOM  15761  N   ALA B 380       -7.476  33.367  45.062  1.00  9.96     -0.346 N
ATOM  15762  HN  ALA B 380       -7.605  32.511  45.601  1.00  0.00      0.163 HD
ATOM  15763  CA  ALA B 380       -6.775  33.288  43.791  1.00 12.18      0.172 C
ATOM  15765  C   ALA B 380       -7.782  33.152  42.655  1.00 15.59      0.240 C
ATOM  15766  O   ALA B 380       -7.933  32.110  42.022  1.00 11.36     -0.271 OA
ATOM  15767  CB  ALA B 380       -5.780  32.105  43.858  1.00  7.19      0.042 C
ATOM  15771  N   ASP B 381       -8.438  34.257  42.310  1.00  8.45     -0.346 N
ATOM  15772  HN  ASP B 381       -8.264  35.095  42.864  1.00  0.00      0.163 HD
ATOM  15773  CA  ASP B 381       -9.380  34.370  41.212  1.00 13.03      0.186 C
ATOM  15775  C   ASP B 381      -10.589  33.460  41.371  1.00 13.55      0.241 C
ATOM  15776  O   ASP B 381      -11.174  32.996  40.378  1.00 15.25     -0.271 OA
ATOM  15777  CB  ASP B 381       -8.692  34.147  39.848  1.00 10.99      0.147 C
ATOM  15780  CG  ASP B 381       -9.563  34.630  38.695  1.00 15.49      0.175 C
ATOM  15781  OD1 ASP B 381      -10.042  35.806  38.732  1.00 17.68     -0.648 OA
ATOM  15782  OD2 ASP B 381       -9.801  33.841  37.757  1.00 13.91     -0.648 OA
ATOM  15783  N   LEU B 382      -11.002  33.138  42.606  1.00 12.48     -0.346 N
ATOM  15784  HN  LEU B 382      -10.472  33.498  43.400  1.00  0.00      0.163 HD
ATOM  15785  CA  LEU B 382      -12.167  32.302  42.877  1.00 11.03      0.177 C
ATOM  15787  C   LEU B 382      -13.080  32.905  43.957  1.00 14.46      0.241 C
ATOM  15788  O   LEU B 382      -13.865  32.218  44.631  1.00 15.33     -0.271 OA
ATOM  15789  CB  LEU B 382      -11.774  30.877  43.362  1.00 10.85      0.038 C
ATOM  15792  CG  LEU B 382      -11.195  30.000  42.235  1.00 17.19     -0.020 C
ATOM  15794  CD1 LEU B 382      -10.714  28.696  42.872  1.00 17.20      0.009 C
ATOM  15798  CD2 LEU B 382      -12.259  29.699  41.187  1.00 16.91      0.009 C
ATOM  15802  N   ALA B 383      -13.120  34.244  44.019  1.00 11.74     -0.346 N
ATOM  15803  HN  ALA B 383      -12.537  34.803  43.396  1.00  0.00      0.163 HD
ATOM  15804  CA  ALA B 383      -14.007  34.901  44.988  1.00 14.66      0.172 C
ATOM  15806  C   ALA B 383      -15.451  34.444  44.942  1.00 15.99      0.243 C
ATOM  15807  O   ALA B 383      -16.038  34.186  45.998  1.00 14.35     -0.271 OA
ATOM  15808  CB  ALA B 383      -13.940  36.428  44.864  1.00 16.60      0.042 C
ATOM  15812  N   PRO B 384      -16.101  34.295  43.786  1.00 17.72     -0.337 N
ATOM  15813  CA  PRO B 384      -17.494  33.897  43.715  1.00 17.41      0.179 C
ATOM  15815  C   PRO B 384      -17.753  32.433  44.044  1.00 18.08      0.241 C
ATOM  15816  O   PRO B 384      -18.923  32.025  44.233  1.00 16.78     -0.271 OA
ATOM  15817  CB  PRO B 384      -17.927  34.169  42.256  1.00 21.82      0.037 C
ATOM  15820  CG  PRO B 384      -16.703  34.458  41.487  1.00 20.36      0.022 C
ATOM  15823  CD  PRO B 384      -15.552  34.651  42.451  1.00 19.38      0.127 C
ATOM  15826  N   SER B 385      -16.711  31.608  44.050  1.00 11.48     -0.344 N
ATOM  15827  HN  SER B 385      -15.786  31.978  43.832  1.00  0.00      0.163 HD
ATOM  15828  CA  SER B 385      -16.850  30.186  44.359  1.00 13.73      0.200 C
ATOM  15830  C   SER B 385      -16.325  29.867  45.766  1.00 14.64      0.243 C
ATOM  15831  O   SER B 385      -16.944  29.021  46.416  1.00 15.07     -0.271 OA
ATOM  15832  CB  SER B 385      -16.012  29.282  43.412  1.00 17.29      0.199 C
ATOM  15835  OG  SER B 385      -16.509  29.449  42.112  1.00 28.58     -0.398 OA
ATOM  15836  HG  SER B 385      -15.997  28.897  41.533  1.00  0.00      0.209 HD
ATOM  15837  N   ASN B 386      -15.243  30.543  46.162  1.00 11.96     -0.345 N
ATOM  15838  HN  ASN B 386      -14.786  31.209  45.539  1.00  0.00      0.163 HD
ATOM  15839  CA  ASN B 386      -14.725  30.303  47.524  1.00 14.32      0.185 C
ATOM  15841  C   ASN B 386      -15.537  31.096  48.559  1.00 17.67      0.241 C
ATOM  15842  O   ASN B 386      -15.523  30.726  49.732  1.00 15.41     -0.271 OA
ATOM  15843  CB  ASN B 386      -13.275  30.743  47.663  1.00 13.04      0.137 C
ATOM  15846  CG  ASN B 386      -12.215  30.008  46.882  1.00 15.06      0.217 C
ATOM  15847  ND2 ASN B 386      -12.354  28.714  46.618  1.00 10.48     -0.370 N
ATOM  15848 1HD2 ASN B 386      -11.637  28.217  46.090  1.00  0.00      0.159 HD
ATOM  15849 2HD2 ASN B 386      -13.200  28.233  46.924  1.00  0.00      0.159 HD
ATOM  15850  OD1 ASN B 386      -11.181  30.596  46.508  1.00  9.21     -0.274 OA
ATOM  15851  N   LEU B 387      -16.208  32.165  48.133  1.00 10.32     -0.346 N
ATOM  15852  HN  LEU B 387      -16.134  32.413  47.146  1.00  0.00      0.163 HD
ATOM  15853  CA  LEU B 387      -17.040  33.003  48.985  1.00 12.47      0.177 C
ATOM  15855  C   LEU B 387      -16.227  33.715  50.074  1.00 14.91      0.241 C
ATOM  15856  O   LEU B 387      -16.484  33.611  51.276  1.00 13.54     -0.271 OA
ATOM  15857  CB  LEU B 387      -18.170  32.187  49.643  1.00 12.11      0.038 C
ATOM  15860  CG  LEU B 387      -19.058  31.409  48.640  1.00 22.30     -0.020 C
ATOM  15862  CD1 LEU B 387      -20.191  30.715  49.385  1.00 22.09      0.009 C
ATOM  15866  CD2 LEU B 387      -19.602  32.378  47.612  1.00 16.70      0.009 C
ATOM  15870  N   THR B 388      -15.248  34.465  49.648  1.00  9.78     -0.344 N
ATOM  15871  HN  THR B 388      -15.129  34.575  48.641  1.00  0.00      0.163 HD
ATOM  15872  CA  THR B 388      -14.310  35.157  50.534  1.00 12.97      0.205 C
ATOM  15874  C   THR B 388      -14.598  36.637  50.707  1.00 14.48      0.243 C
ATOM  15875  O   THR B 388      -13.930  37.244  51.554  1.00 14.90     -0.271 OA
ATOM  15876  CB  THR B 388      -12.864  34.969  49.984  1.00 14.51      0.146 C
ATOM  15878  CG2 THR B 388      -12.452  33.542  50.268  1.00 16.37      0.042 C
ATOM  15882  OG1 THR B 388      -12.879  35.161  48.564  1.00 18.19     -0.393 OA
ATOM  15883  HG1 THR B 388      -11.998  35.046  48.229  1.00  0.00      0.210 HD
ATOM  15884  N   LEU B 389      -15.524  37.204  49.931  1.00 14.74     -0.346 N
ATOM  15885  HN  LEU B 389      -15.982  36.654  49.204  1.00  0.00      0.163 HD
ATOM  15886  CA  LEU B 389      -15.889  38.616  50.117  1.00 13.98      0.177 C
ATOM  15888  C   LEU B 389      -16.967  38.752  51.191  1.00 19.55      0.241 C
ATOM  15889  O   LEU B 389      -17.863  37.900  51.269  1.00 17.89     -0.271 OA
ATOM  15890  CB  LEU B 389      -16.510  39.128  48.791  1.00 14.28      0.038 C
ATOM  15893  CG  LEU B 389      -15.435  39.277  47.691  1.00 22.34     -0.020 C
ATOM  15895  CD1 LEU B 389      -16.127  39.383  46.343  1.00 23.72      0.009 C
ATOM  15899  CD2 LEU B 389      -14.522  40.463  47.979  1.00 19.40      0.009 C
ATOM  15903  N   TRP B 390      -16.941  39.816  51.983  1.00 18.61     -0.346 N
ATOM  15904  HN  TRP B 390      -16.170  40.479  51.906  1.00  0.00      0.163 HD
ATOM  15905  CA  TRP B 390      -17.999  40.055  52.964  1.00 18.98      0.181 C
ATOM  15907  C   TRP B 390      -18.495  41.467  52.667  1.00 18.12      0.241 C
ATOM  15908  O   TRP B 390      -17.887  42.129  51.812  1.00 15.33     -0.271 OA
ATOM  15909  CB  TRP B 390      -17.590  39.813  54.402  1.00 13.38      0.075 C
ATOM  15912  CG  TRP B 390      -16.502  40.711  54.900  1.00 17.42     -0.028 A
ATOM  15913  CD1 TRP B 390      -15.150  40.642  54.589  1.00 17.51      0.096 A
ATOM  15915  CD2 TRP B 390      -16.644  41.745  55.861  1.00 16.79     -0.002 A
ATOM  15916  CE2 TRP B 390      -15.379  42.314  56.079  1.00 19.76      0.042 A
ATOM  15917  CE3 TRP B 390      -17.770  42.267  56.547  1.00 21.51      0.014 A
ATOM  15919  NE1 TRP B 390      -14.505  41.629  55.296  1.00 17.68     -0.365 N
ATOM  15920  HE1 TRP B 390      -13.505  41.821  55.240  1.00  0.00      0.165 HD
ATOM  15921  CZ2 TRP B 390      -15.196  43.374  56.967  1.00 18.44      0.030 A
ATOM  15923  CZ3 TRP B 390      -17.566  43.312  57.423  1.00 20.60      0.001 A
ATOM  15925  CH2 TRP B 390      -16.305  43.878  57.606  1.00 17.52      0.002 A
ATOM  15927  N   SER B 391      -19.522  41.942  53.378  1.00 17.28     -0.344 N
ATOM  15928  HN  SER B 391      -19.896  41.418  54.169  1.00  0.00      0.163 HD
ATOM  15929  CA  SER B 391      -20.098  43.235  52.993  1.00 16.26      0.200 C
ATOM  15931  C   SER B 391      -19.118  44.368  53.187  1.00 16.08      0.242 C
ATOM  15932  O   SER B 391      -19.207  45.386  52.481  1.00 18.97     -0.271 OA
ATOM  15933  CB  SER B 391      -21.415  43.464  53.773  1.00 18.49      0.199 C
ATOM  15936  OG  SER B 391      -21.086  43.582  55.151  1.00 21.08     -0.398 OA
ATOM  15937  HG  SER B 391      -21.894  43.723  55.630  1.00  0.00      0.209 HD
ATOM  15938  N   GLY B 392      -18.171  44.275  54.092  1.00 13.64     -0.350 N
ATOM  15939  HN  GLY B 392      -18.170  43.448  54.689  1.00  0.00      0.163 HD
ATOM  15940  CA  GLY B 392      -17.133  45.252  54.307  1.00 14.91      0.225 C
ATOM  15943  C   GLY B 392      -15.844  45.050  53.542  1.00 16.13      0.236 C
ATOM  15944  O   GLY B 392      -14.895  45.815  53.797  1.00 17.92     -0.272 OA
ATOM  15945  N   SER B 393      -15.715  44.084  52.640  1.00 13.78     -0.344 N
ATOM  15946  HN  SER B 393      -16.488  43.439  52.475  1.00  0.00      0.163 HD
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ATOM  15947  CA  SER B 393     -14.472  43.937  51.881  1.00 11.23      0.200 C
ATOM  15949  C   SER B 393     -14.264  45.137  50.956  1.00 17.06      0.243 C
ATOM  15950  O   SER B 393     -15.192  45.528  50.241  1.00 13.64     -0.271 OA
ATOM  15951  CB  SER B 393     -14.546  42.737  50.903  1.00 15.71      0.199 C
ATOM  15954  OG  SER B 393     -14.557  41.549  51.700  1.00 17.76     -0.398 OA
ATOM  15955  HG  SER B 393     -14.602  40.813  51.101  1.00  0.00      0.209 HD
ATOM  15956  N   LYS B 394     -13.067  45.664  50.922  1.00 12.79     -0.346 N
ATOM  15957  HN  LYS B 394     -12.372  45.326  51.588  1.00  0.00      0.163 HD
ATOM  15958  CA  LYS B 394     -12.670  46.713  49.980  1.00 12.68      0.176 C
ATOM  15960  C   LYS B 394     -11.341  46.252  49.390  1.00 13.43      0.241 C
ATOM  15961  O   LYS B 394     -10.388  46.066  50.146  1.00 11.04     -0.271 OA
ATOM  15962  CB  LYS B 394     -12.406  48.040  50.687  1.00 18.23      0.035 C
ATOM  15965  CG  LYS B 394     -13.658  48.656  51.299  1.00 33.21      0.004 C
ATOM  15968  CD  LYS B 394     -13.295  49.297  52.632  1.00 51.66      0.027 C
ATOM  15971  CE  LYS B 394     -14.427  50.154  53.167  1.00 62.79      0.229 C
ATOM  15974  NZ  LYS B 394     -14.256  50.466  54.613  1.00 71.33     -0.079 N
ATOM  15975  HZ1 LYS B 394     -15.017  51.042  54.973  1.00  0.00      0.274 HD
ATOM  15976  HZ2 LYS B 394     -13.349  50.896  54.794  1.00  0.00      0.274 HD
ATOM  15977  HZ3 LYS B 394     -14.144  49.615  55.164  1.00  0.00      0.274 HD
ATOM  15978  N   ALA B 395     -11.252  46.117  48.087  1.00 10.15     -0.346 N
ATOM  15979  HN  ALA B 395     -12.038  46.394  47.499  1.00  0.00      0.163 HD
ATOM  15980  CA  ALA B 395     -10.043  45.576  47.464  1.00 10.32      0.172 C
ATOM  15982  C   ALA B 395     -8.956  46.629  47.407  1.00 11.52      0.240 C
ATOM  15983  O   ALA B 395     -9.247  47.764  47.031  1.00 12.08     -0.271 OA
ATOM  15984  CB  ALA B 395     -10.381  45.110  46.027  1.00 13.35      0.042 C
ATOM  15988  N   ILE B 396     -7.700  46.235  47.690  1.00  8.72     -0.346 N
ATOM  15989  HN  ILE B 396     -7.504  45.245  47.838  1.00  0.00      0.163 HD
ATOM  15990  CA  ILE B 396     -6.620  47.204  47.787  1.00 10.87      0.180 C
ATOM  15992  C   ILE B 396     -6.134  47.659  46.409  1.00 14.64      0.241 C
ATOM  15993  O   ILE B 396     -5.394  48.642  46.328  1.00 14.42     -0.271 OA
ATOM  15994  CB  ILE B 396     -5.440  46.755  48.659  1.00 11.78      0.013 C
ATOM  15996  CG1 ILE B 396     -4.670  45.617  47.954  1.00 17.71      0.002 C
ATOM  15999  CG2 ILE B 396     -5.922  46.382  50.070  1.00  7.51      0.012 C
ATOM  16003  CD1 ILE B 396     -3.419  45.154  48.652  1.00 15.90      0.005 C
ATOM  16007  N   ASN B 397     -6.600  47.056  45.302  1.00 16.14     -0.346 N
ATOM  16008  HN  ASN B 397     -7.168  46.209  45.338  1.00  0.00      0.163 HD
ATOM  16009  CA  ASN B 397     -6.228  47.713  44.022  1.00 19.03      0.185 C
ATOM  16011  C   ASN B 397     -7.162  48.873  43.764  1.00 20.02      0.241 C
ATOM  16012  O   ASN B 397     -6.867  49.701  42.884  1.00 25.44     -0.271 OA
ATOM  16013  CB  ASN B 397     -6.220  46.744  42.845  1.00 22.65      0.137 C
ATOM  16016  CG  ASN B 397     -7.571  46.096  42.739  1.00 21.94      0.217 C
ATOM  16017  ND2 ASN B 397     -8.286  46.363  41.635  1.00 29.83     -0.370 N
ATOM  16018 1HD2 ASN B 397     -7.944  46.955  40.878  1.00  0.00      0.159 HD
ATOM  16019 2HD2 ASN B 397     -9.203  45.923  41.563  1.00  0.00      0.159 HD
ATOM  16020  OD1 ASN B 397     -7.980  45.389  43.643  1.00 20.86     -0.274 OA
ATOM  16021  N   GLU B 398     -8.254  49.023  44.483  1.00 14.96     -0.346 N
ATOM  16022  HN  GLU B 398     -8.473  48.304  45.172  1.00  0.00      0.163 HD
ATOM  16023  CA  GLU B 398     -9.169  50.146  44.360  1.00 18.09      0.177 C
ATOM  16025  C   GLU B 398     -8.988  51.152  45.508  1.00 23.21      0.241 C
ATOM  16026  O   GLU B 398     -8.967  52.367  45.306  1.00 23.35     -0.271 OA
ATOM  16027  CB  GLU B 398     -10.632  49.691  44.392  1.00 19.28      0.045 C
ATOM  16030  CG  GLU B 398     -10.949  48.574  43.406  1.00 34.49      0.116 C
ATOM  16033  CD  GLU B 398     -12.380  48.098  43.316  1.00 41.85      0.172 C
ATOM  16034  OE1 GLU B 398     -13.182  48.197  44.272  1.00 47.35     -0.648 OA
ATOM  16035  OE2 GLU B 398     -12.746  47.576  42.231  1.00 49.10     -0.648 OA
ATOM  16036  N   ASP B 399     -8.828  50.662  46.720  1.00 13.82     -0.346 N
ATOM  16037  HN  ASP B 399     -8.810  49.651  46.852  1.00  0.00      0.163 HD
ATOM  16038  CA  ASP B 399     -8.673  51.553  47.899  1.00 14.78      0.186 C
ATOM  16040  C   ASP B 399     -7.471  51.042  48.670  1.00 11.92      0.241 C
ATOM  16041  O   ASP B 399     -7.517  49.951  49.265  1.00 13.03     -0.271 OA
ATOM  16042  CB  ASP B 399     -9.961  51.401  48.677  1.00 16.76      0.147 C
ATOM  16045  CG  ASP B 399     -9.973  52.084  50.034  1.00 27.88      0.175 C
ATOM  16046  OD1 ASP B 399     -9.991  52.667  50.983  1.00 34.48     -0.648 OA
ATOM  16047  OD2 ASP B 399     -11.030  52.019  50.674  1.00 27.04     -0.648 OA
ATOM  16048  N   ALA B 400     -6.387  51.827  48.714  1.00 12.53     -0.346 N
ATOM  16049  HN  ALA B 400     -6.411  52.734  48.248  1.00  0.00      0.163 HD
ATOM  16050  CA  ALA B 400     -5.173  51.419  49.410  1.00 14.16      0.172 C
ATOM  16052  C   ALA B 400     -5.407  51.106  50.878  1.00 13.29      0.240 C
ATOM  16053  O   ALA B 400     -4.572  50.394  51.468  1.00 12.53     -0.271 OA
ATOM  16054  CB  ALA B 400     -4.126  52.530  49.309  1.00 20.68      0.042 C
ATOM  16058  N   ALA B 401     -6.457  51.628  51.506  1.00 10.58     -0.346 N
ATOM  16059  HN  ALA B 401     -7.111  52.230  51.005  1.00  0.00      0.163 HD
ATOM  16060  CA  ALA B 401     -6.666  51.326  52.937  1.00 10.41      0.172 C
ATOM  16062  C   ALA B 401     -7.600  50.145  53.134  1.00 11.36      0.240 C
ATOM  16063  O   ALA B 401     -8.158  49.959  54.224  1.00 12.74     -0.271 OA
ATOM  16064  CB  ALA B 401     -7.284  52.541  53.648  1.00 13.24      0.042 C
ATOM  16068  N   GLY B 402     -7.785  49.320  52.103  1.00 12.01     -0.351 N
ATOM  16069  HN  GLY B 402     -7.247  49.479  51.251  1.00  0.00      0.163 HD
ATOM  16070  CA  GLY B 402     -8.711  48.212  52.136  1.00 10.05      0.225 C
ATOM  16073  C   GLY B 402     -8.270  46.963  52.872  1.00 16.11      0.236 C
ATOM  16074  O   GLY B 402     -7.302  47.028  53.624  1.00 12.34     -0.272 OA
ATOM  16075  N   ASN B 403     -8.973  45.849  52.621  1.00  9.81     -0.346 N
ATOM  16076  HN  ASN B 403     -9.667  45.834  51.874  1.00  0.00      0.163 HD
ATOM  16077  CA  ASN B 403     -8.731  44.646  53.437  1.00  9.79      0.185 C
ATOM  16079  C   ASN B 403     -8.971  43.376  52.620  1.00 10.66      0.241 C
ATOM  16080  O   ASN B 403     -9.212  42.302  53.187  1.00 10.35     -0.271 OA
ATOM  16081  CB  ASN B 403     -9.741  44.633  54.598  1.00  9.02      0.137 C
ATOM  16084  CG  ASN B 403     -11.175  44.757  54.150  1.00 19.19      0.217 C
ATOM  16085  ND2 ASN B 403     -12.131  45.116  54.988  1.00 16.67     -0.370 N
ATOM  16086 1HD2 ASN B 403     -13.101  45.200  54.685  1.00  0.00      0.159 HD
ATOM  16087 2HD2 ASN B 403     -11.872  45.323  55.953  1.00  0.00      0.159 HD
ATOM  16088  OD1 ASN B 403     -11.490  44.506  52.979  1.00 12.12     -0.274 OA
ATOM  16089  N   TYR B 404     -8.799  43.536  51.317  1.00 10.11     -0.346 N
ATOM  16090  HN  TYR B 404     -8.542  44.442  50.926  1.00  0.00      0.163 HD
ATOM  16091  CA  TYR B 404     -8.994  42.350  50.444  1.00  8.33      0.180 C
ATOM  16093  C   TYR B 404     -8.071  42.450  49.260  1.00 11.81      0.241 C
ATOM  16094  O   TYR B 404     -7.857  43.565  48.727  1.00 11.23     -0.271 OA
ATOM  16095  CB  TYR B 404     -10.499  42.324  50.009  1.00  7.75      0.073 C
ATOM  16098  CG  TYR B 404     -10.824  41.029  49.253  1.00 10.11     -0.056 A
ATOM  16099  CD1 TYR B 404     -10.621  40.937  47.879  1.00 11.62      0.010 A
ATOM  16101  CD2 TYR B 404     -11.223  39.911  49.945  1.00 12.63      0.010 A
ATOM  16103  CE1 TYR B 404     -10.862  39.731  47.220  1.00  8.44      0.037 A
ATOM  16105  CE2 TYR B 404     -11.488  38.715  49.299  1.00 12.16      0.037 A
ATOM  16107  CZ  TYR B 404     -11.305  38.648  47.938  1.00  9.05      0.065 A
ATOM  16108  OH  TYR B 404     -11.549  37.423  47.323  1.00 14.87     -0.361 OA
ATOM  16109  HH  TYR B 404     -11.422  37.377  46.383  1.00  0.00      0.217 HD
ATOM  16110  N   ILE B 405     -7.555  41.271  48.812  1.00  8.67     -0.346 N
ATOM  16111  HN  ILE B 405     -7.771  40.393  49.287  1.00  0.00      0.163 HD
ATOM  16112  CA  ILE B 405     -6.690  41.289  47.639  1.00  9.68      0.180 C
ATOM  16114  C   ILE B 405     -7.204  40.359  46.539  1.00  8.52      0.241 C
ATOM  16115  O   ILE B 405     -7.383  39.179  46.817  1.00  9.25     -0.271 OA
ATOM  16116  CB  ILE B 405     -5.245  40.824  47.994  1.00 11.67      0.013 C
ATOM  16118  CG1 ILE B 405     -4.675  41.649  49.136  1.00 15.29      0.002 C
ATOM  16121  CG2 ILE B 405     -4.330  40.817  46.770  1.00 12.61      0.012 C
ATOM  16125  CD1 ILE B 405     -3.376  41.305  49.799  1.00 19.83      0.005 C
ATOM  16129  N   HIS B 406     -7.372  40.845  45.301  1.00  9.89     -0.346 N
ATOM  16130  HN  HIS B 406     -7.303  41.849  45.134  1.00  0.00      0.163 HD
ATOM  16131  CA  HIS B 406     -7.655  39.933  44.186  1.00  9.74      0.182 C
ATOM  16133  C   HIS B 406     -6.286  39.397  43.774  1.00  9.79      0.241 C
ATOM  16134  O   HIS B 406     -5.462  40.147  43.231  1.00 11.22     -0.271 OA
ATOM  16135  CB  HIS B 406     -8.300  40.694  43.021  1.00  9.74      0.093 C
ATOM  16138  CG  HIS B 406     -9.722  41.096  43.290  1.00 16.36      0.028 A
ATOM  16139  CD2 HIS B 406     -10.241  42.303  43.708  1.00 19.07      0.114 A
ATOM  16141  ND1 HIS B 406     -10.790  40.245  43.120  1.00 17.10     -0.354 N
ATOM  16142  HD1 HIS B 406     -10.725  39.272  42.820  1.00  0.00      0.166 HD
ATOM  16143  CE1 HIS B 406     -11.934  40.893  43.411  1.00 19.27      0.180 A
ATOM  16145  NE2 HIS B 406     -11.608  42.126  43.775  1.00 19.43     -0.360 N
ATOM  16146  HE2 HIS B 406     -12.274  42.843  44.064  1.00  0.00      0.166 HD
ATOM  16147  N   TYR B 407     -5.917  38.178  44.158  1.00  6.98     -0.346 N
ATOM  16148  HN  TYR B 407     -6.583  37.587  44.656  1.00  0.00      0.163 HD
ATOM  16149  CA  TYR B 407     -4.583  37.673  43.881  1.00  7.14      0.180 C
ATOM  16151  C   TYR B 407     -4.405  37.176  42.443  1.00  8.93      0.241 C
ATOM  16152  O   TYR B 407     -3.259  36.965  42.025  1.00  8.96     -0.271 OA
ATOM  16153  CB  TYR B 407     -4.284  36.518  44.864  1.00  4.84      0.073 C
ATOM  16156  CG  TYR B 407     -3.870  36.898  46.264  1.00  4.94     -0.056 A
ATOM  16157  CD1 TYR B 407     -2.570  37.298  46.499  1.00  8.93      0.010 A
ATOM  16159  CD2 TYR B 407     -4.789  36.862  47.318  1.00  5.02      0.010 A
ATOM  16161  CE1 TYR B 407     -2.125  37.653  47.778  1.00  8.24      0.037 A
ATOM  16163  CE2 TYR B 407     -4.373  37.175  48.611  1.00  6.82      0.037 A
ATOM  16165  CZ  TYR B 407     -3.054  37.579  48.789  1.00  8.99      0.065 A
ATOM  16166  OH  TYR B 407     -2.601  37.853  50.065  1.00  9.62     -0.361 OA
ATOM  16167  HH  TYR B 407     -1.700  38.129  50.187  1.00  0.00      0.217 HD
ATOM  16168  N   GLY B 408     -5.480  37.012  41.664  1.00  8.42     -0.351 N
ATOM  16169  HN  GLY B 408     -6.406  37.295  41.985  1.00  0.00      0.163 HD
ATOM  16170  CA  GLY B 408     -5.293  36.411  40.328  1.00 11.20      0.225 C
ATOM  16173  C   GLY B 408     -5.004  34.926  40.474  1.00  9.79      0.236 C
ATOM  16174  O   GLY B 408     -5.074  34.350  41.573  1.00  9.50     -0.272 OA
ATOM  16175  N   VAL B 409     -4.697  34.227  39.392  1.00  8.62     -0.346 N
ATOM  16176  HN  VAL B 409     -4.558  34.717  38.508  1.00  0.00      0.163 HD
ATOM  16177  CA  VAL B 409     -4.551  32.764  39.428  1.00  6.78      0.180 C
ATOM  16179  C   VAL B 409     -3.116  32.429  39.783  1.00  8.84      0.241 C
ATOM  16180  O   VAL B 409     -2.293  32.052  38.916  1.00  7.35     -0.271 OA
ATOM  16181  CB  VAL B 409     -4.950  32.180  38.048  1.00 13.09      0.009 C
ATOM  16183  CG1 VAL B 409     -5.064  30.664  38.249  1.00 13.32      0.012 C
ATOM  16187  CG2 VAL B 409     -6.276  32.745  37.535  1.00  9.99      0.012 C
ATOM  16191  N   ARG B 410     -2.752  32.640  41.060  1.00  8.68     -0.346 N
ATOM  16192  HN  ARG B 410     -3.489  32.832  41.739  1.00  0.00      0.163 HD
ATOM  16193  CA  ARG B 410     -1.363  32.613  41.544  1.00  5.71      0.176 C
ATOM  16195  C   ARG B 410     -1.389  32.016  42.962  1.00  7.64      0.241 C
ATOM  16196  O   ARG B 410     -1.108  32.708  43.952  1.00  8.29     -0.271 OA
ATOM  16197  CB  ARG B 410     -0.903  34.069  41.696  1.00  5.11      0.036 C
ATOM  16200  CG  ARG B 410     -0.805  34.854  40.393  1.00  9.08      0.023 C
ATOM  16203  CD  ARG B 410     -0.235  36.237  40.630  1.00  9.12      0.138 C
ATOM  16206  NE  ARG B 410     -0.206  37.091  39.432  1.00  9.97     -0.227 N
ATOM  16207  HE  ARG B 410      0.560  36.924  38.779  1.00  0.00      0.177 HD
ATOM  16208  CZ  ARG B 410     -1.037  38.030  39.108  1.00 12.06      0.665 C
ATOM  16209  NH1 ARG B 410     -2.116  38.353  39.816  1.00  8.09     -0.235 N
ATOM  16210 1HH1 ARG B 410     -2.770  39.093  39.561  1.00  0.00      0.174 HD
ATOM  16211 2HH1 ARG B 410     -2.289  37.812  40.663  1.00  0.00      0.174 HD
ATOM  16212  NH2 ARG B 410     -0.806  38.752  37.978  1.00  7.44     -0.235 N
ATOM  16213 1HH2 ARG B 410     -1.460  39.492  37.723  1.00  0.00      0.174 HD
ATOM  16214 2HH2 ARG B 410      0.021  38.504  37.435  1.00  0.00      0.174 HD
ATOM  16215  N   GLU B 411     -1.655  30.707  43.035  1.00  5.96     -0.346 N
ATOM  16216  HN  GLU B 411     -1.745  30.134  42.196  1.00  0.00      0.163 HD
ATOM  16217  CA  GLU B 411     -1.811  30.132  44.377  1.00  6.20      0.177 C
ATOM  16219  C   GLU B 411     -0.579  30.130  45.239  1.00  5.44      0.241 C
ATOM  16220  O   GLU B 411     -0.678  30.336  46.455  1.00  8.51     -0.271 OA
ATOM  16221  CB  GLU B 411     -2.289  28.645  44.204  1.00  7.06      0.045 C
ATOM  16224  CG  GLU B 411     -3.729  28.610  43.628  1.00  7.95      0.116 C
ATOM  16227  CD  GLU B 411     -3.724  28.496  42.109  1.00 15.83      0.172 C
ATOM  16228  OE1 GLU B 411     -2.667  28.473  41.454  1.00  9.57     -0.648 OA
ATOM  16229  OE2 GLU B 411     -4.803  28.459  41.451  1.00 15.34     -0.648 OA
ATOM  16230  N   PHE B 412      0.550  29.737  44.664  1.00  5.29     -0.346 N
ATOM  16231  HN  PHE B 412      0.536  29.496  43.673  1.00  0.00      0.163 HD
ATOM  16232  CA  PHE B 412      1.822  29.634  45.397  1.00  5.16      0.180 C
ATOM  16234  C   PHE B 412      2.283  31.046  45.815  1.00  7.14      0.241 C
ATOM  16235  O   PHE B 412      2.503  31.301  47.006  1.00  6.36     -0.271 OA
ATOM  16236  CB  PHE B 412      2.893  29.004  44.507  1.00  7.69      0.073 C
ATOM  16239  CG  PHE B 412      4.182  28.595  45.168  1.00 10.00     -0.056 A
ATOM  16240  CD1 PHE B 412      4.324  28.625  46.568  1.00  3.17      0.007 A
ATOM  16242  CD2 PHE B 412      5.240  28.182  44.373  1.00 10.52      0.007 A
ATOM  16244  CE1 PHE B 412      5.547  28.239  47.109  1.00 10.14      0.001 A
ATOM  16246  CE2 PHE B 412      6.454  27.762  44.927  1.00  8.38      0.001 A
ATOM  16248  CZ  PHE B 412      6.589  27.814  46.301  1.00 11.88      0.000 A
ATOM  16250  N   GLY B 413      2.191  32.008  44.899  1.00  5.73     -0.351 N
ATOM  16251  HN  GLY B 413      1.864  31.761  43.965  1.00  0.00      0.163 HD
ATOM  16252  CA  GLY B 413      2.537  33.400  45.170  1.00  6.16      0.225 C
ATOM  16255  C   GLY B 413      1.604  33.989  46.225  1.00  8.09      0.236 C
ATOM  16256  O   GLY B 413      2.074  34.600  47.208  1.00  6.64     -0.272 OA
ATOM  16257  N   MET B 414      0.306  33.711  46.104  1.00  5.39     -0.346 N
ATOM  16258  HN  MET B 414     -0.028  33.176  45.303  1.00  0.00      0.163 HD
ATOM  16259  CA  MET B 414     -0.640  34.174  47.122  1.00  5.81      0.177 C
ATOM  16261  CB  MET B 414     -0.249  33.728  48.536  1.00  7.95      0.241 C
ATOM  16262  O   MET B 414     -0.348  34.509  49.496  1.00  7.19     -0.271 OA
ATOM  16263  CB  MET B 414     -2.031  33.569  46.783  1.00  5.95      0.045 C
ATOM  16266  CG  MET B 414     -3.043  33.755  47.953  1.00  8.85      0.076 C
ATOM  16269  SD  MET B 414     -4.715  33.166  47.489  1.00  9.51     -0.173 SA
ATOM  16270  CE  MET B 414     -4.487  31.380  47.506  1.00  7.51      0.089 C
ATOM  16274  N   THR B 415      0.022  32.409  48.641  1.00  4.89     -0.344 N
ATOM  16275  HN  THR B 415      0.043  31.811  47.815  1.00  0.00      0.163 HD
ATOM  16276  CA  THR B 415      0.290  31.851  49.999  1.00  8.05      0.205 C
ATOM  16278  C   THR B 415      1.595  32.397  50.543  1.00  8.98      0.243 C
ATOM  16279  O   THR B 415      1.654  32.761  51.733  1.00  6.52     -0.271 OA
ATOM  16280  CB  THR B 415      0.274  30.317  49.946  1.00  7.06      0.146 C
ATOM  16282  CG2 THR B 415      0.269  29.650  51.326  1.00  7.13      0.042 C
ATOM  16286  OG1 THR B 415     -0.939  29.918  49.280  1.00  9.44     -0.393 OA
ATOM  16287  HG1 THR B 415     -0.936  30.331  48.425  1.00  0.00      0.210 HD
ATOM  16288  N   ALA B 416      2.633  32.534  49.727  1.00  6.60     -0.346 N
ATOM  16289  HN  ALA B 416      2.554  32.270  48.745  1.00  0.00      0.163 HD
ATOM  16290  CA  ALA B 416      3.903  33.073  50.255  1.00  5.98      0.172 C
ATOM  16292  C   ALA B 416      3.849  34.570  50.477  1.00  8.67      0.240 C
ATOM  16293  O   ALA B 416      4.570  35.085  51.336  1.00  7.28     -0.271 OA
ATOM  16294  CB  ALA B 416      5.022  32.698  49.271  1.00 10.04      0.042 C
ATOM  16298  N   ILE B 417      3.049  35.312  49.682  1.00  7.62     -0.346 N
ATOM  16299  HN  ILE B 417      2.606  34.881  48.871  1.00  0.00      0.163 HD
ATOM  16300  CA  ILE B 417      2.811  36.724  49.970  1.00  8.14      0.180 C
ATOM  16302  C   ILE B 417      2.117  36.869  51.323  1.00  7.65      0.241 C
ATOM  16303  O   ILE B 417      2.512  37.687  52.186  1.00  7.00     -0.271 OA
ATOM  16304  CB  ILE B 417      1.925  37.379  48.867  1.00  9.20      0.013 C
ATOM  16306  CG1 ILE B 417      2.861  37.681  47.664  1.00  7.35      0.002 C
ATOM  16309  CG2 ILE B 417      1.284  38.668  49.366  1.00  7.12      0.012 C
ATOM  16313  CD1 ILE B 417      2.031  38.048  46.409  1.00  8.16      0.005 C
ATOM  16317  N   ALA B 418      1.095  36.047  51.605  1.00  6.52     -0.346 N
ATOM  16318  HN  ALA B 418      0.801  35.355  50.915  1.00  0.00      0.163 HD
ATOM  16319  CA  ALA B 418      0.395  36.129  52.889  1.00  6.87      0.172 C
ATOM  16321  C   ALA B 418      1.342  35.778  54.032  1.00  6.68      0.240 C
ATOM  16322  O   ALA B 418      1.184  36.379  55.132  1.00  6.14     -0.271 OA
ATOM  16323  CB  ALA B 418     -0.852  35.190  52.826  1.00  6.48      0.042 C
ATOM  16327  N   ASN B 419      2.321  34.883  53.827  1.00  5.10     -0.346 N
ATOM  16328  HN  ASN B 419      2.371  34.369  52.947  1.00  0.00      0.163 HD
ATOM  16329  CA  ASN B 419      3.321  34.649  54.880  1.00  2.84      0.185 C
ATOM  16331  C   ASN B 419      4.133  35.937  55.143  1.00  7.88      0.241 C
ATOM  16332  O   ASN B 419      4.386  36.224  56.304  1.00  8.87     -0.271 OA
ATOM  16333  CB  ASN B 419      4.386  33.568  54.475  1.00  5.75      0.137 C
ATOM  16336  CG  ASN B 419      3.814  32.164  54.427  1.00 13.26      0.217 C
ATOM  16337  ND2 ASN B 419      4.458  31.193  53.812  1.00  8.97     -0.370 N
ATOM  16338 1HD2 ASN B 419      5.346  31.359  53.339  1.00  0.00      0.159 HD
ATOM  16339 2HD2 ASN B 419      4.073  30.249  53.780  1.00  0.00      0.159 HD
ATOM  16340  OD1 ASN B 419      2.732  31.962  55.003  1.00  8.99     -0.274 OA
ATOM  16341  N   GLY B 420      4.447  36.714  54.131  1.00  5.95     -0.351 N
ATOM  16342  HN  GLY B 420      4.200  36.425  53.185  1.00  0.00      0.163 HD
ATOM  16343  CA  GLY B 420      5.152  38.002  54.335  1.00  4.04      0.225 C
ATOM  16346  C   GLY B 420      4.231  38.976  55.060  1.00  6.43      0.236 C
ATOM  16347  O   GLY B 420      4.688  39.754  55.925  1.00  8.30     -0.272 OA
ATOM  16348  N   ILE B 421      2.941  38.979  54.770  1.00  5.92     -0.346 N
ATOM  16349  HN  ILE B 421      2.595  38.343  54.052  1.00  0.00      0.163 HD
ATOM  16350  CA  ILE B 421      1.983  39.876  55.454  1.00  7.89      0.180 C
ATOM  16352  C   ILE B 421      2.017  39.560  56.944  1.00  8.66      0.241 C
ATOM  16353  O   ILE B 421      2.021  40.440  57.846  1.00  8.20     -0.271 OA
ATOM  16354  CB  ILE B 421      0.560  39.694  54.862  1.00  7.12      0.013 C
ATOM  16356  CG1 ILE B 421      0.616  40.328  53.423  1.00  9.21      0.002 C
ATOM  16359  CG2 ILE B 421     -0.466  40.447  55.676  1.00 12.63      0.012 C
ATOM  16363  CD1 ILE B 421     -0.697  40.121  52.634  1.00 13.46      0.005 C
ATOM  16367  N   SER B 422      1.901  38.264  57.236  1.00  7.32     -0.344 N
ATOM  16368  HN  SER B 422      1.829  37.567  56.495  1.00  0.00      0.163 HD
ATOM  16369  CA  SER B 422      1.880  37.864  58.650  1.00 11.68      0.200 C
ATOM  16371  C   SER B 422      3.201  38.173  59.321  1.00  9.91      0.243 C
ATOM  16372  O   SER B 422      3.204  38.642  60.490  1.00 10.07     -0.271 OA
ATOM  16373  CB  SER B 422      1.413  36.402  58.718  1.00 11.05      0.199 C
ATOM  16376  OG ASER B 422      2.474  35.529  58.568  0.50 12.53     -0.398 OA
ATOM  16377  HG ASER B 422      2.185  34.625  58.610  1.00  0.00      0.209 HD
ATOM  16378  N   LEU B 423      4.358  37.988  58.716  1.00  7.67     -0.346 N
ATOM  16379  HN  LEU B 423      4.359  37.604  57.771  1.00  0.00      0.163 HD
ATOM  16380  CA  LEU B 423      5.648  38.312  59.348  1.00  9.81      0.177 C
ATOM  16382  C   LEU B 423      5.826  39.811  59.608  1.00 12.96      0.241 C
ATOM  16383  O   LEU B 423      6.483  40.231  60.584  1.00 12.21     -0.271 OA
ATOM  16384  CB  LEU B 423      6.771  37.836  58.405  1.00  7.24      0.038 C
ATOM  16387  CG  LEU B 423      6.977  36.304  58.410  1.00 11.89     -0.020 C
ATOM  16389  CD1 LEU B 423      7.827  35.894  57.198  1.00 11.16      0.009 C
ATOM  16393  CD2 LEU B 423      7.681  35.822  59.675  1.00 14.08      0.009 C
ATOM  16397  N   HIS B 424      5.218  40.644  58.756  1.00  8.68     -0.346 N
ATOM  16398  HN  HIS B 424      4.667  40.256  57.990  1.00  0.00      0.163 HD
ATOM  16399  CA  HIS B 424      5.322  42.102  58.893  1.00  7.69      0.182 C
ATOM  16401  C   HIS B 424      4.694  42.596  60.193  1.00 11.79      0.241 C
ATOM  16402  O   HIS B 424      5.334  43.448  60.830  1.00 10.23     -0.271 OA
ATOM  16403  CB  HIS B 424      4.615  42.846  57.735  1.00 10.60      0.093 C
ATOM  16406  CG  HIS B 424      4.855  44.342  57.771  1.00 10.48      0.028 A
ATOM  16407  CD2 HIS B 424      5.803  45.111  57.174  1.00  8.59      0.114 A
ATOM  16409  ND1 HIS B 424      4.057  45.165  58.519  1.00  9.30     -0.354 N
ATOM  16410  HD1 HIS B 424      3.252  44.866  59.069  1.00  0.00      0.166 HD
ATOM  16411  CE1 HIS B 424      4.504  46.435  58.414  1.00 12.00      0.180 A
ATOM  16413  NE2 HIS B 424      5.566  46.430  57.573  1.00  9.29     -0.360 N
ATOM  16414  HE2 HIS B 424      6.101  47.248  57.281  1.00  0.00      0.166 HD
ATOM  16415  N   GLY B 425      3.527  42.083  60.534  1.00  9.54     -0.351 N
ATOM  16416  HN  GLY B 425      3.117  41.356  59.947  1.00  0.00      0.163 HD
ATOM  16417  CA  GLY B 425      2.795  42.526  61.736  1.00 11.26      0.225 C
ATOM  16420  C   GLY B 425      1.707  43.532  61.308  1.00 10.89     -0.235 C
ATOM  16421  O   GLY B 425      1.885  44.205  60.298  1.00  9.91     -0.272 OA
ATOM  16422  N   GLY B 426      0.582  43.583  62.049  1.00  8.56     -0.351 N
ATOM  16423  HN  GLY B 426      0.459  42.939  62.831  1.00  0.00      0.163 HD
ATOM  16424  CA  GLY B 426     -0.458  44.553  61.738  1.00  8.51      0.225 C
ATOM  16427  C   GLY B 426     -1.720  43.937  61.159  1.00  9.53      0.236 C
ATOM  16428  O   GLY B 426     -2.769  44.554  61.108  1.00 12.32     -0.272 OA
ATOM  16429  N   PHE B 427     -1.600  42.697  60.628  1.00  9.73     -0.346 N
ATOM  16430  HN  PHE B 427     -0.717  42.198  60.735  1.00  0.00      0.163 HD
ATOM  16431  CA  PHE B 427     -2.689  42.053  59.910  1.00  7.87      0.180 C
ATOM  16433  C   PHE B 427     -2.893  40.586  60.216  1.00  6.79      0.241 C
ATOM  16434  O   PHE B 427     -2.032  39.889  60.776  1.00 12.10     -0.271 OA
ATOM  16435  CB  PHE B 427     -2.355  42.092  58.367  1.00 11.89      0.073 C
ATOM  16438  CG  PHE B 427     -2.288  43.514  57.861  1.00 12.95      0.056 A
ATOM  16439  CD1 PHE B 427     -3.464  44.203  57.623  1.00 10.77      0.007 A
ATOM  16441  CD2 PHE B 427     -1.060  44.135  57.678  1.00 12.54      0.007 A
ATOM  16443  CE1 PHE B 427     -3.453  45.515  57.144  1.00 12.45      0.001 A
ATOM  16445  CE2 PHE B 427     -1.028  45.453  57.225  1.00  8.95      0.001 A
ATOM  16447  CZ  PHE B 427     -2.204  46.108  56.958  1.00 14.49      0.000 A
ATOM  16449  N   LEU B 428     -4.062  40.078  59.852  1.00  8.96     -0.346 N
ATOM  16450  HN  LEU B 428     -4.752  40.703  59.435  1.00  0.00      0.163 HD
ATOM  16451  CA  LEU B 428     -4.417  38.658  60.018  1.00  9.06      0.177 C
ATOM  16453  C   LEU B 428     -4.855  38.201  58.637  1.00  9.18      0.243 C
ATOM  16454  O   LEU B 428     -5.937  38.566  58.177  1.00 10.94     -0.271 OA
ATOM  16455  CB  LEU B 428     -5.591  38.575  60.970  1.00 12.15      0.038 C
ATOM  16458  CG  LEU B 428     -6.417  37.304  61.150  1.00 27.62     -0.020 C
ATOM  16460  CD1 LEU B 428     -5.855  36.043  60.547  1.00 22.05      0.009 C
ATOM  16464  CD2 LEU B 428     -6.761  37.044  62.617  1.00 21.72      0.009 C
ATOM  16468  N   PRO B 429     -3.979  37.535  57.878  1.00 10.53     -0.337 N
ATOM  16469  CA  PRO B 429     -4.319  37.276  56.484  1.00  8.30      0.179 C
ATOM  16471  C   PRO B 429     -5.128  35.998  56.368  1.00  8.42      0.241 C
ATOM  16472  O   PRO B 429     -4.918  35.061  57.176  1.00  8.91     -0.271 OA
ATOM  16473  CB  PRO B 429     -2.952  37.149  55.796  1.00  6.10      0.037 C
ATOM  16476  CG  PRO B 429     -2.035  36.733  56.907  1.00 11.56      0.022 C
ATOM  16479  CD  PRO B 429     -2.582  37.202  58.227  1.00  7.07      0.127 C
ATOM  16482  N   TYR B 430     -6.014  35.964  55.382  1.00  7.09     -0.346 N
ATOM  16483  HN  TYR B 430     -6.239  36.811  54.860  1.00  0.00      0.163 HD
ATOM  16484  CA  TYR B 430     -6.667  34.693  55.051  1.00  7.27      0.180 C
ATOM  16486  C   TYR B 430     -6.513  34.562  53.539  1.00  8.36      0.241 C
ATOM  16487  O   TYR B 430     -6.476  35.579  52.819  1.00  6.78     -0.271 OA
ATOM  16488  CB  TYR B 430     -8.123  34.511  55.455  1.00 10.71      0.073 C
ATOM  16491  CG  TYR B 430     -9.177  35.458  54.914  1.00 10.26     -0.056 A
ATOM  16492  CD1 TYR B 430     -9.776  35.244  53.686  1.00  8.09      0.010 A
ATOM  16494  CD2 TYR B 430     -9.589  36.554  55.658  1.00 11.76      0.010 A
ATOM  16496  CE1 TYR B 430     -10.779  36.074  53.212  1.00 12.32      0.037 A
ATOM  16498  CE2 TYR B 430     -10.599  37.410  55.209  1.00 14.99      0.037 A
ATOM  16500  CZ  TYR B 430     -11.184  37.148  53.987  1.00 14.31      0.065 A
ATOM  16501  OH  TYR B 430     -12.161  38.003  53.507  1.00 14.55     -0.361 OA
ATOM  16502  HH  TYR B 430     -12.439  38.740  54.039  1.00  0.00      0.217 HD
ATOM  16503  N   THR B 431     -6.332  33.326  53.073  1.00  6.79     -0.344 N
ATOM  16504  HN  THR B 431     -6.336  32.522  53.700  1.00  0.00      0.163 HD
ATOM  16505  CA  THR B 431     -6.125  33.158  51.617  1.00  6.19      0.205 C
ATOM  16507  C   THR B 431     -7.096  32.043  51.158  1.00 10.07      0.243 C
ATOM  16508  O   THR B 431     -7.572  31.328  52.023  1.00  8.84     -0.271 OA
ATOM  16509  CB  THR B 431     -4.699  32.716  51.268  1.00  7.63      0.146 C
ATOM  16511  CG2 THR B 431     -3.698  33.850  51.541  1.00  8.11      0.042 C
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ATOM  16515  OG1 THR B 431      -4.326  31.548  52.015  1.00  9.95      -0.393 OA
ATOM  16516  HG1 THR B 431      -3.442  31.274  51.799  1.00  0.00       0.210 HD
ATOM  16517  N   SER B 432      -7.348  31.873  49.861  1.00  7.61      -0.344 N
ATOM  16518  HN  SER B 432      -6.882  32.436  49.149  1.00  0.00       0.163 HD
ATOM  16519  CA  SER B 432      -8.329  30.837  49.501  1.00  8.47       0.200 C
ATOM  16521  C   SER B 432      -8.163  30.407  48.031  1.00  8.65       0.243 C
ATOM  16522  O   SER B 432      -7.859  31.179  47.141  1.00  8.80      -0.271 OA
ATOM  16523  CB  SER B 432      -9.718  31.472  49.659  1.00 13.23       0.199 C
ATOM  16526  OG  SER B 432     -10.772  30.536  49.522  1.00 13.98      -0.398 OA
ATOM  16527  HG  SER B 432     -11.631  30.929  49.620  1.00  0.00       0.209 HD
ATOM  16528  N   THR B 433      -8.490  29.159  47.803  1.00  7.43      -0.344 N
ATOM  16529  HN  THR B 433      -8.720  28.573  48.606  1.00  0.00       0.163 HD
ATOM  16530  CA  THR B 433      -8.548  28.546  46.466  1.00  6.76       0.205 C
ATOM  16532  C   THR B 433      -9.250  27.186  46.371  1.00 10.22       0.243 C
ATOM  16533  O   THR B 433      -9.697  26.843  47.787  1.00  9.44      -0.271 OA
ATOM  16534  CB  THR B 433      -7.155  28.361  45.839  1.00  8.91       0.146 C
ATOM  16536  CG2 THR B 433      -6.303  27.391  46.674  1.00  6.64       0.042 C
ATOM  16540  OG1 THR B 433      -7.365  27.775  44.534  1.00  9.37      -0.393 OA
ATOM  16541  HG1 THR B 433      -6.505  27.661  44.147  1.00  0.00       0.210 HD
ATOM  16542  N   PHE B 434      -9.514  26.445  45.619  1.00  7.48      -0.346 N
ATOM  16543  HN  PHE B 434      -9.343  26.827  44.689  1.00  0.00       0.163 HD
ATOM  16544  CA  PHE B 434     -10.046  25.089  45.743  1.00  9.24       0.180 C
ATOM  16546  C   PHE B 434      -8.986  24.235  46.421  1.00 10.68       0.241 C
ATOM  16547  O   PHE B 434      -7.791  24.411  46.190  1.00  9.51      -0.271 OA
ATOM  16548  CB  PHE B 434     -10.301  24.461  44.352  1.00  7.81       0.073 C
ATOM  16551  CG  PHE B 434     -11.445  25.079  43.589  1.00 15.10      -0.056 A
ATOM  16552  CD1 PHE B 434     -12.454  25.789  44.217  1.00 12.06       0.007 A
ATOM  16554  CD2 PHE B 434     -11.533  24.870  42.211  1.00 22.35       0.007 A
ATOM  16556  CE1 PHE B 434     -13.495  26.343  43.496  1.00 13.59       0.001 A
ATOM  16558  CE2 PHE B 434     -12.612  25.380  41.492  1.00 16.01       0.001 A
ATOM  16560  CZ  PHE B 434     -13.585  26.124  42.138  1.00 16.00       0.000 A
ATOM  16562  N   LEU B 435      -9.434  23.223  47.187  1.00  5.77      -0.346 N
ATOM  16563  HN  LEU B 435     -10.434  23.036  47.257  1.00  0.00       0.163 HD
ATOM  16564  CA  LEU B 435      -8.478  22.396  47.916  1.00  6.72       0.177 C
ATOM  16566  C   LEU B 435      -7.459  21.721  47.011  1.00  7.73       0.241 C
ATOM  16567  O   LEU B 435      -6.316  21.565  47.433  1.00  6.78      -0.271 OA
ATOM  16568  CB  LEU B 435      -9.265  21.336  48.739  1.00  6.50       0.038 C
ATOM  16571  CG  LEU B 435      -8.373  20.316  49.498  1.00 10.50      -0.020 C
ATOM  16573  CD1 LEU B 435      -7.443  21.029  50.485  1.00  9.78       0.009 C
ATOM  16577  CD2 LEU B 435      -9.268  19.301  50.229  1.00  9.96       0.009 C
ATOM  16581  N   MET B 436      -7.870  21.299  45.798  1.00  6.74      -0.346 N
ATOM  16582  HN  MET B 436      -8.829  21.432  45.478  1.00  0.00       0.163 HD
ATOM  16583  CA  MET B 436      -6.843  20.627  44.951  1.00  9.13       0.177 C
ATOM  16585  C   MET B 436      -5.620  21.517  44.786  1.00  8.30       0.241 C
ATOM  16586  O   MET B 436      -4.507  21.011  44.767  1.00  9.71      -0.271 OA
ATOM  16587  CB  MET B 436      -7.438  20.294  43.591  1.00  8.39       0.045 C
ATOM  16590  CG  MET B 436      -6.473  19.559  42.641  1.00 10.09       0.076 C
ATOM  16593  SD  MET B 436      -5.898  17.986  43.317  1.00 12.58      -0.173 SA
ATOM  16594  CE  MET B 436      -7.404  17.047  43.309  1.00  7.50       0.089 C
ATOM  16598  N   PHE B 437      -5.788  22.850  44.642  1.00  6.10      -0.346 N
ATOM  16599  HN  PHE B 437      -6.716  23.250  44.778  1.00  0.00       0.163 HD
ATOM  16600  CA  PHE B 437      -4.693  23.723  44.300  1.00  4.79       0.180 C
ATOM  16602  C   PHE B 437      -3.899  24.135  45.526  1.00  9.89       0.241 C
ATOM  16603  O   PHE B 437      -2.865  24.781  45.397  1.00 10.94      -0.271 OA
ATOM  16604  CB  PHE B 437      -5.203  24.868  43.390  1.00  9.89       0.073 C
ATOM  16607  CG  PHE B 437      -5.997  24.256  42.224  1.00 12.40      -0.056 A
ATOM  16608  CD1 PHE B 437      -5.427  23.242  41.456  1.00 14.43       0.007 A
ATOM  16610  CD2 PHE B 437      -7.272  24.680  41.930  1.00 13.89       0.007 A
ATOM  16612  CE1 PHE B 437      -6.128  22.652  40.398  1.00 16.79       0.001 A
ATOM  16614  CE2 PHE B 437      -7.986  24.112  40.886  1.00 20.75       0.001 A
ATOM  16616  CZ  PHE B 437      -7.409  23.113  40.121  1.00 18.84       0.000 A
ATOM  16618  N   VAL B 438      -4.093  23.474  46.673  1.00  7.72      -0.346 N
ATOM  16619  HN  VAL B 438      -4.935  22.915  46.816  1.00  0.00       0.163 HD
ATOM  16620  CA  VAL B 438      -3.063  23.564  47.750  1.00  7.70       0.180 C
ATOM  16622  C   VAL B 438      -1.799  22.869  47.224  1.00 10.04       0.241 C
ATOM  16623  O   VAL B 438      -0.673  23.244  47.604  1.00  8.09      -0.271 OA
ATOM  16624  CB  VAL B 438      -3.531  22.872  49.037  1.00 10.73       0.009 C
ATOM  16626  CG1 VAL B 438      -3.621  21.351  48.865  1.00  9.03       0.012 C
ATOM  16630  CG2 VAL B 438      -2.562  23.189  50.189  1.00 11.87       0.012 C
ATOM  16634  N   GLU B 439      -1.913  21.923  46.262  1.00  6.88      -0.346 N
ATOM  16635  HN  GLU B 439      -2.840  21.637  45.946  1.00  0.00       0.163 HD
ATOM  16636  CA  GLU B 439      -0.737  21.309  45.673  1.00  7.35       0.177 C
ATOM  16638  C   GLU B 439       0.107  22.346  44.906  1.00  8.52       0.241 C
ATOM  16639  O   GLU B 439       1.317  22.169  44.960  1.00 10.66      -0.271 OA
ATOM  16640  CB  GLU B 439      -1.112  20.136  44.731  1.00  3.49       0.045 C
ATOM  16643  CG  GLU B 439      -1.733  19.028  45.612  1.00  8.67       0.116 C
ATOM  16646  CD  GLU B 439      -1.642  17.648  44.973  1.00 13.89       0.172 C
ATOM  16647  OE1 GLU B 439      -1.411  17.573  43.763  1.00  8.80      -0.648 OA
ATOM  16648  OE2 GLU B 439      -1.791  16.659  45.708  1.00  8.88      -0.648 OA
ATOM  16649  N   TYR B 440      -0.466  23.380  44.271  1.00  4.95      -0.346 N
ATOM  16650  HN  TYR B 440      -1.482  23.457  44.226  1.00  0.00       0.163 HD
ATOM  16651  CA  TYR B 440       0.374  24.390  43.648  1.00  6.84       0.180 C
ATOM  16653  C   TYR B 440       1.117  25.194  44.730  1.00  8.23       0.241 C
ATOM  16654  O   TYR B 440       2.235  25.696  44.498  1.00 12.30      -0.271 OA
ATOM  16655  CB  TYR B 440      -0.505  25.372  42.846  1.00  4.47       0.073 C
ATOM  16658  CG  TYR B 440      -0.831  24.834  41.444  1.00  8.13      -0.056 A
ATOM  16659  CD1 TYR B 440      -1.380  23.590  41.253  1.00  5.57       0.010 A
ATOM  16661  CD2 TYR B 440      -0.606  25.667  40.339  1.00  9.25       0.010 A
ATOM  16663  CE1 TYR B 440      -1.743  23.148  39.964  1.00  7.68       0.037 A
ATOM  16665  CE2 TYR B 440      -0.922  25.224  39.056  1.00  7.55       0.037 A
ATOM  16667  CZ  TYR B 440      -1.450  23.960  38.895  1.00  8.33       0.065 A
ATOM  16668  OH  TYR B 440      -1.788  23.547  37.615  1.00  9.05      -0.361 OA
ATOM  16669  HH  TYR B 440      -2.152  22.676  37.504  1.00  0.00       0.217 HD
ATOM  16670  N   ALA B 441       0.489  25.375  45.882  1.00  6.30      -0.346 N
ATOM  16671  HN  ALA B 441      -0.416  24.937  46.054  1.00  0.00       0.163 HD
ATOM  16672  CA  ALA B 441       1.121  26.219  46.909  1.00  7.18       0.172 C
ATOM  16674  C   ALA B 441       1.764  25.417  48.038  1.00  8.99       0.240 C
ATOM  16675  O   ALA B 441       1.999  26.028  49.080  1.00  7.12      -0.271 OA
ATOM  16676  CB  ALA B 441      -0.017  27.033  47.534  1.00  8.53       0.042 C
ATOM  16680  N   ARG B 442       1.969  24.113  47.866  1.00  5.32      -0.346 N
ATOM  16681  HN  ARG B 442       1.895  23.704  46.934  1.00  0.00       0.163 HD
ATOM  16682  CA  ARG B 442       2.302  23.260  49.019  1.00  5.00       0.176 C
ATOM  16684  C   ARG B 442       3.441  23.693  49.891  1.00  6.21       0.241 C
ATOM  16685  O   ARG B 442       3.332  23.674  51.132  1.00  8.35      -0.271 OA
ATOM  16686  CB  ARG B 442       2.565  21.838  48.395  1.00  7.23       0.036 C
ATOM  16689  CG  ARG B 442       2.542  20.741  49.490  1.00 14.23       0.023 C
ATOM  16692  CD  ARG B 442       1.180  20.818  50.177  1.00 15.77       0.138 C
ATOM  16695  NE  ARG B 442       0.863  19.888  51.269  1.00 11.27      -0.227 N
ATOM  16696  HE  ARG B 442       0.118  19.201  51.155  1.00  0.00       0.177 HD
ATOM  16697  CZ  ARG B 442       1.559  19.944  52.422  1.00 31.73       0.665 C
ATOM  16698  NH1 ARG B 442       2.537  20.805  52.539  1.00 27.07      -0.235 N
ATOM  16699 1HH1 ARG B 442       3.064  20.847  53.401  1.00  0.00       0.174 HD
ATOM  16700 2HH1 ARG B 442       2.664  21.410  51.728  1.00  0.00       0.174 HD
ATOM  16701  NH2 ARG B 442       1.396  19.168  53.462  1.00 21.20      -0.235 N
ATOM  16702 1HH2 ARG B 442       1.923  19.210  54.334  1.00  0.00       0.174 HD
ATOM  16703 2HH2 ARG B 442       0.633  18.497  53.371  1.00  0.00       0.174 HD
ATOM  16704  N   ASN B 443       4.600  24.101  49.314  1.00  7.15      -0.346 N
ATOM  16705  HN  ASN B 443       4.675  24.148  48.300  1.00  0.00       0.163 HD
ATOM  16706  CA  ASN B 443       5.754  24.477  50.158  1.00  5.14       0.185 C
ATOM  16708  C   ASN B 443       5.562  25.809  50.900  1.00  6.85       0.241 C
ATOM  16709  O   ASN B 443       6.153  25.954  51.961  1.00  7.30      -0.271 OA
ATOM  16710  CB  ASN B 443       7.060  24.438  49.374  1.00  5.53       0.137 C
ATOM  16713  CG  ASN B 443       8.266  24.325  50.324  1.00 10.12       0.217 C
ATOM  16714  ND2 ASN B 443       8.382  23.203  51.042  1.00  8.32      -0.370 N
ATOM  16715 1HD2 ASN B 443       7.725  22.423  51.031  1.00  0.00       0.159 HD
ATOM  16716 2HD2 ASN B 443       9.181  23.128  51.671  1.00  0.00       0.159 HD
ATOM  16717  OD1 ASN B 443       9.051  25.257  50.337  1.00 10.21      -0.274 OA
ATOM  16718  N   ALA B 444       4.739  26.724  50.422  1.00  6.63      -0.346 N
ATOM  16719  HN  ALA B 444       4.297  26.568  49.516  1.00  0.00       0.163 HD
ATOM  16720  CA  ALA B 444       4.444  27.954  51.154  1.00  4.79       0.172 C
ATOM  16722  C   ALA B 444       3.545  27.641  52.353  1.00  6.25       0.240 C
ATOM  16723  O   ALA B 444       3.647  28.243  53.445  1.00  7.50      -0.271 OA
ATOM  16724  CB  ALA B 444       3.785  28.971  50.203  1.00  5.84       0.042 C
ATOM  16728  N   VAL B 445       2.681  26.607  52.213  1.00  4.91      -0.346 N
ATOM  16729  HN  VAL B 445       2.591  26.137  51.312  1.00  0.00       0.163 HD
ATOM  16730  CA  VAL B 445       1.874  26.162  53.355  1.00  4.15       0.180 C
ATOM  16732  C   VAL B 445       2.838  25.570  54.379  1.00  7.40       0.241 C
ATOM  16733  O   VAL B 445       2.761  25.900  55.563  1.00  7.22      -0.271 OA
ATOM  16734  CB  VAL B 445       0.822  25.119  52.888  1.00 11.25       0.009 C
ATOM  16736  CG1 VAL B 445       0.109  24.537  54.095  1.00 12.98       0.012 C
ATOM  16740  CG2 VAL B 445      -0.246  25.759  51.965  1.00 10.36       0.012 C
ATOM  16744  N   ARG B 446       3.752  24.683  53.980  1.00  7.41      -0.346 N
ATOM  16745  HN  ARG B 446       3.775  24.381  53.006  1.00  0.00       0.163 HD
ATOM  16746  CA  ARG B 446       4.732  24.136  54.945  1.00  5.60       0.176 C
ATOM  16748  C   ARG B 446       5.519  25.252  55.618  1.00  6.17       0.241 C
ATOM  16749  O   ARG B 446       5.829  25.215  56.803  1.00  5.69      -0.271 OA
ATOM  16750  CB  ARG B 446       5.705  23.241  54.123  1.00  4.62       0.036 C
ATOM  16753  CG  ARG B 446       6.559  22.423  55.151  1.00  6.91       0.023 C
ATOM  16756  CD  ARG B 446       7.592  21.576  54.369  1.00  7.73       0.138 C
ATOM  16759  NE  ARG B 446       8.025  20.480  55.268  1.00  8.96      -0.227 N
ATOM  16760  HE  ARG B 446       7.385  19.703  55.429  1.00  0.00       0.177 HD
ATOM  16761  CZ  ARG B 446       9.215  20.461  55.879  1.00 11.15       0.665 C
ATOM  16762  NH1 ARG B 446      10.115  21.407  55.658  1.00 11.42      -0.235 N
ATOM  16763 1HH1 ARG B 446       9.893  22.207  55.106  1.00  0.00       0.174 HD
ATOM  16764 2HH1 ARG B 446      11.022  21.393  56.164  1.00  0.00       0.174 HD
ATOM  16765  NH2 ARG B 446       9.508  19.407  56.659  1.00  8.66      -0.235 N
ATOM  16766 1HH2 ARG B 446       8.812  18.675  56.799  1.00  0.00       0.174 HD
ATOM  16767 2HH2 ARG B 446      10.441  19.393  57.125  1.00  0.00       0.174 HD
ATOM  16768  N   MET B 447       5.930  26.283  54.850  1.00  9.95      -0.346 N
ATOM  16769  HN  MET B 447       5.690  26.295  53.859  1.00  0.00       0.163 HD
ATOM  16770  CA  MET B 447       6.718  27.393  55.412  1.00  8.50       0.177 C
ATOM  16772  C   MET B 447       5.960  28.208  56.443  1.00  6.64       0.241 C
ATOM  16773  O   MET B 447       6.555  28.636  57.442  1.00  6.57      -0.271 OA
ATOM  16774  CB  MET B 447       7.287  28.337  54.348  1.00  5.94       0.045 C
ATOM  16777  CG  MET B 447       8.352  27.667  53.444  1.00  8.60       0.076 C
ATOM  16780  SD  MET B 447       9.830  27.109  54.395  1.00 11.53      -0.173 SA
ATOM  16781  CE  MET B 447      10.501  28.702  54.848  1.00 16.23       0.089 C
ATOM  16785  N   ALA B 448       4.643  28.341  56.295  1.00  5.11      -0.346 N
ATOM  16786  HN  ALA B 448       4.171  27.980  55.466  1.00  0.00       0.163 HD
ATOM  16787  CA  ALA B 448       3.879  29.029  57.370  1.00  8.09       0.172 C
ATOM  16789  C   ALA B 448       3.941  28.203  58.646  1.00  8.21       0.240 C
ATOM  16790  O   ALA B 448       4.019  28.789  59.737  1.00  9.67      -0.271 OA
ATOM  16791  CB  ALA B 448       2.424  29.142  56.901  1.00  8.16       0.042 C
ATOM  16795  N   ALA B 449       3.814  26.871  58.480  1.00  7.44      -0.346 N
ATOM  16796  HN  ALA B 449       3.701  26.453  57.556  1.00  0.00       0.163 HD
ATOM  16797  CA  ALA B 449       3.848  26.034  59.728  1.00  4.78       0.172 C
ATOM  16799  C   ALA B 449       5.224  26.006  60.374  1.00  8.45       0.240 C
ATOM  16800  O   ALA B 449       5.391  26.137  61.612  1.00  8.96      -0.271 OA
ATOM  16801  CB  ALA B 449       3.436  24.638  59.339  1.00  5.17       0.042 C
ATOM  16805  N   LEU B 450       6.298  25.893  59.565  1.00  7.20      -0.346 N
ATOM  16806  HN  LEU B 450       6.150  25.721  58.571  1.00  0.00       0.163 HD
ATOM  16807  CA  LEU B 450       7.668  26.009  60.067  1.00  8.24       0.177 C
ATOM  16809  C   LEU B 450       7.981  27.348  60.700  1.00 11.15       0.241 C
ATOM  16810  O   LEU B 450       8.637  27.353  61.765  1.00  6.43      -0.271 OA
ATOM  16811  CB  LEU B 450       8.659  25.774  58.880  1.00  7.36       0.038 C
ATOM  16814  CG  LEU B 450      10.158  25.695  59.205  1.00 13.72      -0.020 C
ATOM  16816  CD1 LEU B 450      10.474  24.719  60.316  1.00 23.32       0.009 C
ATOM  16820  CD2 LEU B 450      10.928  25.317  57.935  1.00 16.91       0.009 C
ATOM  16824  N   MET B 451       7.512  28.487  60.188  1.00  8.55      -0.346 N
ATOM  16825  HN  MET B 451       6.915  28.438  59.363  1.00  0.00       0.163 HD
ATOM  16826  CA  MET B 451       7.812  29.802  60.752  1.00  7.26       0.177 C
ATOM  16828  C   MET B 451       6.819  30.207  61.841  1.00  8.02       0.241 C
ATOM  16829  O   MET B 451       6.959  31.262  62.436  1.00  9.58      -0.271 OA
ATOM  16830  CB  MET B 451       7.722  30.914  59.667  1.00  6.77       0.045 C
ATOM  16833  CG  MET B 451       8.834  30.674  58.632  1.00  7.08       0.076 C
ATOM  16836  SD  MET B 451       8.970  32.136  57.521  1.00 12.58      -0.173 SA
ATOM  16837  CE  MET B 451       7.622  31.891  56.386  1.00 12.95       0.089 C
ATOM  16841  N   LYS B 452       5.897  29.324  62.135  1.00  7.97      -0.346 N
ATOM  16842  HN  LYS B 452       5.882  28.455  61.601  1.00  0.00       0.163 HD
ATOM  16843  CA  LYS B 452       4.888  29.501  63.177  1.00  9.56       0.176 C
ATOM  16845  C   LYS B 452       4.083  30.761  62.953  1.00 11.80       0.241 C
ATOM  16846  O   LYS B 452       3.850  31.524  63.890  1.00  9.24      -0.271 OA
ATOM  16847  CB  LYS B 452       5.621  29.580  64.529  1.00 14.07       0.035 C
ATOM  16850  CG  LYS B 452       6.334  28.258  64.855  1.00 19.42       0.004 C
ATOM  16853  CD  LYS B 452       6.665  28.273  66.356  1.00 29.29       0.027 C
ATOM  16856  CE  LYS B 452       7.906  27.456  66.654  1.00 44.22       0.229 C
ATOM  16859  NZ  LYS B 452       9.055  27.899  65.816  1.00 65.56      -0.079 N
ATOM  16860  HZ1 LYS B 452       9.890  27.349  66.017  1.00  0.00       0.274 HD
ATOM  16861  HZ2 LYS B 452       9.230  28.899  65.918  1.00  0.00       0.274 HD
ATOM  16862  HZ3 LYS B 452       8.824  27.882  64.823  1.00  0.00       0.274 HD
ATOM  16863  N   GLN B 453       3.576  30.972  61.736  1.00  9.18      -0.346 N
ATOM  16864  HN  GLN B 453       3.690  30.270  61.005  1.00  0.00       0.163 HD
ATOM  16865  CA  GLN B 453       2.851  32.225  61.454  1.00 10.69       0.177 C
ATOM  16867  C   GLN B 453       1.349  31.977  61.385  1.00 10.27       0.241 C
ATOM  16868  O   GLN B 453       0.929  30.937  60.871  1.00 10.07      -0.271 OA
ATOM  16869  CB  GLN B 453       3.296  32.666  60.028  1.00 12.07       0.044 C
ATOM  16872  CG  GLN B 453       4.735  33.182  60.044  1.00 12.84       0.105 C
ATOM  16875  CD  GLN B 453       5.031  34.224  61.098  1.00 20.16       0.215 C
ATOM  16876  OE1 GLN B 453       4.353  35.346  60.928  1.00 16.02      -0.370 O
ATOM  16877 1HE2 GLN B 453       3.699  35.495  60.159  1.00  0.00       0.159 HD
ATOM  16878 2HE2 GLN B 453       4.553  36.049  61.639  1.00  0.00       0.159 HD
ATOM  16879  OE1 GLN B 453       5.827  34.043  62.034  1.00 20.52      -0.274 OA
ATOM  16880  NE2 GLN B 453       0.547  32.902  61.823  1.00  9.16      -0.346 N
ATOM  16881  HN  ARG B 454       0.943  33.754  62.221  1.00  0.00       0.163 HD
ATOM  16882  CA  ARG B 454      -0.905  32.757  61.762  1.00  9.34       0.176 C
ATOM  16884  C   ARG B 454      -1.405  33.138  60.388  1.00 16.11       0.241 C
ATOM  16885  O   ARG B 454      -1.061  34.182  59.827  1.00 13.46      -0.271 OA
ATOM  16886  CB  ARG B 454      -1.467  33.727  62.858  1.00 12.21       0.036 C
ATOM  16889  CG  ARG B 454      -2.999  33.782  62.765  1.00 14.04       0.023 C
ATOM  16892  CD  ARG B 454      -3.586  34.526  63.969  1.00 21.28       0.138 C
ATOM  16895  NE  ARG B 454      -3.120  35.928  63.956  1.00 22.13      -0.227 N
ATOM  16896  HE  ARG B 454      -2.354  36.193  63.337  1.00  0.00       0.177 HD
ATOM  16897  CZ  ARG B 454      -3.684  36.863  64.744  1.00 39.89       0.665 C
ATOM  16898  NH1 ARG B 454      -4.703  36.578  65.552  1.00 31.72      -0.235 N
ATOM  16899 1HH1 ARG B 454      -5.043  35.616  65.550  1.00  0.00       0.174 HD
ATOM  16900 2HH1 ARG B 454      -5.130  37.286  66.149  1.00  0.00       0.174 HD
ATOM  16901  NH2 ARG B 454      -3.242  38.114  64.746  1.00 26.80      -0.235 N
ATOM  16902 1HH2 ARG B 454      -2.461  38.332  64.127  1.00  0.00       0.174 HD
ATOM  16903 2HH2 ARG B 454      -3.669  38.822  65.343  1.00  0.00       0.174 HD
ATOM  16904  N   GLN B 455      -2.152  32.261  59.753  1.00 10.52      -0.346 N
ATOM  16905  HN  GLN B 455      -2.322  31.352  60.183  1.00  0.00       0.163 HD
ATOM  16906  CA  GLN B 455      -2.749  32.552  58.442  1.00 10.05       0.177 C
ATOM  16908  C   GLN B 455      -3.944  31.588  58.377  1.00 11.73       0.241 C
ATOM  16909  O   GLN B 455      -3.719  30.411  58.709  1.00 11.70      -0.271 OA
ATOM  16910  CB  GLN B 455      -1.799  32.187  57.280  1.00  9.87       0.044 C
ATOM  16913  CG  GLN B 455      -2.433  32.408  55.914  1.00 11.90       0.105 C
ATOM  16916  CD  GLN B 455      -1.579  32.133  54.703  1.00 13.29       0.215 C
ATOM  16917  OE1 GLN B 455      -0.270  32.228  54.817  1.00  9.51      -0.370 O
ATOM  16918 1HE2 GLN B 455       0.308  32.042  53.997  1.00  0.00       0.159 HD
ATOM  16919 2HE2 GLN B 455       0.123  32.459  55.730  1.00  0.00       0.159 HD
ATOM  16920  OE1 GLN B 455      -2.054  31.854  53.600  1.00 11.91      -0.274 OA
ATOM  16921  NE2 GLN B 455      -5.106  32.070  57.954  1.00  8.46      -0.346 N
ATOM  16922  HN  VAL B 456      -5.209  33.056  57.715  1.00  0.00       0.163 HD
ATOM  16923  CA  VAL B 456      -6.239  31.144  57.840  1.00  6.82       0.180 C
ATOM  16925  C   VAL B 456      -6.332  30.787  56.342  1.00  7.23       0.241 C
ATOM  16926  O   VAL B 456      -6.416  31.682  55.507  1.00  9.44      -0.271 OA
ATOM  16927  CB  VAL B 456      -7.558  31.735  58.332  1.00 11.17       0.009 C
ATOM  16929  CG1 VAL B 456      -8.692  30.693  58.192  1.00  8.22       0.012 C
ATOM  16933  CG2 VAL B 456      -7.436  32.071  59.827  1.00 11.84       0.012 C
ATOM  16937  N   MET B 457      -6.289  29.512  56.034  1.00  5.45      -0.346 N
ATOM  16938  HN  MET B 457      -6.235  28.825  56.783  1.00  0.00       0.163 HD
ATOM  16939  CA  MET B 457      -6.315  29.040  54.648  1.00  7.84       0.177 C
ATOM  16941  C   MET B 457      -7.667  28.388  54.373  1.00  9.21       0.241 C
ATOM  16942  O   MET B 457      -8.012  27.368  54.943  1.00 11.96      -0.271 OA
ATOM  16943  CB  MET B 457      -5.148  28.041  54.423  1.00 10.91       0.045 C
ATOM  16946  CG  MET B 457      -3.789  28.747  54.749  1.00 14.69       0.076 C
ATOM  16949  SD  MET B 457      -2.558  27.505  55.158  1.00 23.95      -0.173 SA
ATOM  16950  CE  MET B 457      -1.042  28.479  55.250  1.00 15.77       0.089 C
ATOM  16954  N   VAL B 458      -8.451  28.996  53.505  1.00  6.24      -0.346 N
ATOM  16955  HN  VAL B 458      -8.079  29.815  53.024  1.00  0.00       0.163 HD
ATOM  16956  CA  VAL B 458      -9.814  28.581  53.183  1.00  6.96       0.180 C
ATOM  16958  C   VAL B 458      -9.867  27.750  51.915  1.00  9.66       0.241 C
ATOM  16959  O   VAL B 458      -9.683  28.300  50.811  1.00 10.56      -0.271 OA
ATOM  16960  CB  VAL B 458     -10.644  29.880  53.028  1.00 11.46       0.009 C
ATOM  16962  CG1 VAL B 458     -12.098  29.570  52.733  1.00 14.68       0.012 C
ATOM  16966  CG2 VAL B 458     -10.524  30.733  54.312  1.00 11.92       0.012 C
ATOM  16970  N   TYR B 459      -9.971  26.442  52.057  1.00  5.57      -0.346 N
ATOM  16971  HN  TYR B 459     -10.072  26.033  52.986  1.00  0.00       0.163 HD
ATOM  16972  CA  TYR B 459      -9.941  25.582  50.874  1.00  6.87       0.180 C
ATOM  16974  C   TYR B 459     -11.323  24.971  50.665  1.00 10.97       0.241 C
ATOM  16975  O   TYR B 459     -11.796  24.190  51.511  1.00 11.49      -0.271 OA
ATOM  16976  CB  TYR B 459      -8.899  24.438  51.065  1.00  4.73       0.073 C
ATOM  16979  CG  TYR B 459      -7.484  24.963  51.206  1.00 10.32      -0.056 A
ATOM  16980  CD1 TYR B 459      -7.024  25.894  50.270  1.00 14.23       0.010 A
ATOM  16982  CD2 TYR B 459      -6.623  24.546  52.189  1.00 10.25       0.010 A
ATOM  16984  CE1 TYR B 459      -5.710  26.397  50.387  1.00 13.59       0.037 A
ATOM  16986  CE2 TYR B 459      -5.315  25.010  52.288  1.00  7.55       0.037 A
ATOM  16988  CZ  TYR B 459      -4.891  25.946  51.376  1.00 11.46       0.065 A
ATOM  16989  OH  TYR B 459      -3.616  26.482  51.451  1.00 12.55      -0.361 OA
ATOM  16990  HH  TYR B 459      -3.044  26.167  52.141  1.00  0.00       0.217 HD
ATOM  16991  N   THR B 460     -11.994  25.304  49.571  1.00 11.39      -0.344 N
ATOM  16992  HN  THR B 460     -11.568  25.908  48.868  1.00  0.00       0.163 HD
ATOM  16993  CA  THR B 460     -13.365  24.791  49.382  1.00  6.79       0.205 C
ATOM  16995  C   THR B 460     -13.384  23.666  48.328  1.00 12.89       0.243 C
ATOM  16996  O   THR B 460     -12.337  23.477  47.716  1.00 10.86      -0.271 OA
ATOM  16997  CB  THR B 460     -14.270  25.955  48.957  1.00  9.13       0.146 C
ATOM  16999  OG1 THR B 460     -14.134  27.214  49.797  1.00  9.74      -0.393 OA
ATOM  17000  HG1 THR B 460     -14.458  27.069  47.354  1.00  0.00       0.210 HD
ATOM  17001  N   HIS B 461     -14.530  23.058  47.998  1.00  9.46      -0.346 N
ATOM  17002  HN  HIS B 461     -15.378  23.534  48.492  1.00  0.00       0.163 HD
ATOM  17003  CA  HIS B 461     -14.640  22.024  46.974  1.00 10.46       0.182 C
ATOM  17005  C   HIS B 461     -13.731  20.862  47.366  1.00  7.70       0.241 C
ATOM  17006  O   HIS B 461     -12.736  20.487  46.706  1.00 10.02      -0.271 OA
ATOM  17007  CB  HIS B 461     -14.265  22.575  45.569  1.00 10.69      -0.093 C
ATOM  17014  CG  HIS B 461     -15.256  23.634  45.094  1.00 13.44       0.028 A
ATOM  17015  CD2 HIS B 461     -16.044  23.761  43.986  1.00 10.41       0.114 A
ATOM  17017  ND1 HIS B 461     -15.442  24.751  45.829  1.00 11.10      -0.354 N
ATOM  17018  HD1 HIS B 461     -14.984  24.949  46.719  1.00  0.00       0.166 HD
ATOM  17019  CE1 HIS B 461     -16.323  25.567  45.213  1.00 15.09       0.180 A
ATOM  17021  NE2 HIS B 461     -16.727  24.962  44.102  1.00 14.21      -0.360 N
ATOM  17022  HE2 HIS B 461     -17.421  25.320  43.446  1.00  0.00       0.166 HD
ATOM  17023  N   ASP B 462     -14.073  20.303  48.531  1.00 10.10      -0.345 N
ATOM  17024  HN  ASP B 462     -14.978  20.523  48.946  1.00  0.00       0.163 HD
ATOM  17025  CA  ASP B 462     -13.167  19.378  49.222  1.00  8.11       0.186 C
ATOM  17027  C   ASP B 462     -13.216  17.930  48.890  1.00  8.63       0.241 C
ATOM  17028  O   ASP B 462     -12.377  17.203  49.423  1.00  9.66      -0.271 OA
ATOM  17029  CB  ASP B 462     -13.450  19.551  50.755  1.00  8.16       0.147 C
ATOM  17032  CG  ASP B 462     -14.726  18.865  51.193  1.00 10.95       0.175 C
ATOM  17033  OD1 ASP B 462     -15.744  18.929  50.490  1.00  9.58      -0.648 OA
ATOM  17034  OD2 ASP B 462     -14.710  18.217  52.280  1.00 11.54      -0.648 OA
ATOM  17035  N   SER B 463     -14.121  17.507  47.978  1.00  8.63      -0.344 N
ATOM  17036  HN  SER B 463     -14.744  18.157  47.500  1.00  0.00       0.163 HD
ATOM  17037  CA  SER B 463     -14.160  16.070  47.713  1.00  9.43       0.200 C
ATOM  17039  C   SER B 463     -14.823  15.732  46.384  1.00  9.38       0.243 C
ATOM  17040  O   SER B 463     -15.283  16.662  45.702  1.00  9.73      -0.271 OA
ATOM  17041  CB  SER B 463     -14.972  15.387  48.843  1.00 11.20       0.199 C
ATOM  17044  OG  SER B 463     -16.348  15.636  48.701  1.00 11.82      -0.398 OA
ATOM  17045  HG  SER B 463     -16.846  15.217  49.394  1.00  0.00       0.209 HD
ATOM  17046  N   ILE B 464     -15.160  14.468  46.183  1.00 11.34      -0.346 N
ATOM  17047  HN  ILE B 464     -14.846  13.750  46.836  1.00  0.00       0.163 HD
ATOM  17048  CA  ILE B 464     -16.000  14.085  45.002  1.00 12.36       0.180 C
ATOM  17050  C   ILE B 464     -17.333  14.797  45.141  1.00 13.01       0.241 C
ATOM  17051  O   ILE B 464     -18.050  14.914  44.150  1.00 15.46      -0.271 OA
ATOM  17052  CB  ILE B 464     -16.273  12.584  44.916  1.00 11.52       0.013 C
ATOM  17054  CG1 ILE B 464     -16.636  12.091  46.350  1.00 12.04       0.002 C
ATOM  17057  CG2 ILE B 464     -15.030  11.829  44.443  1.00  9.38       0.012 C
ATOM  17061  CD1 ILE B 464     -17.197  10.652  46.292  1.00 16.71       0.005 C
ATOM  17065  N   GLY B 465     -17.746  15.300  46.327  1.00 10.23      -0.351 N
ATOM  17066  HN  GLY B 465     -17.203  15.142  47.176  1.00  0.00       0.163 HD
ATOM  17067  CA  GLY B 465     -18.985  16.074  46.369  1.00 12.08       0.225 C
ATOM  17070  O   GLY B 465     -18.978  17.313  45.486  1.00 12.92      -0.272 OA
ATOM  17071  N   LEU B 466     -20.055  17.915  45.265  1.00 12.04      -0.272 OA
ATOM  17072  N   LEU B 466     -17.868  17.778  44.879  1.00 10.55      -0.346 N
ATOM  17073  HN  LEU B 466     -16.964  17.344  45.067  1.00  0.00       0.163 HD
ATOM  17074  CA  LEU B 466     -17.959  18.907  43.950  1.00 12.15       0.177 C
ATOM  17076  C   LEU B 466     -18.564  18.499  42.615  1.00 13.08       0.240 C
ATOM  17077  O   LEU B 466     -19.014  19.362  41.811  1.00 13.06      -0.271 OA
ATOM  17078  CB  LEU B 466     -16.637  19.652  43.708  1.00 10.36       0.038 C
ATOM  17081  CG  LEU B 466     -15.547  18.802  43.030  1.00 11.89      -0.020 C
ATOM  17083  CD1 LEU B 466     -15.614  18.943  41.503  1.00 11.50       0.009 C
ATOM  17087  CD2 LEU B 466     -14.170  19.314  43.512  1.00 10.81       0.009 C
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ATOM  17091  N   GLY B 467     -18.553  17.212  42.321  1.00 12.86    -0.351 N
ATOM  17092  HN  GLY B 467     -18.069  16.565  42.943  1.00  0.00     0.163 HD
ATOM  17093  CA  GLY B 467     -19.208  16.697  41.142  1.00 13.87     0.225 C
ATOM  17096  C   GLY B 467     -18.524  16.783  39.804  1.00 14.44     0.236 C
ATOM  17097  O   GLY B 467     -17.448  16.264  39.591  1.00 12.82    -0.272 OA
ATOM  17098  N   GLU B 468     -19.228  17.383  38.825  1.00  9.86    -0.346 N
ATOM  17099  HN  GLU B 468     -20.026  17.964  39.080  1.00  0.00     0.163 HD
ATOM  17100  CA  GLU B 468     -18.888  17.231  37.399  1.00 10.32     0.177 C
ATOM  17102  C   GLU B 468     -17.508  17.681  36.981  1.00 12.06     0.241 C
ATOM  17103  O   GLU B 468     -17.014  17.177  35.946  1.00 12.82    -0.271 OA
ATOM  17104  CB  GLU B 468     -19.973  18.011  36.602  1.00 12.01     0.045 C
ATOM  17107  CG  GLU B 468     -21.340  17.322  36.729  1.00 14.55     0.116 C
ATOM  17110  CD  GLU B 468     -22.264  17.917  37.760  1.00 23.66     0.172 C
ATOM  17111  OE1 GLU B 468     -21.803  18.452  38.788  1.00 16.48    -0.648 OA
ATOM  17112  OE2 GLU B 468     -23.506  17.835  37.559  1.00 18.84    -0.648 OA
ATOM  17113  N   ASP B 469     -16.850  18.640  37.650  1.00 11.44    -0.346 N
ATOM  17114  HN  ASP B 469     -17.264  19.090  38.467  1.00  0.00     0.163 HD
ATOM  17115  CA  ASP B 469     -15.501  19.027  37.166  1.00 10.55     0.186 C
ATOM  17117  C   ASP B 469     -14.563  17.817  37.078  1.00 14.20     0.241 C
ATOM  17118  O   ASP B 469     -13.545  17.890  36.388  1.00 16.84    -0.271 OA
ATOM  17119  CB  ASP B 469     -14.932  20.142  38.066  1.00  9.57     0.147 C
ATOM  17122  CG  ASP B 469     -15.458  21.493  37.626  1.00 23.68     0.175 C
ATOM  17123  OD1 ASP B 469     -16.075  21.607  36.541  1.00 20.91    -0.648 OA
ATOM  17124  OD2 ASP B 469     -15.303  22.468  38.359  1.00 19.78    -0.648 OA
ATOM  17125  N   GLY B 470     -14.754  16.759  37.880  1.00  9.27    -0.351 N
ATOM  17126  HN  GLY B 470     -15.441  16.813  38.632  1.00  0.00     0.163 HD
ATOM  17127  CA  GLY B 470     -13.997  15.543  37.689  1.00  8.52     0.225 C
ATOM  17130  C   GLY B 470     -12.666  15.414  38.388  1.00  9.61     0.238 C
ATOM  17131  O   GLY B 470     -12.342  16.192  39.291  1.00 11.79    -0.272 OA
ATOM  17132  N   PRO B 471     -11.919  14.358  38.043  1.00  9.72    -0.337 N
ATOM  17133  CA  PRO B 471     -10.797  13.915  38.823  1.00  8.52     0.179 C
ATOM  17135  C   PRO B 471      -9.594  14.818  38.915  1.00 10.65     0.241 C
ATOM  17136  O   PRO B 471      -8.839  14.688  39.876  1.00  8.29    -0.271 OA
ATOM  17137  CB  PRO B 471     -10.465  12.517  38.269  1.00  7.68     0.037 C
ATOM  17140  CG  PRO B 471     -10.961  12.584  36.818  1.00 13.91     0.022 C
ATOM  17143  CD  PRO B 471     -12.256  13.363  36.989  1.00 12.69     0.127 C
ATOM  17146  N   THR B 472      -9.408  15.779  38.019  1.00  8.44    -0.344 N
ATOM  17147  HN  THR B 472     -10.047  15.867  37.229  1.00  0.00     0.163 HD
ATOM  17148  CA  THR B 472      -8.300  16.706  38.157  1.00  6.31     0.205 C
ATOM  17150  C   THR B 472      -8.604  17.695  39.293  1.00  9.07     0.243 C
ATOM  17151  O   THR B 472      -7.671  18.336  39.746  1.00 11.62    -0.271 OA
ATOM  17152  CB  THR B 472      -8.023  17.553  36.903  1.00  9.39     0.146 C
ATOM  17154  CG2 THR B 472      -7.763  16.580  35.735  1.00  7.95     0.042 C
ATOM  17158  OG1 THR B 472      -9.205  18.286  36.552  1.00 13.52    -0.393 OA
ATOM  17159  HG1 THR B 472      -9.365  18.885  37.271  1.00  0.00     0.210 HD
ATOM  17160  N   HIS B 473      -9.870  17.938  39.601  1.00  7.72    -0.346 N
ATOM  17161  HN  HIS B 473     -10.608  17.463  39.082  1.00  0.00     0.163 HD
ATOM  17162  CA  HIS B 473     -10.234  18.870  40.666  1.00  8.48     0.182 C
ATOM  17164  C   HIS B 473     -10.725  18.181  41.954  1.00  9.85     0.241 C
ATOM  17165  O   HIS B 473     -10.658  18.872  42.990  1.00  9.71    -0.271 OA
ATOM  17166  CB  HIS B 473     -11.450  19.679  40.155  1.00  7.24     0.093 C
ATOM  17169  CG  HIS B 473     -11.109  20.776  39.191  1.00 14.31     0.028 A
ATOM  17170  CD2 HIS B 473     -11.471  22.082  39.165  1.00 14.64     0.114 A
ATOM  17172  ND1 HIS B 473     -10.362  20.540  38.061  1.00 15.24    -0.354 N
ATOM  17173  HD1 HIS B 473      -9.967  19.637  37.799  1.00  0.00     0.166 HD
ATOM  17174  CE1 HIS B 473     -10.233  21.650  37.369  1.00 15.04     0.180 A
ATOM  17176  NE2 HIS B 473     -10.881  22.592  38.018  1.00 21.02    -0.360 N
ATOM  17177  HE2 HIS B 473     -10.942  23.565  37.719  1.00  0.00     0.166 HD
ATOM  17178  N   GLN B 474     -11.182  16.930  41.945  1.00  9.54    -0.346 N
ATOM  17179  HN  GLN B 474     -11.173  16.394  41.077  1.00  0.00     0.163 HD
ATOM  17180  CA  GLN B 474     -11.703  16.311  43.187  1.00  9.55     0.177 C
ATOM  17182  C   GLN B 474     -10.614  15.800  44.112  1.00 10.22     0.243 C
ATOM  17183  O   GLN B 474      -9.882  14.848  43.808  1.00 11.19    -0.271 OA
ATOM  17184  CB  GLN B 474     -12.579  15.066  42.821  1.00  7.35     0.044 C
ATOM  17187  CG  GLN B 474     -13.821  15.521  42.009  1.00  9.55     0.105 C
ATOM  17190  CD  GLN B 474     -14.402  14.377  41.192  1.00 16.85     0.215 C
ATOM  17191  NE2 GLN B 474     -15.677  14.526  40.806  1.00 11.30    -0.370 N
ATOM  17192 1HE2 GLN B 474     -16.242  15.353  41.000  1.00  0.00     0.159 HD
ATOM  17193 2HE2 GLN B 474     -16.067  13.759  40.258  1.00  0.00     0.159 HD
ATOM  17194  OE1 GLN B 474     -13.720  13.380  40.958  1.00 11.91    -0.274 OA
ATOM  17195  N   PRO B 475     -10.431  16.426  45.266  1.00 11.81    -0.337 N
ATOM  17196  CA  PRO B 475      -9.450  16.021  46.239  1.00  9.47     0.179 C
ATOM  17198  C   PRO B 475      -9.693  14.595  46.717  1.00 13.77     0.241 C
ATOM  17199  O   PRO B 475     -10.841  14.174  46.866  1.00 10.23    -0.271 OA
ATOM  17200  CB  PRO B 475      -9.597  17.008  47.412  1.00  8.09     0.037 C
ATOM  17203  CG  PRO B 475     -10.225  18.219  46.743  1.00  9.04     0.022 C
ATOM  17206  CD  PRO B 475     -11.246  17.544  45.798  1.00  9.38     0.127 C
ATOM  17209  N   VAL B 476      -8.601  13.864  46.953  1.00  9.10    -0.346 N
ATOM  17210  HN  VAL B 476      -7.684  14.255  46.735  1.00  0.00     0.163 HD
ATOM  17211  CA  VAL B 476      -8.686  12.519  47.516  1.00  7.61     0.180 C
ATOM  17213  C   VAL B 476      -7.678  12.446  48.668  1.00  7.66     0.241 C
ATOM  17214  O   VAL B 476      -7.981  12.113  49.835  1.00 10.06    -0.271 OA
ATOM  17215  CB  VAL B 476      -8.387  11.389  46.510  1.00 12.38     0.009 C
ATOM  17217  CG1 VAL B 476      -8.418   9.995  47.205  1.00 10.31     0.012 C
ATOM  17221  CG2 VAL B 476      -9.499  11.378  45.436  1.00  9.59     0.012 C
ATOM  17225  N   GLU B 477      -6.427  12.765  48.324  1.00  4.82    -0.346 N
ATOM  17226  HN  GLU B 477      -6.235  13.153  47.400  1.00  0.00     0.163 HD
ATOM  17227  CA  GLU B 477      -5.324  12.556  49.280  1.00  8.41     0.177 C
ATOM  17229  C   GLU B 477      -4.770  13.848  49.875  1.00 10.26     0.241 C
ATOM  17230  O   GLU B 477      -3.815  13.770  50.662  1.00  8.31    -0.271 OA
ATOM  17231  CB  GLU B 477      -4.216  11.770  48.554  1.00  8.85     0.045 C
ATOM  17234  CG  GLU B 477      -3.400  12.466  47.454  1.00  8.27     0.116 C
ATOM  17237  CD  GLU B 477      -4.031  12.580  46.073  1.00 12.42     0.172 C
ATOM  17238  OE1 GLU B 477      -5.281  12.593  45.916  1.00 10.86    -0.648 OA
ATOM  17239  OE2 GLU B 477      -3.296  12.677  45.035  1.00 11.44    -0.648 OA
ATOM  17240  N   GLN B 478      -5.366  14.987  49.562  1.00  7.49    -0.346 N
ATOM  17241  HN  GLN B 478      -6.232  14.982  49.024  1.00  0.00     0.163 HD
ATOM  17242  CA  GLN B 478      -4.765  16.273  50.000  1.00  8.14     0.177 C
ATOM  17244  C   GLN B 478      -4.979  16.510  51.498  1.00  9.09     0.241 C
ATOM  17245  O   GLN B 478      -4.099  17.092  52.154  1.00  8.76    -0.271 OA
ATOM  17246  CB  GLN B 478      -5.414  17.418  49.212  1.00 10.55     0.044 C
ATOM  17249  CG  GLN B 478      -4.806  17.436  47.786  1.00  7.59     0.105 C
ATOM  17252  CD  GLN B 478      -5.341  16.315  46.919  1.00 12.04     0.215 C
ATOM  17253  NE2 GLN B 478      -4.488  15.861  45.991  1.00  8.70    -0.370 N
ATOM  17254 1HE2 GLN B 478      -3.568  16.267  45.821  1.00  0.00     0.159 HD
ATOM  17255 2HE2 GLN B 478      -4.848  15.106  45.407  1.00  0.00     0.159 HD
ATOM  17256  OE1 GLN B 478      -6.457  15.823  47.125  1.00  7.84    -0.274 OA
ATOM  17257  N   VAL B 479      -6.148  16.151  51.999  1.00  7.03    -0.346 N
ATOM  17258  HN  VAL B 479      -6.864  15.715  51.419  1.00  0.00     0.163 HD
ATOM  17259  CA  VAL B 479      -6.373  16.410  53.442  1.00  6.37     0.180 C
ATOM  17261  C   VAL B 479      -5.367  15.627  54.281  1.00 10.10     0.241 C
ATOM  17262  O   VAL B 479      -4.849  16.131  55.271  1.00  8.76    -0.271 OA
ATOM  17263  CB  VAL B 479      -7.801  16.087  53.853  1.00  8.29     0.009 C
ATOM  17265  CG1 VAL B 479      -8.032  16.299  55.380  1.00 14.63     0.012 C
ATOM  17269  CG2 VAL B 479      -8.680  17.110  53.103  1.00 11.54     0.012 C
ATOM  17273  N   ALA B 480      -5.151  14.343  53.967  1.00  6.26    -0.346 N
ATOM  17274  HN  ALA B 480      -5.658  13.938  53.180  1.00  0.00     0.163 HD
ATOM  17275  CA  ALA B 480      -4.213  13.498  54.713  1.00  9.83     0.172 C
ATOM  17277  C   ALA B 480      -2.802  14.104  54.682  1.00 12.51     0.240 C
ATOM  17278  O   ALA B 480      -2.077  14.047  55.682  1.00 10.36    -0.271 OA
ATOM  17279  CB  ALA B 480      -4.177  12.099  54.109  1.00  6.61     0.042 C
ATOM  17283  N   SER B 481      -2.404  14.711  53.566  1.00  8.11    -0.344 N
ATOM  17284  HN  SER B 481      -3.025  14.724  52.757  1.00  0.00     0.163 HD
ATOM  17285  CA  SER B 481      -1.101  15.358  53.475  1.00  8.63     0.200 C
ATOM  17287  C   SER B 481      -1.014  16.587  54.411  1.00 10.95     0.243 C
ATOM  17288  O   SER B 481       0.067  16.760  54.975  1.00 12.50    -0.271 OA
ATOM  17289  CB  SER B 481      -0.772  15.941  52.080  1.00 14.03     0.199 C
ATOM  17292  OG ASER B 481       0.544  16.477  52.145  0.70 20.28    -0.398 OA
ATOM  17293  HG ASER B 481       0.746  16.835  51.289  1.00  0.00     0.209 HD
ATOM  17294  N   LEU B 482      -2.070  17.391  54.561  1.00  6.06    -0.346 N
ATOM  17295  HN  LEU B 482      -2.902  17.247  53.989  1.00  0.00     0.163 HD
ATOM  17296  CA  LEU B 482      -2.041  18.482  55.546  1.00  4.32     0.177 C
ATOM  17298  C   LEU B 482      -2.012  18.003  56.985  1.00  7.31     0.241 C
ATOM  17299  O   LEU B 482      -1.307  18.533  57.877  1.00  6.51    -0.271 OA
ATOM  17300  CB  LEU B 482      -3.336  19.369  55.391  1.00  8.98     0.038 C
ATOM  17303  CG  LEU B 482      -3.386  20.165  54.075  1.00 14.54    -0.020 C
ATOM  17305  CD1 LEU B 482      -4.777  20.757  53.836  1.00 14.51     0.009 C
ATOM  17309  CD2 LEU B 482      -2.333  21.278  54.118  1.00 12.58     0.009 C
ATOM  17313  N   ARG B 483      -2.754  16.927  57.255  1.00  6.11    -0.346 N
ATOM  17314  HN  ARG B 483      -3.271  16.465  56.507  1.00  0.00     0.163 HD
ATOM  17315  CA  ARG B 483      -2.829  16.405  58.629  1.00  7.52     0.176 C
ATOM  17317  C   ARG B 483      -1.491  15.878  59.136  1.00 12.34     0.241 C
ATOM  17318  O   ARG B 483      -1.272  15.886  60.353  1.00 11.22    -0.271 OA
ATOM  17319  CB  ARG B 483      -3.819  15.218  58.729  1.00  9.30     0.036 C
ATOM  17322  CG  ARG B 483      -5.300  15.639  58.615  1.00  7.89     0.023 C
ATOM  17325  CD  ARG B 483      -6.167  14.372  58.878  1.00 12.59     0.138 C
ATOM  17328  NE  ARG B 483      -7.585  14.844  58.923  1.00 11.46    -0.227 N
ATOM  17329  HE  ARG B 483      -7.839  15.627  59.526  1.00  0.00     0.177 HD
ATOM  17330  CZ  ARG B 483      -8.523  14.249  58.180  1.00 16.13     0.665 C
ATOM  17331  NH1 ARG B 483      -8.234  13.210  57.385  1.00  8.87    -0.235 N
ATOM  17332 1HH1 ARG B 483      -7.276  12.862  57.359  1.00  0.00     0.174 HD
ATOM  17333 2HH1 ARG B 483      -8.950  12.756  56.818  1.00  0.00     0.174 HD
ATOM  17334  NH2 ARG B 483      -9.767  14.701  58.214  1.00  9.39    -0.235 N
ATOM  17335 1HH2 ARG B 483      -9.987  15.492  58.819  1.00  0.00     0.174 HD
ATOM  17336 2HH2 ARG B 483     -10.483  14.247  57.647  1.00  0.00     0.174 HD
ATOM  17337  N   VAL B 484      -0.626  15.409  58.240  1.00  7.91    -0.346 N
ATOM  17338  HN  VAL B 484      -0.836  15.408  57.242  1.00  0.00     0.163 HD
ATOM  17339  CA  VAL B 484       0.666  14.885  58.769  1.00 10.54     0.180 C
ATOM  17341  C   VAL B 484       1.757  15.945  58.656  1.00 14.36     0.241 C
ATOM  17342  O   VAL B 484       2.919  15.621  58.839  1.00 10.43    -0.271 OA
ATOM  17343  CB  VAL B 484       1.091  13.578  58.116  1.00 11.82     0.009 C
ATOM  17345  CG1 VAL B 484      -0.009  12.524  58.301  1.00 13.09     0.012 C
ATOM  17349  CG2 VAL B 484       1.357  13.701  56.611  1.00 12.59     0.012 C
ATOM  17353  N   THR B 485       1.398  17.197  58.396  1.00  8.30    -0.344 N
ATOM  17354  HN  THR B 485       0.418  17.423  58.224  1.00  0.00     0.163 HD
ATOM  17355  CA  THR B 485       2.427  18.265  58.357  1.00  6.68     0.205 C
ATOM  17357  C   THR B 485       2.580  18.770  59.789  1.00  6.74     0.246 C
ATOM  17358  O   THR B 485       1.590  19.224  60.389  1.00  8.23    -0.271 OA
ATOM  17359  CB  THR B 485       1.925  19.384  57.450  1.00  7.97     0.146 C
ATOM  17361  CG2 THR B 485       2.890  20.601  57.427  1.00  6.51     0.042 C
ATOM  17365  OG1 THR B 485       1.792  18.891  56.081  1.00 10.17    -0.393 OA
ATOM  17366  HG1 THR B 485       1.479  19.588  55.516  1.00  0.00     0.210 HD
ATOM  17367  N   PRO B 486       3.787  18.858  60.320  1.00  8.02    -0.337 N
ATOM  17368  CA  PRO B 486       3.992  19.345  61.693  1.00  7.70     0.179 C
ATOM  17370  C   PRO B 486       3.540  20.802  61.823  1.00  6.78     0.241 C
ATOM  17371  O   PRO B 486       3.740  21.619  60.946  1.00  8.65    -0.271 OA
ATOM  17372  CB  PRO B 486       5.509  19.237  61.929  1.00  7.95     0.037 C
ATOM  17375  CG  PRO B 486       5.922  18.128  60.997  1.00  9.54     0.022 C
ATOM  17378  CD  PRO B 486       5.050  18.364  59.750  1.00  7.90     0.127 C
ATOM  17381  N   ASN B 487       2.963  21.080  62.976  1.00  7.10    -0.346 N
ATOM  17382  HN  ASN B 487       2.847  20.329  63.656  1.00  0.00     0.163 HD
ATOM  17383  CA  ASN B 487       2.482  22.416  63.324  1.00  9.40     0.185 C
ATOM  17385  C   ASN B 487       1.363  22.906  62.392  1.00 10.52     0.241 C
ATOM  17386  O   ASN B 487       1.002  24.093  62.414  1.00 16.07    -0.271 OA
ATOM  17387  CB  ASN B 487       3.618  23.442  63.401  1.00  9.58     0.137 C
ATOM  17390  CG  ASN B 487       3.169  24.633  64.259  1.00 20.64     0.217 C
ATOM  17391  ND2 ASN B 487       3.535  25.829  63.858  1.00  9.27    -0.370 N
ATOM  17392 1HD2 ASN B 487       4.118  25.955  63.030  1.00  0.00     0.159 HD
ATOM  17393 2HD2 ASN B 487       3.237  26.620  64.428  1.00  0.00     0.159 HD
ATOM  17394  OD1 ASN B 487       2.459  24.480  65.268  1.00 11.73    -0.274 OA
ATOM  17395  N   MET B 488       0.679  22.067  61.613  1.00  8.27    -0.346 N
ATOM  17396  HN  MET B 488       0.918  21.076  61.605  1.00  0.00     0.163 HD
ATOM  17397  CA  MET B 488      -0.421  22.560  60.762  1.00  8.30     0.177 C
ATOM  17399  C   MET B 488      -1.720  22.252  61.499  1.00 14.24     0.241 C
ATOM  17400  O   MET B 488      -1.772  21.191  62.143  1.00 11.29    -0.271 OA
ATOM  17401  CB  MET B 488      -0.430  21.760  59.432  1.00  9.24     0.045 C
ATOM  17404  CG  MET B 488      -1.660  22.046  58.565  1.00 13.28     0.076 C
ATOM  17407  SD  MET B 488      -1.648  23.792  58.005  1.00 23.66    -0.173 SA
ATOM  17408  CE  MET B 488      -0.080  23.909  57.314  1.00 19.26     0.089 C
ATOM  17412  N   SER B 489      -2.759  23.084  61.554  1.00  8.53    -0.344 N
ATOM  17413  HN  SER B 489      -2.657  24.027  61.179  1.00  0.00     0.163 HD
ATOM  17414  CA  SER B 489      -4.033  22.690  62.131  1.00  6.70     0.200 C
ATOM  17416  C   SER B 489      -5.037  22.543  60.978  1.00 11.26     0.243 C
ATOM  17417  O   SER B 489      -5.039  23.386  60.050  1.00 11.30    -0.271 OA
ATOM  17418  CB  SER B 489      -4.560  23.764  63.152  1.00  9.60     0.199 C
ATOM  17421  OG  SER B 489      -5.787  23.254  63.663  1.00 11.91    -0.398 OA
ATOM  17422  HG  SER B 489      -6.105  23.903  64.280  1.00  0.00     0.209 HD
ATOM  17423  N   THR B 490      -5.767  21.433  60.879  1.00  6.88    -0.344 N
ATOM  17424  HN  THR B 490      -5.713  20.726  61.613  1.00  0.00     0.163 HD
ATOM  17425  CA  THR B 490      -6.649  21.216  59.725  1.00  7.96     0.205 C
ATOM  17427  C   THR B 490      -8.067  20.877  60.203  1.00  7.76     0.243 C
ATOM  17428  O   THR B 490      -8.152  19.984  61.044  1.00  7.62    -0.271 OA
ATOM  17429  CB  THR B 490      -6.128  19.980  58.949  1.00 12.92     0.146 C
ATOM  17431  CG2 THR B 490      -6.994  19.757  57.708  1.00 13.63     0.042 C
ATOM  17435  OG1 THR B 490      -4.796  20.243  58.497  1.00 11.69    -0.393 OA
ATOM  17436  HG1 THR B 490      -4.258  20.381  59.268  1.00  0.00     0.210 HD
ATOM  17437  N   TRP B 491      -9.070  21.636  59.792  1.00  6.48    -0.346 N
ATOM  17438  HN  TRP B 491      -8.876  22.381  59.123  1.00  0.00     0.163 HD
ATOM  17439  CA  TRP B 491     -10.443  21.453  60.254  1.00  7.88     0.181 C
ATOM  17441  C   TRP B 491     -11.310  21.033  59.066  1.00  6.52     0.241 C
ATOM  17442  O   TRP B 491     -11.327  21.750  58.046  1.00  6.16    -0.271 OA
ATOM  17443  CB  TRP B 491     -11.029  22.755  60.890  1.00  6.07     0.075 C
ATOM  17446  CG  TRP B 491     -10.349  23.010  62.220  1.00  6.95    -0.028 A
ATOM  17447  CD1 TRP B 491      -9.045  23.416  62.402  1.00  9.82     0.096 A
ATOM  17449  CD2 TRP B 491     -10.887  22.790  63.530  1.00  7.65    -0.002 A
ATOM  17450  CE2 TRP B 491      -9.881  23.127  64.459  1.00 10.00     0.042 A
ATOM  17451  CE3 TRP B 491     -12.132  22.377  63.992  1.00 10.93     0.014 A
ATOM  17453  NE1 TRP B 491      -8.768  23.479  63.753  1.00  7.98    -0.365 N
ATOM  17454  HE1 TRP B 491      -7.872  23.747  64.160  1.00  0.00     0.165 HD
ATOM  17455  CZ2 TRP B 491     -10.040  23.001  65.849  1.00 18.63     0.030 A
ATOM  17457  CZ3 TRP B 491     -12.304  22.274  65.383  1.00 12.47     0.001 A
ATOM  17459  CH2 TRP B 491     -11.281  22.553  66.275  1.00 13.42     0.002 A
ATOM  17461  N   ARG B 492     -12.171  20.018  59.256  1.00  4.56    -0.346 N
ATOM  17462  HN  ARG B 492     -12.183  19.515  60.143  1.00  0.00     0.163 HD
ATOM  17463  CA  ARG B 492     -13.110  19.632  58.161  1.00  7.25     0.176 C
ATOM  17465  C   ARG B 492     -14.507  19.606  58.780  1.00 10.56     0.243 C
ATOM  17466  O   ARG B 492     -15.013  18.561  59.182  1.00  9.51    -0.271 OA
ATOM  17467  CB  ARG B 492     -12.714  18.229  57.631  1.00  5.48     0.036 C
ATOM  17470  CG  ARG B 492     -13.653  17.937  56.401  1.00  6.44     0.023 C
ATOM  17473  CD  ARG B 492     -13.139  16.707  55.644  1.00 10.86     0.138 C
ATOM  17476  NE  ARG B 492     -13.886  16.515  54.384  1.00 12.32    -0.227 N
ATOM  17477  HE  ARG B 492     -13.712  17.169  53.621  1.00  0.00     0.177 HD
ATOM  17478  CZ  ARG B 492     -14.786  15.526  54.179  1.00  9.76     0.665 C
ATOM  17479  NH1 ARG B 492     -15.025  14.612  55.110  1.00  6.48    -0.235 N
ATOM  17480 1HH1 ARG B 492     -14.555  14.722  56.009  1.00  0.00     0.174 HD
ATOM  17481 2HH1 ARG B 492     -15.704  13.866  54.955  1.00  0.00     0.174 HD
ATOM  17482  NH2 ARG B 492     -15.391  15.384  53.022  1.00  9.81    -0.235 N
ATOM  17483 1HH2 ARG B 492     -15.207  16.087  52.306  1.00  0.00     0.174 HD
ATOM  17484 2HH2 ARG B 492     -16.070  14.638  52.867  1.00  0.00     0.174 HD
ATOM  17485  N   PRO B 493     -15.162  20.765  58.951  1.00  8.27    -0.337 N
ATOM  17486  CA  PRO B 493     -16.389  20.886  59.700  1.00  9.45     0.179 C
ATOM  17488  C   PRO B 493     -17.592  20.191  59.074  1.00 10.38     0.241 C
ATOM  17489  O   PRO B 493     -17.704  20.172  57.826  1.00  9.64    -0.271 OA
ATOM  17490  CB  PRO B 493     -16.659  22.398  59.785  1.00 10.30     0.037 C
ATOM  17493  CG  PRO B 493     -15.865  22.987  58.661  1.00 11.52     0.022 C
ATOM  17496  CD  PRO B 493     -14.645  22.082  58.501  1.00  6.79     0.127 C
ATOM  17499  N   CYS B 494     -18.462  19.628  59.949  1.00  9.05    -0.345 N
ATOM  17500  HN  CYS B 494     -18.349  19.707  60.960  1.00  0.00     0.163 HD
ATOM  17501  CA  CYS B 494     -19.590  18.890  59.331  1.00  9.22     0.186 C
ATOM  17503  C   CYS B 494     -20.833  19.760  59.103  1.00 12.07     0.242 C
ATOM  17504  O   CYS B 494     -21.792  19.254  58.506  1.00  8.83    -0.271 OA
ATOM  17505  CB  CYS B 494     -20.009  17.679  60.164  1.00  9.14     0.121 C
ATOM  17508  SG  CYS B 494     -20.830  18.071  61.736  1.00 11.22    -0.095 SA
ATOM  17509  N   ASP B 495     -20.873  20.971  59.615  1.00  9.74    -0.345 N
ATOM  17510  HN  ASP B 495     -20.078  21.337  60.139  1.00  0.00     0.163 HD
ATOM  17511  CA  ASP B 495     -22.088  21.795  59.420  1.00  9.93     0.186 C
ATOM  17513  C   ASP B 495     -21.742  23.225  59.767  1.00  9.70     0.241 C
ATOM  17514  O   ASP B 495     -20.554  23.550  60.013  1.00  8.18    -0.271 OA
ATOM  17515  CB  ASP B 495     -23.227  21.223  60.312  1.00 11.31     0.147 C
ATOM  17518  CG  ASP B 495     -22.964  21.376  61.809  1.00 12.01     0.175 C
ATOM  17519  OD1 ASP B 495     -22.068  22.126  62.272  1.00 10.64    -0.648 OA
ATOM  17520  OD2 ASP B 495     -23.670  20.733  62.619  1.00 10.15    -0.648 OA
ATOM  17521  N   GLN B 496     -22.712  24.159  59.729  1.00 10.26    -0.346 N
ATOM  17522  HN  GLN B 496     -23.682  23.879  59.582  1.00  0.00     0.163 HD
ATOM  17523  CA  GLN B 496     -22.381  25.570  59.898  1.00  8.52     0.177 C
ATOM  17525  C   GLN B 496     -21.870  25.924  61.285  1.00 10.81     0.241 C
ATOM  17526  O   GLN B 496     -21.166  26.920  61.472  1.00 11.45    -0.271 OA
ATOM  17527  CB  GLN B 496     -23.637  26.431  59.546  1.00  8.68     0.044 C
ATOM  17530  CG  GLN B 496     -24.790  26.256  60.562  1.00  9.25     0.105 C
ATOM  17533  CD  GLN B 496     -25.801  27.385  60.417  1.00 14.01     0.215 C
ATOM  17534  NE2 GLN B 496     -26.916  27.346  61.159  1.00 11.00    -0.370 N
ATOM  17535 1HE2 GLN B 496     -27.593  28.102  61.062  1.00  0.00     0.159 HD
ATOM  17536 2HE2 GLN B 496     -27.092  26.558  61.783  1.00  0.00     0.159 HD
ATOM  17537  OE1 GLN B 496     -25.586  28.347  59.655  1.00 11.64    -0.274 OA
ATOM  17538  N   VAL B 497     -22.240  25.132  62.296  1.00  9.24    -0.346 N
ATOM  17539  HN  VAL B 497     -22.859  24.341  62.119  1.00  0.00     0.163 HD
ATOM  17540  CA  VAL B 497     -21.764  25.391  63.655  1.00  6.57     0.180 C
ATOM  17542  C   VAL B 497     -20.292  24.992  63.775  1.00  8.77     0.241 C
ATOM  17543  O   VAL B 497     -19.456  25.765  64.274  1.00  9.72    -0.271 OA
ATOM  17544  CB  VAL B 497     -22.600  24.577  64.685  1.00 10.60     0.009 C
ATOM  17546  CG1 VAL B 497     -22.163  24.944  66.094  1.00 15.77     0.012 C
ATOM  17550  CG2 VAL B 497     -24.084  24.933  64.468  1.00 10.98     0.012 C
ATOM  17554  N   GLU B 498     -19.944  23.726  63.399  1.00  8.75    -0.346 N
ATOM  17555  HN  GLU B 498     -20.641  23.038  63.115  1.00  0.00     0.163 HD
ATOM  17556  CA  GLU B 498     -18.488  23.407  63.427  1.00  6.30     0.177 C
ATOM  17558  C   GLU B 498     -17.703  24.391  62.551  1.00  9.29     0.241 C
ATOM  17559  O   GLU B 498     -16.519  24.650  62.864  1.00  9.61    -0.271 OA
ATOM  17560  CB  GLU B 498     -18.182  22.007  62.912  1.00  7.88     0.045 C
ATOM  17563  CG  GLU B 498     -18.768  20.941  63.860  1.00 10.94     0.116 C
ATOM  17566  CD  GLU B 498     -18.266  19.534  63.568  1.00 12.57     0.172 C
ATOM  17567  OE1 GLU B 498     -17.654  19.272  62.525  1.00  8.22    -0.648 OA
ATOM  17568  OE2 GLU B 498     -18.554  18.638  64.402  1.00 12.03    -0.648 OA
ATOM  17569  N   SER B 499     -18.277  24.893  61.466  1.00  7.97    -0.344 N
ATOM  17570  HN  SER B 499     -19.237  24.638  61.233  1.00  0.00     0.163 HD
ATOM  17571  CA  SER B 499     -17.525  25.825  60.591  1.00  7.94     0.200 C
ATOM  17573  C   SER B 499     -17.172  27.114  61.343  1.00  9.86     0.243 C
ATOM  17574  O   SER B 499     -16.102  27.711  61.219  1.00 10.24    -0.271 OA
ATOM  17575  CB  SER B 499     -18.387  26.181  59.356  1.00  9.77     0.199 C
ATOM  17578  OG  SER B 499     -18.563  25.036  58.513  1.00 10.15    -0.398 OA
ATOM  17579  HG  SER B 499     -19.092  25.255  57.755  1.00  0.00     0.209 HD
ATOM  17580  N   ALA B 500     -18.108  27.645  62.127  1.00  7.50    -0.346 N
ATOM  17581  HN  ALA B 500     -19.021  27.194  62.185  1.00  0.00     0.163 HD
ATOM  17582  CA  ALA B 500     -17.863  28.856  62.906  1.00 10.65     0.172 C
ATOM  17584  C   ALA B 500     -16.850  28.578  64.027  1.00 10.55     0.240 C
ATOM  17585  O   ALA B 500     -16.017  29.444  64.300  1.00 10.90    -0.271 OA
ATOM  17586  CB  ALA B 500     -19.159  29.407  63.511  1.00 12.78     0.042 C
ATOM  17590  N   VAL B 501     -16.886  27.427  64.659  1.00  8.82    -0.346 N
ATOM  17591  HN  VAL B 501     -17.634  26.771  64.437  1.00  0.00     0.163 HD
ATOM  17592  CA  VAL B 501     -15.902  27.049  65.664  1.00  6.45     0.180 C
ATOM  17594  C   VAL B 501     -14.490  26.979  65.062  1.00  9.80     0.241 C
ATOM  17595  O   VAL B 501     -13.497  27.453  65.665  1.00  9.29    -0.271 OA
ATOM  17596  CB  VAL B 501     -16.245  25.733  66.373  1.00  7.89     0.009 C
ATOM  17598  CG1 VAL B 501     -15.106  25.330  67.371  1.00  9.64     0.012 C
ATOM  17602  CG2 VAL B 501     -17.478  25.894  67.268  1.00 10.19     0.012 C
ATOM  17606  N   ALA B 502     -14.363  26.404  63.873  1.00  8.10    -0.346 N
ATOM  17607  HN  ALA B 502     -15.201  26.033  63.425  1.00  0.00     0.163 HD
ATOM  17608  CA  ALA B 502     -13.090  26.274  63.171  1.00  8.54     0.172 C
ATOM  17610  C   ALA B 502     -12.520  27.638  62.791  1.00  9.44     0.240 C
ATOM  17611  O   ALA B 502     -11.322  27.888  62.959  1.00 10.04    -0.271 OA
ATOM  17612  CB  ALA B 502     -13.288  25.425  61.901  1.00  8.68     0.042 C
ATOM  17616  N   TRP B 503     -13.359  28.571  62.360  1.00 10.08    -0.346 N
ATOM  17617  HN  TRP B 503     -14.348  28.342  62.266  1.00  0.00     0.163 HD
ATOM  17618  CA  TRP B 503     -12.902  29.933  62.012  1.00  8.73     0.181 C
ATOM  17620  C   TRP B 503     -12.411  30.614  63.284  1.00 10.02     0.241 C
ATOM  17621  O   TRP B 503     -11.399  31.293  63.327  1.00  9.44    -0.271 OA
ATOM  17622  CB  TRP B 503     -14.047  30.717  61.343  1.00  7.68     0.075 C
ATOM  17625  CG  TRP B 503     -13.844  30.990  59.892  1.00 12.15    -0.028 A
ATOM  17626  CD1 TRP B 503     -14.502  30.456  58.808  1.00 13.51     0.096 A
ATOM  17628  CD2 TRP B 503     -12.883  31.914  59.347  1.00 14.10    -0.002 A
ATOM  17629  CE2 TRP B 503     -13.020  31.898  57.946  1.00 13.56     0.042 A
ATOM  17630  CE3 TRP B 503     -11.942  32.746  59.943  1.00 10.22     0.014 A
ATOM  17632  NE1 TRP B 503     -13.994  30.978  57.644  1.00 13.31    -0.365 N
ATOM  17633  HE1 TRP B 503     -14.293  30.723  56.703  1.00  0.00     0.165 HD
ATOM  17634  CZ2 TRP B 503     -12.207  32.691  57.132  1.00 16.07     0.030 A
ATOM  17636  CZ3 TRP B 503     -11.121  33.541  59.155  1.00 17.15     0.001 A
ATOM  17638  CH2 TRP B 503     -11.278  33.510  57.756  1.00 13.45     0.002 A
ATOM  17640  N   LYS B 504     -13.126  30.449  64.418  1.00  9.19    -0.346 N
ATOM  17641  HN  LYS B 504     -13.985  29.900  64.399  1.00  0.00     0.163 HD
ATOM  17642  CA  LYS B 504     -12.675  31.056  65.682  1.00  9.96     0.176 C
ATOM  17644  C   LYS B 504     -11.329  30.490  66.107  1.00 11.74     0.241 C
ATOM  17645  O   LYS B 504     -10.430  31.206  66.591  1.00 11.23    -0.271 OA
ATOM  17646  CB  LYS B 504     -13.713  30.808  66.797  1.00 10.27     0.035 C
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ATOM  17649  CG  LYS B 504     -13.358  31.494  68.125  1.00  9.94     0.004 C
ATOM  17652  CD  LYS B 504     -14.408  31.089  69.162  1.00 15.10     0.027 C
ATOM  17655  CE  LYS B 504     -14.187  31.969  70.399  1.00 19.48     0.229 C
ATOM  17658  NZ  LYS B 504     -13.171  31.433  71.316  1.00 20.62    -0.079 N
ATOM  17659  HZ1 LYS B 504     -13.024  32.018  72.138  1.00  0.00     0.274 HD
ATOM  17660  HZ2 LYS B 504     -12.292  31.267  70.827  1.00  0.00     0.274 HD
ATOM  17661  HZ3 LYS B 504     -13.395  30.476  71.587  1.00  0.00     0.274 HD
ATOM  17662  N   TYR B 505     -11.171  29.166  66.041  1.00  8.49    -0.346 N
ATOM  17663  HN  TYR B 505     -11.966  28.589  65.767  1.00  0.00     0.163 HD
ATOM  17664  CA  TYR B 505      -9.899  28.513  66.347  1.00 10.12     0.180 C
ATOM  17666  C   TYR B 505      -8.791  29.074  65.458  1.00 10.92     0.241 C
ATOM  17667  O   TYR B 505      -7.728  29.298  66.017  1.00 11.04    -0.271 OA
ATOM  17668  CB  TYR B 505     -10.005  26.993  66.112  1.00  7.95     0.073 C
ATOM  17671  CG  TYR B 505      -8.860  26.171  66.661  1.00 11.94    -0.056 A
ATOM  17672  CD1 TYR B 505      -8.926  25.692  67.964  1.00 16.67     0.010 A
ATOM  17674  CD2 TYR B 505      -7.733  25.845  65.910  1.00 12.19     0.010 A
ATOM  17676  CE1 TYR B 505      -7.920  24.905  68.503  1.00 18.73     0.037 A
ATOM  17678  CE2 TYR B 505      -6.713  25.071  66.462  1.00 13.60     0.037 A
ATOM  17680  CZ  TYR B 505      -6.809  24.612  67.743  1.00 16.92     0.065 A
ATOM  17681  OH  TYR B 505      -5.812  23.809  68.309  1.00 20.64    -0.361 OA
ATOM  17682  HH  TYR B 505      -5.879  23.489  69.201  1.00  0.00     0.217 HD
ATOM  17683  N   GLY B 506      -8.995  29.197  64.153  1.00  9.73    -0.351 N
ATOM  17684  HN  GLY B 506      -9.907  28.955  63.766  1.00  0.00     0.163 HD
ATOM  17685  CA  GLY B 506      -7.932  29.676  63.247  1.00  8.15     0.225 C
ATOM  17688  C   GLY B 506      -7.549  31.136  63.544  1.00  9.78     0.236 C
ATOM  17689  O   GLY B 506      -6.387  31.518  63.415  1.00 12.85    -0.272 OA
ATOM  17690  N   VAL B 507      -8.501  32.033  63.829  1.00  9.62    -0.346 N
ATOM  17691  HN  VAL B 507      -9.483  31.759  63.857  1.00  0.00     0.163 HD
ATOM  17692  CA  VAL B 507      -8.101  33.426  64.101  1.00 12.28     0.180 C
ATOM  17694  C   VAL B 507      -7.415  33.537  65.450  1.00  9.96     0.241 C
ATOM  17695  O   VAL B 507      -6.511  34.377  65.603  1.00 12.62    -0.271 OA
ATOM  17696  CB  VAL B 507      -9.243  34.459  63.976  1.00 13.42     0.009 C
ATOM  17698  CG1 VAL B 507      -9.855  34.420  62.574  1.00 13.38     0.012 C
ATOM  17702  CG2 VAL B 507     -10.273  34.322  65.039  1.00 17.47     0.012 C
ATOM  17706  N   GLU B 508      -7.686  32.671  66.437  1.00  9.20    -0.346 N
ATOM  17707  HN  GLU B 508      -8.376  31.939  66.269  1.00  0.00     0.163 HD
ATOM  17708  CA  GLU B 508      -7.039  32.731  67.733  1.00 11.95     0.177 C
ATOM  17710  C   GLU B 508      -5.728  31.966  67.826  1.00 17.47     0.241 C
ATOM  17711  O   GLU B 508      -4.978  32.079  68.811  1.00 15.21    -0.271 OA
ATOM  17712  CB  GLU B 508      -7.961  32.135  68.858  1.00 14.61     0.045 C
ATOM  17715  CG  GLU B 508      -9.154  33.085  69.004  1.00 14.92     0.116 C
ATOM  17718  CD  GLU B 508     -10.153  32.660  70.063  1.00 25.24     0.172 C
ATOM  17719  OE1 GLU B 508     -10.318  31.465  70.330  1.00 18.11    -0.648 OA
ATOM  17720  OE2 GLU B 508     -10.818  33.516  70.681  1.00 24.56    -0.648 OA
ATOM  17721  N   ARG B 509      -5.407  31.229  66.749  1.00  9.18    -0.346 N
ATOM  17722  HN  ARG B 509      -6.001  31.226  65.920  1.00  0.00     0.163 HD
ATOM  17723  CA  ARG B 509      -4.185  30.434  66.799  1.00 12.08     0.176 C
ATOM  17725  C   ARG B 509      -3.018  31.367  66.509  1.00 18.61     0.241 C
ATOM  17726  O   ARG B 509      -2.831  31.693  65.347  1.00 24.76    -0.271 OA
ATOM  17727  CB  ARG B 509      -4.321  29.252  65.831  1.00 15.86     0.036 C
ATOM  17730  CG  ARG B 509      -3.175  28.298  65.875  1.00 19.38     0.023 C
ATOM  17733  CD  ARG B 509      -3.301  27.064  64.945  1.00 18.71     0.138 C
ATOM  17736  NE  ARG B 509      -2.170  26.300  65.480  1.00 24.51    -0.227 N
ATOM  17737  HE  ARG B 509      -2.124  26.293  66.499  1.00  0.00     0.177 HD
ATOM  17738  CZ  ARG B 509      -1.220  25.634  64.912  1.00 23.52     0.665 C
ATOM  17739  NH1 ARG B 509      -1.214  25.518  63.605  1.00 13.04    -0.235 N
ATOM  17740 1HH1 ARG B 509      -1.934  25.921  63.005  1.00  0.00     0.174 HD
ATOM  17741 2HH1 ARG B 509      -0.464  24.992  63.157  1.00  0.00     0.174 HD
ATOM  17742  NH2 ARG B 509      -0.287  25.111  65.690  1.00 25.49    -0.235 N
ATOM  17743 1HH2 ARG B 509      -0.292  25.201  66.706  1.00  0.00     0.174 HD
ATOM  17744 2HH2 ARG B 509       0.463  24.585  65.242  1.00  0.00     0.174 HD
ATOM  17745  N   GLN B 510      -2.166  31.641  67.482  1.00 14.74    -0.346 N
ATOM  17746  HN  GLN B 510      -2.276  31.209  68.399  1.00  0.00     0.163 HD
ATOM  17747  CA  GLN B 510      -1.064  32.570  67.230  1.00 22.40     0.177 C
ATOM  17749  C   GLN B 510       0.227  31.966  66.693  1.00 19.76     0.241 C
ATOM  17750  O   GLN B 510       1.075  32.699  66.198  1.00 23.30    -0.271 OA
ATOM  17751  CB  GLN B 510      -0.623  33.198  68.593  1.00 24.34     0.044 C
ATOM  17754  CG  GLN B 510      -1.774  33.900  69.298  1.00 46.92     0.105 C
ATOM  17757  CD  GLN B 510      -1.676  35.408  69.168  1.00 60.33     0.215 C
ATOM  17758  NE2 GLN B 510      -2.070  36.103  70.234  1.00 66.24    -0.370 N
ATOM  17759 1HE2 GLN B 510      -2.004  37.117  70.147  1.00  0.00     0.159 HD
ATOM  17760 2HE2 GLN B 510      -2.427  35.675  71.089  1.00  0.00     0.159 HD
ATOM  17761  OE1 GLN B 510      -1.244  35.926  68.133  1.00 69.57    -0.274 OA
ATOM  17762  N   ASP B 511       0.445  30.694  66.889  1.00 15.59    -0.346 N
ATOM  17763  HN  ASP B 511      -0.294  30.113  67.285  1.00  0.00     0.163 HD
ATOM  17764  CA  ASP B 511       1.734  30.090  66.549  1.00 18.10     0.186 C
ATOM  17766  C   ASP B 511       1.712  29.141  65.363  1.00 13.11     0.241 C
ATOM  17767  O   ASP B 511       2.629  28.301  65.264  1.00 11.80    -0.271 OA
ATOM  17768  CB  ASP B 511       2.267  29.343  67.787  1.00 22.37     0.147 C
ATOM  17771  CG  ASP B 511       1.257  28.332  68.280  1.00 36.87     0.175 C
ATOM  17772  OD1 ASP B 511       0.118  28.262  67.766  1.00 39.21    -0.648 OA
ATOM  17773  OD2 ASP B 511       1.576  27.575  69.215  1.00 42.63    -0.648 OA
ATOM  17774  N   GLY B 512       0.736  29.309  64.466  1.00 11.53    -0.351 N
ATOM  17775  HN  GLY B 512      -0.008  29.993  64.602  1.00  0.00     0.163 HD
ATOM  17776  CA  GLY B 512       0.793  28.459  63.279  1.00  8.48     0.225 C
ATOM  17779  C   GLY B 512      -0.502  28.660  62.486  1.00 10.73     0.238 C
ATOM  17780  O   GLY B 512      -1.440  29.294  62.966  1.00 11.07    -0.272 OA
ATOM  17781  N   PRO B 513      -0.487  28.128  61.270  1.00 10.02    -0.337 N
ATOM  17782  CA  PRO B 513      -1.608  28.294  60.370  1.00  8.63     0.179 C
ATOM  17784  C   PRO B 513      -2.762  27.329  60.611  1.00  9.36     0.241 C
ATOM  17785  O   PRO B 513      -2.590  26.291  61.264  1.00 10.43    -0.271 OA
ATOM  17786  CB  PRO B 513      -0.934  28.159  58.992  1.00  6.70     0.037 C
ATOM  17789  CG  PRO B 513       0.099  27.072  59.234  1.00  9.83     0.022 C
ATOM  17792  CD  PRO B 513       0.661  27.461  60.621  1.00  6.82     0.127 C
ATOM  17795  N   THR B 514      -3.911  27.636  60.007  1.00  9.80    -0.344 N
ATOM  17796  HN  THR B 514      -3.976  28.483  59.442  1.00  0.00     0.163 HD
ATOM  17797  CA  THR B 514      -5.094  26.755  60.152  1.00  7.80     0.205 C
ATOM  17799  C   THR B 514      -5.791  26.602  58.801  1.00  9.64     0.243 C
ATOM  17800  O   THR B 514      -6.113  27.647  58.195  1.00  8.86    -0.271 OA
ATOM  17801  CB  THR B 514      -6.064  27.409  61.141  1.00 10.70     0.146 C
ATOM  17803  CG2 THR B 514      -7.287  26.511  61.386  1.00 13.24     0.042 C
ATOM  17807  OG1 THR B 514      -5.402  27.658  62.403  1.00  8.92    -0.393 OA
ATOM  17808  HG1 THR B 514      -6.004  28.064  63.016  1.00  0.00     0.210 HD
ATOM  17809  N   ALA B 515      -5.980  25.381  58.315  1.00  5.77    -0.346 N
ATOM  17810  HN  ALA B 515      -5.671  24.565  58.843  1.00  0.00     0.163 HD
ATOM  17811  CA  ALA B 515      -6.639  25.214  57.009  1.00  6.95     0.172 C
ATOM  17813  C   ALA B 515      -8.087  24.754  57.240  1.00  8.77     0.240 C
ATOM  17814  O   ALA B 515      -8.304  23.863  58.069  1.00 11.86    -0.271 OA
ATOM  17815  CB  ALA B 515      -5.897  24.077  56.259  1.00  8.38     0.042 C
ATOM  17819  N   LEU B 516      -9.054  25.387  56.606  1.00  9.25    -0.346 N
ATOM  17820  HN  LEU B 516      -8.821  26.196  56.031  1.00  0.00     0.163 HD
ATOM  17821  CA  LEU B 516     -10.440  24.968  56.701  1.00 10.15     0.177 C
ATOM  17823  C   LEU B 516     -10.819  24.203  55.435  1.00 11.18     0.241 C
ATOM  17824  O   LEU B 516     -10.524  24.688  54.339  1.00 10.01    -0.271 OA
ATOM  17825  CB  LEU B 516     -11.359  26.199  56.783  1.00  9.89     0.038 C
ATOM  17828  CG  LEU B 516     -10.982  27.174  57.909  1.00 16.78    -0.020 C
ATOM  17830  CD1 LEU B 516     -11.947  28.374  57.933  1.00 19.36     0.009 C
ATOM  17834  CD2 LEU B 516     -10.944  26.526  59.263  1.00 12.10     0.009 C
ATOM  17838  N   ILE B 517     -11.363  22.994  55.586  1.00  7.02    -0.346 N
ATOM  17839  HN  ILE B 517     -11.572  22.663  56.528  1.00  0.00     0.163 HD
ATOM  17840  CA  ILE B 517     -11.671  22.123  54.444  1.00 10.07     0.180 C
ATOM  17842  C   ILE B 517     -13.190  22.147  54.243  1.00  9.88     0.241 C
ATOM  17843  O   ILE B 517     -13.879  21.665  55.123  1.00  8.22    -0.271 OA
ATOM  17844  CB  ILE B 517     -11.202  20.697  54.783  1.00  8.36     0.013 C
ATOM  17846  CG1 ILE B 517      -9.724  20.675  55.173  1.00 11.67     0.002 C
ATOM  17849  CG2 ILE B 517     -11.453  19.729  53.615  1.00  5.95     0.012 C
ATOM  17853  CD1 ILE B 517      -8.784  21.273  54.143  1.00 11.58     0.005 C
ATOM  17857  N   LEU B 518     -13.667  22.850  53.230  1.00  9.82    -0.346 N
ATOM  17858  HN  LEU B 518     -13.020  23.158  52.504  1.00  0.00     0.163 HD
ATOM  17859  CA  LEU B 518     -15.068  23.203  53.103  1.00  7.86     0.177 C
ATOM  17861  C   LEU B 518     -15.748  22.628  51.866  1.00  7.79     0.241 C
ATOM  17862  O   LEU B 518     -15.097  22.409  50.872  1.00 12.05    -0.271 OA
ATOM  17863  CB  LEU B 518     -15.173  24.741  53.036  1.00  5.21     0.038 C
ATOM  17866  CG  LEU B 518     -14.470  25.401  54.229  1.00 12.78    -0.020 C
ATOM  17868  CD1 LEU B 518     -14.379  26.905  53.985  1.00  9.43     0.009 C
ATOM  17872  CD2 LEU B 518     -15.247  25.128  55.527  1.00 12.38     0.009 C
ATOM  17876  N   SER B 519     -17.053  22.401  51.991  1.00  7.22    -0.344 N
ATOM  17877  HN  SER B 519     -17.550  22.711  52.826  1.00  0.00     0.163 HD
ATOM  17878  CA  SER B 519     -17.770  21.706  50.927  1.00  7.29     0.200 C
ATOM  17880  C   SER B 519     -18.417  22.645  49.937  1.00 13.09     0.243 C
ATOM  17881  O   SER B 519     -18.656  23.799  50.281  1.00  9.97    -0.271 OA
ATOM  17882  CB  SER B 519     -18.854  20.811  51.601  1.00  9.94     0.199 C
ATOM  17885  OG  SER B 519     -19.945  21.653  52.025  1.00 12.46    -0.398 OA
ATOM  17886  HG  SER B 519     -20.606  21.108  52.436  1.00  0.00     0.209 HD
ATOM  17887  N   ARG B 520     -18.607  22.072  48.748  1.00  9.02    -0.346 N
ATOM  17888  HN  ARG B 520     -18.232  21.148  48.535  1.00  0.00     0.163 HD
ATOM  17889  CA  ARG B 520     -19.386  22.837  47.753  1.00 12.40     0.176 C
ATOM  17891  C   ARG B 520     -20.862  22.586  48.015  1.00 14.94     0.241 C
ATOM  17892  O   ARG B 520     -21.670  23.510  47.877  1.00 18.34    -0.271 OA
ATOM  17893  CB  ARG B 520     -19.069  22.300  46.342  1.00 10.81     0.036 C
ATOM  17896  CG  ARG B 520     -19.835  23.110  45.271  1.00 11.70     0.023 C
ATOM  17899  CD  ARG B 520     -19.691  22.364  43.915  1.00 16.48     0.138 C
ATOM  17902  NE  ARG B 520     -20.336  23.228  42.893  1.00 22.83    -0.227 N
ATOM  17903  HE  ARG B 520     -20.190  24.235  42.966  1.00  0.00     0.177 HD
ATOM  17904  CZ  ARG B 520     -21.088  22.788  41.892  1.00 31.71     0.665 C
ATOM  17905  NH1 ARG B 520     -21.265  21.481  41.701  1.00 25.62    -0.235 N
ATOM  17906 1HH1 ARG B 520     -20.849  20.804  42.341  1.00  0.00     0.174 HD
ATOM  17907 2HH1 ARG B 520     -21.843  21.143  40.932  1.00  0.00     0.174 HD
ATOM  17908  NH2 ARG B 520     -21.630  23.671  41.058  1.00 32.88    -0.235 N
ATOM  17909 1HH2 ARG B 520     -21.495  24.671  41.204  1.00  0.00     0.174 HD
ATOM  17910 2HH2 ARG B 520     -22.208  23.333  40.289  1.00  0.00     0.174 HD
ATOM  17911  N   GLN B 521     -21.245  21.377  48.371  1.00 12.61    -0.346 N
ATOM  17912  HN  GLN B 521     -20.512  20.686  48.532  1.00  0.00     0.163 HD
ATOM  17913  CA  GLN B 521     -22.625  20.938  48.555  1.00 15.76     0.177 C
ATOM  17915  C   GLN B 521     -23.154  21.138  49.965  1.00 15.93     0.241 C
ATOM  17916  O   GLN B 521     -22.392  21.311  50.910  1.00 10.79    -0.271 OA
ATOM  17917  CB  GLN B 521     -22.807  19.488  48.109  1.00 14.58     0.044 C
ATOM  17920  CG  GLN B 521     -22.430  18.429  49.150  1.00 13.21     0.105 C
ATOM  17923  CD  GLN B 521     -20.961  18.120  49.306  1.00 18.60     0.215 C
ATOM  17924  NE2 GLN B 521     -20.055  18.900  48.751  1.00  7.85    -0.370 N
ATOM  17925 1HE2 GLN B 521     -20.404  19.708  48.236  1.00  0.00     0.159 HD
ATOM  17926 2HE2 GLN B 521     -19.062  18.691  48.856  1.00  0.00     0.159 HD
ATOM  17927  OE1 GLN B 521     -20.533  17.128  49.938  1.00 14.39    -0.274 OA
ATOM  17928  N   ASN B 522     -24.487  21.185  50.116  1.00 11.26    -0.346 N
ATOM  17929  HN  ASN B 522     -25.087  20.976  49.318  1.00  0.00     0.163 HD
ATOM  17930  CA  ASN B 522     -25.094  21.528  51.393  1.00 13.26     0.185 C
ATOM  17932  C   ASN B 522     -24.943  20.447  52.448  1.00 12.33     0.241 C
ATOM  17933  O   ASN B 522     -25.053  19.282  52.083  1.00 14.75    -0.271 OA
ATOM  17934  CB  ASN B 522     -26.612  21.742  51.188  1.00 16.11     0.137 C
ATOM  17937  CG  ASN B 522     -26.845  22.903  50.230  1.00 20.37     0.217 C
ATOM  17938  ND2 ASN B 522     -27.891  22.781  49.421  1.00 25.95    -0.370 N
ATOM  17939 1HD2 ASN B 522     -28.477  21.946  49.420  1.00  0.00     0.159 HD
ATOM  17940 2HD2 ASN B 522     -28.047  23.558  48.779  1.00  0.00     0.159 HD
ATOM  17941  OD1 ASN B 522     -26.139  23.908  50.231  1.00 17.77    -0.274 OA
ATOM  17942  N   LEU B 523     -24.762  20.816  53.686  1.00  8.41    -0.346 N
ATOM  17943  HN  LEU B 523     -24.763  21.814  53.897  1.00  0.00     0.163 HD
ATOM  17944  CA  LEU B 523     -24.556  19.870  54.795  1.00 13.45     0.177 C
ATOM  17946  C   LEU B 523     -25.641  20.025  55.852  1.00 15.47     0.241 C
ATOM  17947  O   LEU B 523     -25.892  21.151  56.295  1.00 12.42    -0.271 OA
ATOM  17948  CB  LEU B 523     -23.204  20.138  55.470  1.00 11.98     0.038 C
ATOM  17951  CG  LEU B 523     -21.956  20.226  54.557  1.00 15.77    -0.020 C
ATOM  17953  CD1 LEU B 523     -20.675  20.387  55.387  1.00 14.27     0.009 C
ATOM  17957  CD2 LEU B 523     -21.844  18.950  53.725  1.00 14.60     0.009 C
ATOM  17961  N   ALA B 524     -26.271  18.935  56.289  1.00 14.73    -0.346 N
ATOM  17962  HN  ALA B 524     -26.052  18.018  55.899  1.00  0.00     0.163 HD
ATOM  17963  CA  ALA B 524     -27.289  19.076  57.345  1.00 17.16     0.172 C
ATOM  17965  C   ALA B 524     -26.687  19.466  58.685  1.00 17.45     0.240 C
ATOM  17966  O   ALA B 524     -25.608  19.006  59.072  1.00 16.58    -0.271 OA
ATOM  17967  CB  ALA B 524     -28.002  17.723  57.491  1.00 14.09     0.042 C
ATOM  17971  N   GLN B 525     -27.416  20.255  59.475  1.00 11.30    -0.346 N
ATOM  17972  HN  GLN B 525     -28.325  20.600  59.165  1.00  0.00     0.163 HD
ATOM  17973  CA  GLN B 525     -26.898  20.617  60.784  1.00 11.34     0.177 C
ATOM  17975  C   GLN B 525     -27.200  19.491  61.777  1.00 15.18     0.241 C
ATOM  17976  O   GLN B 525     -28.326  18.949  61.834  1.00 15.44    -0.271 OA
ATOM  17977  CB  GLN B 525     -27.604  21.902  61.266  1.00  8.68     0.044 C
ATOM  17980  CG  GLN B 525     -27.079  22.305  62.665  1.00  9.23     0.105 C
ATOM  17983  CD  GLN B 525     -27.271  23.776  62.933  1.00 17.20     0.215 C
ATOM  17984  NE2 GLN B 525     -27.717  24.101  64.148  1.00 13.85    -0.370 N
ATOM  17985 1HE2 GLN B 525     -27.920  23.388  64.849  1.00  0.00     0.159 HD
ATOM  17986 2HE2 GLN B 525     -27.847  25.096  64.329  1.00  0.00     0.159 HD
ATOM  17987  OE1 GLN B 525     -27.025  24.638  62.086  1.00 15.63    -0.274 OA
ATOM  17988  N   GLN B 526     -26.302  19.247  62.715  1.00 13.66    -0.346 N
ATOM  17989  HN  GLN B 526     -25.425  19.767  62.697  1.00  0.00     0.163 HD
ATOM  17990  CA  GLN B 526     -26.510  18.267  63.776  1.00 13.43     0.177 C
ATOM  17992  C   GLN B 526     -26.988  18.928  65.048  1.00 13.44     0.241 C
ATOM  17993  O   GLN B 526     -26.516  20.005  65.375  1.00 13.09    -0.271 OA
ATOM  17994  CB  GLN B 526     -25.199  17.513  64.099  1.00 12.70     0.044 C
ATOM  17997  CG  GLN B 526     -24.690  16.807  62.816  1.00 12.07     0.105 C
ATOM  18000  CD  GLN B 526     -25.583  15.696  62.348  1.00 15.00     0.215 C
ATOM  18001  NE2 GLN B 526     -25.598  15.447  61.046  1.00 20.36    -0.370 N
ATOM  18002 1HE2 GLN B 526     -25.005  15.978  60.408  1.00  0.00     0.159 HD
ATOM  18003 2HE2 GLN B 526     -26.205  14.692  60.728  1.00  0.00     0.159 HD
ATOM  18004  OE1 GLN B 526     -26.298  15.056  63.118  1.00 24.11    -0.274 OA
ATOM  18005  N   GLU B 527     -27.781  18.202  65.845  1.00 13.98    -0.346 N
ATOM  18006  HN  GLU B 527     -28.072  17.262  65.576  1.00  0.00     0.163 HD
ATOM  18007  CA  GLU B 527     -28.223  18.791  67.118  1.00 14.35     0.177 C
ATOM  18009  C   GLU B 527     -27.181  18.571  68.206  1.00 16.61     0.241 C
ATOM  18010  O   GLU B 527     -26.498  17.535  68.166  1.00 14.38    -0.271 OA
ATOM  18011  CB  GLU B 527     -29.460  17.995  67.584  1.00 26.87     0.045 C
ATOM  18014  CG  GLU B 527     -30.657  18.292  66.686  1.00 56.26     0.116 C
ATOM  18017  CD  GLU B 527     -31.832  17.430  67.132  1.00 70.67     0.172 C
ATOM  18018  OE1 GLU B 527     -31.660  16.192  67.158  1.00 80.08    -0.648 OA
ATOM  18019  OE2 GLU B 527     -32.879  18.020  67.462  1.00 80.73    -0.648 OA
ATOM  18020  N   ARG B 528     -26.989  19.539  69.077  1.00 11.69    -0.346 N
ATOM  18021  HN  ARG B 528     -27.540  20.395  69.013  1.00  0.00     0.163 HD
ATOM  18022  CA  ARG B 528     -25.999  19.397  70.127  1.00 11.77     0.176 C
ATOM  18024  C   ARG B 528     -26.533  19.952  71.450  1.00 12.16     0.241 C
ATOM  18025  O   ARG B 528     -27.153  21.022  71.428  1.00 14.17    -0.271 OA
ATOM  18026  CB  ARG B 528     -24.664  20.128  69.841  1.00  9.64     0.036 C
ATOM  18029  CG  ARG B 528     -23.976  19.707  68.528  1.00 12.76     0.023 C
ATOM  18032  CD  ARG B 528     -22.692  20.469  68.213  1.00  9.76     0.138 C
ATOM  18035  NE  ARG B 528     -22.167  19.946  66.937  1.00 12.52    -0.227 N
ATOM  18036  HE  ARG B 528     -21.400  19.276  66.998  1.00  0.00     0.177 HD
ATOM  18037  CZ  ARG B 528     -22.586  20.254  65.728  1.00 13.33     0.665 C
ATOM  18038  NH1 ARG B 528     -23.512  21.165  65.428  1.00 10.13    -0.235 N
ATOM  18039 1HH1 ARG B 528     -23.837  21.404  64.491  1.00  0.00     0.174 HD
ATOM  18040 2HH1 ARG B 528     -23.943  21.657  66.211  1.00  0.00     0.174 HD
ATOM  18041  NH2 ARG B 528     -22.017  19.604  64.693  1.00  8.77    -0.235 N
ATOM  18042 1HH2 ARG B 528     -22.342  19.843  63.756  1.00  0.00     0.174 HD
ATOM  18043 2HH2 ARG B 528     -21.309  18.907  64.923  1.00  0.00     0.174 HD
ATOM  18044  N   THR B 529     -26.105  19.336  72.553  1.00 11.55    -0.344 N
ATOM  18045  HN  THR B 529     -25.623  18.438  72.503  1.00  0.00     0.163 HD
ATOM  18046  CA  THR B 529     -26.352  19.997  73.844  1.00 15.81     0.205 C
ATOM  18048  C   THR B 529     -25.279  21.057  74.024  1.00 19.34     0.243 C
ATOM  18049  O   THR B 529     -24.308  21.186  73.259  1.00 16.89    -0.271 OA
ATOM  18050  CB  THR B 529     -26.240  18.963  74.985  1.00 21.42     0.146 C
ATOM  18052  CG2 THR B 529     -27.176  17.788  74.738  1.00 20.73     0.042 C
ATOM  18056  OG1 THR B 529     -24.907  18.416  74.981  1.00 19.66    -0.393 OA
ATOM  18057  HG1 THR B 529     -24.323  19.149  75.135  1.00  0.00     0.210 HD
ATOM  18058  N   GLU B 530     -25.339  21.807  75.125  1.00 13.32    -0.346 N
ATOM  18059  HN  GLU B 530     -26.116  21.663  75.770  1.00  0.00     0.163 HD
ATOM  18060  CA  GLU B 530     -24.360  22.809  75.446  1.00 12.16     0.177 C
ATOM  18062  C   GLU B 530     -22.992  22.176  75.686  1.00 16.36     0.241 C
ATOM  18063  O   GLU B 530     -22.025  22.808  75.317  1.00 18.02    -0.271 OA
ATOM  18064  CB  GLU B 530     -24.795  23.617  76.697  1.00 23.72     0.045 C
ATOM  18067  CG  GLU B 530     -25.443  24.942  76.367  1.00 55.55     0.116 C
ATOM  18070  CD  GLU B 530     -26.505  25.013  75.293  1.00 68.09     0.172 C
ATOM  18071  OE1 GLU B 530     -27.540  24.309  75.374  1.00 75.67    -0.648 OA
ATOM  18072  OE2 GLU B 530     -26.340  25.813  74.330  1.00 73.31    -0.648 OA
ATOM  18073  N   GLU B 531     -22.922  20.972  76.277  1.00 16.36    -0.346 N
ATOM  18074  HN  GLU B 531     -23.785  20.508  76.559  1.00  0.00     0.163 HD
ATOM  18075  CA  GLU B 531     -21.658  20.314  76.525  1.00 18.20     0.177 C
ATOM  18077  C   GLU B 531     -21.015  19.895  75.211  1.00 17.65     0.241 C
ATOM  18078  O   GLU B 531     -19.837  20.113  75.007  1.00 22.40    -0.271 OA
ATOM  18079  CB  GLU B 531     -21.860  19.049  77.380  1.00 22.89     0.045 C
ATOM  18082  CG  GLU B 531     -22.049  19.461  78.849  1.00 27.29     0.116 C
ATOM  18085  CD  GLU B 531     -23.453  19.977  79.095  1.00 35.84     0.172 C
ATOM  18086  OE1 GLU B 531     -24.403  19.601  78.365  1.00 32.77    -0.648 OA
ATOM  18087  OE2 GLU B 531     -23.590  20.787  80.033  1.00 42.43    -0.648 OA
ATOM  18088  N   GLN B 532     -21.845  19.382  74.288  1.00 14.95    -0.346 N
ATOM  18089  HN  GLN B 532     -22.838  19.254  74.485  1.00  0.00     0.163 HD
ATOM  18090  CA  GLN B 532     -21.281  19.014  72.997  1.00 15.42     0.177 C
ATOM  18092  C   GLN B 532     -20.845  20.234  72.225  1.00 17.80     0.241 C
ATOM  18093  O   GLN B 532     -19.875  20.135  71.463  1.00 13.93    -0.271 OA
ATOM  18094  CB  GLN B 532     -22.250  18.224  72.119  1.00 11.04     0.044 C
ATOM  18097  CG  GLN B 532     -22.605  16.882  72.760  1.00 11.88     0.105 C
ATOM  18100  CD  GLN B 532     -23.749  16.221  72.039  1.00 15.90     0.215 C
ATOM  18101  NE2 GLN B 532     -23.623  14.972  71.617  1.00 21.76    -0.370 N
ATOM  18102 1HE2 GLN B 532     -22.759  14.443  71.735  1.00  0.00     0.159 HD
ATOM  18103 2HE2 GLN B 532     -24.398  14.524  71.128  1.00  0.00     0.159 HD
ATOM  18104  OE1 GLN B 532     -24.786  16.856  71.897  1.00 22.64    -0.274 OA
ATOM  18105  N   LEU B 533     -21.558  21.360  72.361  1.00 17.18    -0.346 N
ATOM  18106  HN  LEU B 533     -22.380  21.386  72.965  1.00  0.00     0.163 HD
ATOM  18107  CA  LEU B 533     -21.134  22.550  71.627  1.00 18.24     0.177 C
ATOM  18109  C   LEU B 533     -19.768  23.050  72.081  1.00 18.27     0.241 C
ATOM  18110  O   LEU B 533     -18.893  23.427  71.274  1.00 15.26    -0.271 OA
ATOM  18111  CB  LEU B 533     -22.233  23.611  71.828  1.00 18.59     0.038 C
ATOM  18114  CG  LEU B 533     -22.095  24.933  71.124  1.00 18.58    -0.020 C
ATOM  18116  CD1 LEU B 533     -22.337  24.780  69.617  1.00 19.10     0.009 C
ATOM  18120  CD2 LEU B 533     -23.190  25.855  71.676  1.00 26.05     0.009 C
ATOM  18124  N   ALA B 534     -19.474  22.981  73.375  1.00 17.80    -0.346 N
ATOM  18125  HN  ALA B 534     -20.195  22.669  74.025  1.00  0.00     0.163 HD
ATOM  18126  CA  ALA B 534     -18.177  23.330  73.895  1.00 19.00     0.172 C
ATOM  18128  C   ALA B 534     -17.084  22.334  73.455  1.00 21.29     0.240 C
ATOM  18129  O   ALA B 534     -15.948  22.754  73.290  1.00 23.64    -0.271 OA
ATOM  18130  CB  ALA B 534     -18.190  23.383  75.416  1.00 20.01     0.042 C
ATOM  18134  N   ASN B 535     -17.413  21.066  73.222  1.00 13.47    -0.346 N
ATOM  18135  HN  ASN B 535     -18.391  20.782  73.284  1.00  0.00     0.163 HD
ATOM  18136  CA  ASN B 535     -16.398  20.074  72.879  1.00 14.19     0.185 C
ATOM  18138  C   ASN B 535     -15.971  20.124  71.427  1.00 14.39     0.241 C
ATOM  18139  O   ASN B 535     -15.015  19.436  71.052  1.00 12.14    -0.271 OA
ATOM  18140  CB  ASN B 535     -16.895  18.667  73.244  1.00 10.90     0.137 C
ATOM  18143  CG  ASN B 535     -16.795  18.439  74.778  1.00 18.73     0.217 C
ATOM  18144  ND2 ASN B 535     -17.553  17.448  75.206  1.00 20.75    -0.370 N
ATOM  18145 1HD2 ASN B 535     -17.487  17.298  76.213  1.00  0.00     0.159 HD
ATOM  18146 2HD2 ASN B 535     -18.174  16.882  74.628  1.00  0.00     0.159 HD
ATOM  18147  OD1 ASN B 535     -16.052  19.116  75.469  1.00 19.35    -0.274 OA
ATOM  18148  N   ILE B 536     -16.653  20.900  70.584  1.00 12.41    -0.346 N
ATOM  18149  HN  ILE B 536     -17.443  21.449  70.923  1.00  0.00     0.163 HD
ATOM  18150  CA  ILE B 536     -16.268  20.965  69.168  1.00 10.48     0.180 C
ATOM  18152  C   ILE B 536     -14.828  21.456  69.068  1.00 15.67     0.241 C
ATOM  18153  O   ILE B 536     -14.030  20.912  68.315  1.00 11.64    -0.271 OA
ATOM  18154  CB  ILE B 536     -17.177  21.925  68.341  1.00  9.30     0.013 C
ATOM  18156  CG1 ILE B 536     -18.636  21.454  68.365  1.00 14.87     0.002 C
ATOM  18159  CG2 ILE B 536     -16.643  21.947  66.895  1.00  8.87     0.012 C
ATOM  18163  CD1 ILE B 536     -19.615  22.398  67.647  1.00 12.68     0.005 C
ATOM  18167  N   ALA B 537     -14.434  22.418  69.929  1.00 12.30    -0.346 N
ATOM  18168  HN  ALA B 537     -15.105  22.795  70.598  1.00  0.00     0.163 HD
ATOM  18169  CA  ALA B 537     -13.072  22.928  69.922  1.00 13.26     0.172 C
ATOM  18171  C   ALA B 537     -12.024  21.955  70.417  1.00 13.73     0.240 C
ATOM  18172  O   ALA B 537     -10.812  22.164  70.219  1.00 14.03    -0.271 OA
ATOM  18173  CB  ALA B 537     -12.995  24.260  70.698  1.00 18.28     0.042 C
ATOM  18177  N   ARG B 538     -12.420  20.816  70.979  1.00  9.44    -0.346 N
ATOM  18178  HN  ARG B 538     -13.415  20.682  71.161  1.00  0.00     0.163 HD
ATOM  18179  CA  ARG B 538     -11.503  19.759  71.343  1.00  9.19     0.176 C
ATOM  18181  C   ARG B 538     -11.170  18.889  70.117  1.00  7.50     0.240 C
ATOM  18182  O   ARG B 538     -10.409  17.937  70.273  1.00 12.04    -0.271 OA
ATOM  18183  CB  ARG B 538     -12.112  18.865  72.423  1.00 12.25     0.036 C
ATOM  18186  CG  ARG B 538     -12.265  19.769  73.685  1.00 16.69     0.023 C
ATOM  18189  CD  ARG B 538     -12.617  18.835  74.838  1.00 21.03     0.138 C
ATOM  18192  NE  ARG B 538     -12.923  19.604  76.012  1.00 36.83    -0.227 N
ATOM  18193  HE  ARG B 538     -13.653  20.309  75.911  1.00  0.00     0.177 HD
ATOM  18194  CZ  ARG B 538     -12.365  19.504  77.214  1.00 47.60     0.665 C
ATOM  18195  NH1 ARG B 538     -11.390  18.647  77.476  1.00 44.43    -0.235 N
ATOM  18196 1HH1 ARG B 538     -10.962  18.570  78.399  1.00  0.00     0.174 HD
ATOM  18197 2HH1 ARG B 538     -11.006  18.012  76.776  1.00  0.00     0.174 HD
ATOM  18198  NH2 ARG B 538     -12.866  20.333  78.127  1.00 47.08    -0.235 N
ATOM  18199 1HH2 ARG B 538     -12.438  20.256  79.050  1.00  0.00     0.174 HD
ATOM  18200 2HH2 ARG B 538     -13.617  20.993  77.925  1.00  0.00     0.174 HD
ATOM  18201  N   GLY B 539     -11.719  19.191  68.940  1.00  8.24    -0.351 N
ATOM  18202  HN  GLY B 539     -12.431  19.918  68.864  1.00  0.00     0.163 HD
ATOM  18203  CA  GLY B 539     -11.270  18.448  67.759  1.00  8.34     0.225 C
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ATOM  18206  C   GLY B 539      -11.983  17.181  67.430  1.00  9.02     0.235 C
ATOM  18207  O   GLY B 539      -12.221  16.844  66.269  1.00  8.19    -0.272 OA
ATOM  18208  N   GLY B 540      -12.353  16.350  68.423  1.00  9.61    -0.351 N
ATOM  18209  HN  GLY B 540      -12.064  16.571  69.376  1.00  0.00     0.163 HD
ATOM  18210  CA  GLY B 540      -13.143  15.156  68.198  1.00  7.67     0.225 C
ATOM  18213  C   GLY B 540      -14.010  15.044  69.495  1.00 10.96     0.236 C
ATOM  18214  O   GLY B 540      -13.526  15.368  70.591  1.00  9.28    -0.272 OA
ATOM  18215  N   TYR B 541      -15.253  14.626  69.316  1.00  7.67    -0.346 N
ATOM  18216  HN  TYR B 541      -15.564  14.313  68.397  1.00  0.00     0.163 HD
ATOM  18217  CA  TYR B 541      -16.177  14.618  70.454  1.00  9.41     0.180 C
ATOM  18219  C   TYR B 541      -17.314  13.637  70.137  1.00  8.13     0.241 C
ATOM  18220  O   TYR B 541      -17.580  13.336  68.970  1.00 10.43    -0.271 OA
ATOM  18221  CB  TYR B 541      -16.708  16.036  70.721  1.00  8.81     0.073 C
ATOM  18224  CG  TYR B 541      -17.555  16.609  69.598  1.00 12.58    -0.056 A
ATOM  18225  CD1 TYR B 541      -16.937  17.234  68.521  1.00  7.91     0.010 A
ATOM  18227  CD2 TYR B 541      -18.944  16.536  69.614  1.00 12.39     0.010 A
ATOM  18229  CE1 TYR B 541      -17.700  17.781  67.488  1.00 10.74     0.037 A
ATOM  18231  CE2 TYR B 541      -19.735  17.082  68.605  1.00 11.29     0.037 A
ATOM  18233  CZ  TYR B 541      -19.077  17.670  67.515  1.00  8.46     0.065 A
ATOM  18234  OH  TYR B 541      -19.811  18.200  66.515  1.00  9.06    -0.361 OA
ATOM  18235  HH  TYR B 541      -20.758  18.124  66.534  1.00  0.00     0.217 HD
ATOM  18236  N   VAL B 542      -17.946  13.150  71.196  1.00  9.37    -0.346 N
ATOM  18237  HN  VAL B 542      -17.645  13.406  72.136  1.00  0.00     0.163 HD
ATOM  18238  CA  VAL B 542      -19.095  12.230  71.004  1.00  7.36     0.180 C
ATOM  18240  C   VAL B 542      -20.321  13.066  70.605  1.00 13.16     0.241 C
ATOM  18241  O   VAL B 542      -20.799  13.939  71.340  1.00 11.84    -0.271 OA
ATOM  18242  CB  VAL B 542      -19.412  11.517  72.335  1.00 12.76     0.009 C
ATOM  18244  CG1 VAL B 542      -20.595  10.570  72.179  1.00 12.98     0.012 C
ATOM  18248  CG2 VAL B 542      -18.184  10.722  72.803  1.00 12.60     0.012 C
ATOM  18252  N   LEU B 543      -20.834  12.754  69.428  1.00  8.04    -0.346 N
ATOM  18253  HN  LEU B 543      -20.412  11.987  68.904  1.00  0.00     0.163 HD
ATOM  18254  CA  LEU B 543      -21.966  13.446  68.842  1.00  8.12     0.177 C
ATOM  18256  C   LEU B 543      -23.244  12.633  69.105  1.00 13.86     0.241 C
ATOM  18257  O   LEU B 543      -24.252  13.259  69.418  1.00 12.19    -0.271 OA
ATOM  18258  CB  LEU B 543      -21.751  13.591  67.312  1.00 11.60     0.038 C
ATOM  18261  CG  LEU B 543      -22.916  14.280  66.570  1.00 16.32    -0.020 C
ATOM  18263  CD1 LEU B 543      -23.009  15.728  67.055  1.00 12.33     0.009 C
ATOM  18267  CD2 LEU B 543      -22.747  14.187  65.059  1.00 17.28     0.009 C
ATOM  18271  N   LYS B 544      -23.221  11.332  68.932  1.00 15.29    -0.346 N
ATOM  18272  HN  LYS B 544      -22.367  10.904  68.574  1.00  0.00     0.163 HD
ATOM  18273  CA  LYS B 544      -24.374  10.460  69.231  1.00 13.34     0.176 C
ATOM  18275  C   LYS B 544      -23.834   9.325  70.106  1.00 14.63     0.241 C
ATOM  18276  O   LYS B 544      -22.753   8.781  69.836  1.00 13.57    -0.271 OA
ATOM  18277  CB  LYS B 544      -25.039   9.842  68.006  1.00 15.54     0.035 C
ATOM  18280  CG  LYS B 544      -25.613  10.848  67.021  1.00 17.38     0.004 C
ATOM  18283  CD  LYS B 544      -26.881  11.488  67.577  1.00 22.89     0.027 C
ATOM  18286  CE  LYS B 544      -27.620  12.135  66.401  1.00 35.45     0.229 C
ATOM  18289  NZ  LYS B 544      -28.460  13.278  66.876  1.00 37.10    -0.079 N
ATOM  18290  HZ1 LYS B 544      -28.952  13.709  66.093  1.00  0.00     0.274 HD
ATOM  18291  HZ2 LYS B 544      -27.912  13.959  67.401  1.00  0.00     0.274 HD
ATOM  18292  HZ3 LYS B 544      -29.101  12.995  67.618  1.00  0.00     0.274 HD
ATOM  18293  N   ASP B 545      -24.571   8.933  71.141  1.00 14.90    -0.346 N
ATOM  18294  HN  ASP B 545      -25.478   9.364  71.318  1.00  0.00     0.163 HD
ATOM  18295  CA  ASP B 545      -24.067   7.869  72.033  1.00 16.70     0.186 C
ATOM  18297  C   ASP B 545      -25.148   6.866  72.388  1.00 17.98     0.241 C
ATOM  18298  O   ASP B 545      -26.307   7.180  72.192  1.00 21.16    -0.271 OA
ATOM  18299  CB  ASP B 545      -23.534   8.533  73.306  1.00 15.70     0.147 C
ATOM  18302  CG  ASP B 545      -22.445   7.665  73.943  1.00 21.45     0.175 C
ATOM  18303  OD1 ASP B 545      -21.999   6.637  73.382  1.00 23.00    -0.648 OA
ATOM  18304  OD2 ASP B 545      -21.986   8.004  75.048  1.00 25.94    -0.648 OA
ATOM  18305  N   CYS B 546      -24.839   5.744  72.982  1.00 20.01    -0.345 N
ATOM  18306  HN  CYS B 546      -23.852   5.561  73.161  1.00  0.00     0.163 HD
ATOM  18307  CA  CYS B 546      -25.796   4.740  73.405  1.00 19.11     0.186 C
ATOM  18309  C   CYS B 546      -25.820   4.741  74.940  1.00 22.49     0.241 C
ATOM  18310  O   CYS B 546      -24.922   5.322  75.540  1.00 22.60    -0.271 OA
ATOM  18311  CB  CYS B 546      -25.224   3.387  72.954  1.00 18.97     0.121 C
ATOM  18314  SG  CYS B 546      -23.472   3.191  73.400  1.00 29.24    -0.095 SA
ATOM  18315  N   ALA B 547      -26.822   4.135  75.562  1.00 19.81    -0.346 N
ATOM  18316  HN  ALA B 547      -27.606   3.762  75.026  1.00  0.00     0.163 HD
ATOM  18317  CA  ALA B 547      -26.800   4.001  77.034  1.00 24.89     0.172 C
ATOM  18319  C   ALA B 547      -25.834   2.870  77.315  1.00 24.96     0.240 C
ATOM  18320  O   ALA B 547      -25.944   1.863  76.578  1.00 33.35    -0.271 OA
ATOM  18321  CB  ALA B 547      -28.167   3.605  77.577  1.00 23.41     0.042 C
ATOM  18325  N   GLY B 548      -24.913   2.919  78.238  1.00 25.34    -0.351 N
ATOM  18326  HN  GLY B 548      -24.825   3.750  78.823  1.00  0.00     0.163 HD
ATOM  18327  CA  GLY B 548      -24.006   1.787  78.437  1.00 21.38     0.225 C
ATOM  18330  C   GLY B 548      -22.751   1.961  77.589  1.00 26.17     0.236 C
ATOM  18331  O   GLY B 548      -22.604   3.010  76.940  1.00 30.37    -0.272 OA
ATOM  18332  N   GLN B 549      -21.856   0.986  77.540  1.00 23.02    -0.346 N
ATOM  18333  HN  GLN B 549      -22.007   0.121  78.059  1.00  0.00     0.163 HD
ATOM  18334  CA  GLN B 549      -20.635   1.164  76.725  1.00 27.72     0.177 C
ATOM  18336  C   GLN B 549      -20.903   0.770  75.284  1.00 26.36     0.243 C
ATOM  18337  O   GLN B 549      -21.653  -0.186  75.016  1.00 23.12    -0.271 OA
ATOM  18338  CB  GLN B 549      -19.485   0.373  77.338  1.00 38.24     0.044 C
ATOM  18341  CG  GLN B 549      -18.128   0.724  76.746  1.00 64.06     0.105 C
ATOM  18344  CD  GLN B 549      -16.966  -0.161  77.114  1.00 71.93     0.215 C
ATOM  18345  NE2 GLN B 549      -15.733   0.330  76.974  1.00 75.12    -0.370 N
ATOM  18346 1HE2 GLN B 549      -15.579   1.276  76.625  1.00  0.00     0.159 HD
ATOM  18347 2HE2 GLN B 549      -14.946  -0.269  77.223  1.00  0.00     0.159 HD
ATOM  18348  OE1 GLN B 549      -17.152  -1.304  77.536  1.00 82.91    -0.274 OA
ATOM  18349  N   PRO B 550      -20.312   1.469  74.308  1.00 23.45    -0.337 N
ATOM  18350  CA  PRO B 550      -20.561   1.135  72.924  1.00 21.77     0.179 C
ATOM  18352  C   PRO B 550      -19.909  -0.188  72.506  1.00 15.86     0.241 C
ATOM  18353  O   PRO B 550      -18.843  -0.532  72.985  1.00 19.07    -0.271 OA
ATOM  18354  CB  PRO B 550      -19.936   2.299  72.138  1.00 22.73     0.037 C
ATOM  18357  CG  PRO B 550      -18.966   2.948  73.057  1.00 26.90     0.022 C
ATOM  18360  CD  PRO B 550      -19.442   2.656  74.462  1.00 27.08     0.127 C
ATOM  18363  N   GLU B 551      -20.545  -0.896  71.606  1.00 16.02    -0.346 N
ATOM  18364  HN  GLU B 551      -21.484  -0.606  71.332  1.00  0.00     0.163 HD
ATOM  18365  CA  GLU B 551      -19.967  -2.086  70.976  1.00 20.45     0.177 C
ATOM  18367  C   GLU B 551      -19.276  -1.667  69.658  1.00 18.66     0.241 C
ATOM  18368  O   GLU B 551      -18.491  -2.410  69.068  1.00 18.39    -0.271 OA
ATOM  18369  CB  GLU B 551      -21.110  -3.036  70.553  1.00 23.50     0.045 C
ATOM  18372  CG  GLU B 551      -22.117  -3.286  71.652  1.00 45.05     0.116 C
ATOM  18375  CD  GLU B 551      -23.269  -4.194  71.287  1.00 40.98     0.172 C
ATOM  18376  OE1 GLU B 551      -23.943  -4.009  70.263  1.00 45.13    -0.648 OA
ATOM  18377  OE2 GLU B 551      -23.517  -5.142  72.067  1.00 61.59    -0.648 OA
ATOM  18378  N   LEU B 552      -19.669  -0.495  69.131  1.00 18.43    -0.346 N
ATOM  18379  HN  LEU B 552      -20.313   0.108  69.643  1.00  0.00     0.163 HD
ATOM  18380  CA  LEU B 552      -19.170  -0.091  67.824  1.00 16.73     0.177 C
ATOM  18382  C   LEU B 552      -19.074   1.418  67.682  1.00 14.61     0.241 C
ATOM  18383  O   LEU B 552      -19.982   2.088  68.154  1.00 14.25    -0.271 OA
ATOM  18384  CB  LEU B 552      -20.168  -0.550  66.769  1.00 19.73     0.038 C
ATOM  18387  CG  LEU B 552      -19.782  -0.098  65.334  1.00 26.74    -0.020 C
ATOM  18389  CD1 LEU B 552      -19.058  -1.241  64.666  1.00 22.41     0.009 C
ATOM  18393  CD2 LEU B 552      -21.038   0.332  64.619  1.00 37.49     0.009 C
ATOM  18397  N   ILE B 553      -17.953   1.914  67.153  1.00 12.46    -0.346 N
ATOM  18398  HN  ILE B 553      -17.210   1.305  66.812  1.00  0.00     0.163 HD
ATOM  18399  CA  ILE B 553      -17.839   3.378  67.085  1.00  8.34     0.180 C
ATOM  18401  C   ILE B 553      -17.643   3.836  65.639  1.00 14.74     0.241 C
ATOM  18402  O   ILE B 553      -16.766   3.292  64.968  1.00 12.10    -0.271 OA
ATOM  18403  CB  ILE B 553      -16.647   3.869  67.930  1.00 12.01     0.013 C
ATOM  18405  CG1 ILE B 553      -16.822   3.480  69.404  1.00 15.90     0.002 C
ATOM  18408  CG2 ILE B 553      -16.505   5.403  67.784  1.00 13.11     0.012 C
ATOM  18412  CD1 ILE B 553      -15.691   3.844  70.332  1.00 16.38     0.005 C
ATOM  18416  N   PHE B 554      -18.386   4.851  65.223  1.00 10.19    -0.346 N
ATOM  18417  HN  PHE B 554      -19.096   5.236  65.846  1.00  0.00     0.163 HD
ATOM  18418  CA  PHE B 554      -18.213   5.428  63.901  1.00 10.65     0.180 C
ATOM  18420  C   PHE B 554      -17.401   6.716  64.120  1.00 12.96     0.241 C
ATOM  18421  O   PHE B 554      -17.671   7.447  65.098  1.00 11.60    -0.271 OA
ATOM  18422  CB  PHE B 554      -19.577   5.826  63.280  1.00  8.36     0.073 C
ATOM  18425  CG  PHE B 554      -20.413   4.691  62.802  1.00 14.14    -0.056 A
ATOM  18426  CD1 PHE B 554      -20.059   4.017  61.635  1.00 16.06     0.007 A
ATOM  18428  CD2 PHE B 554      -21.535   4.266  63.496  1.00 22.60     0.007 A
ATOM  18430  CE1 PHE B 554      -20.813   2.956  61.163  1.00 15.17     0.001 A
ATOM  18432  CE2 PHE B 554      -22.288   3.191  63.024  1.00 22.91     0.001 A
ATOM  18434  CZ  PHE B 554      -21.909   2.530  61.866  1.00 18.49     0.000 A
ATOM  18436  N   ILE B 555      -16.385   6.924  63.281  1.00  9.89    -0.346 N
ATOM  18437  HN  ILE B 555      -16.138   6.208  62.598  1.00  0.00     0.163 HD
ATOM  18438  CA  ILE B 555      -15.622   8.172  63.334  1.00  7.21     0.180 C
ATOM  18440  C   ILE B 555      -15.849   8.829  61.968  1.00  8.84     0.241 C
ATOM  18441  O   ILE B 555      -15.555   8.173  60.983  1.00 12.02    -0.271 OA
ATOM  18442  CB  ILE B 555      -14.118   7.966  63.570  1.00 13.25     0.013 C
ATOM  18444  CG1 ILE B 555      -13.906   7.168  64.866  1.00 15.47     0.002 C
ATOM  18447  CG2 ILE B 555      -13.348   9.299  63.656  1.00 11.44     0.012 C
ATOM  18451  CD1 ILE B 555      -12.492   6.557  64.945  1.00 18.34     0.005 C
ATOM  18455  N   ALA B 556      -16.382  10.055  61.957  1.00  7.31    -0.346 N
ATOM  18456  HN  ALA B 556      -16.644  10.540  62.815  1.00  0.00     0.163 HD
ATOM  18457  CA  ALA B 556      -16.568  10.666  60.618  1.00  7.79     0.172 C
ATOM  18459  C   ALA B 556      -16.225  12.133  60.673  1.00  7.94     0.240 C
ATOM  18460  O   ALA B 556      -16.109  12.791  61.717  1.00 10.12    -0.271 OA
ATOM  18461  CB  ALA B 556      -18.027  10.454  60.183  1.00  8.28     0.042 C
ATOM  18465  N   THR B 557      -16.084  12.773  59.489  1.00  8.67    -0.344 N
ATOM  18466  HN  THR B 557      -16.230  12.252  58.624  1.00  0.00     0.163 HD
ATOM  18467  CA  THR B 557      -15.732  14.177  59.414  1.00  7.75     0.205 C
ATOM  18469  C   THR B 557      -16.567  14.801  58.281  1.00  8.86     0.243 C
ATOM  18470  O   THR B 557      -17.015  14.065  57.392  1.00  7.77    -0.271 OA
ATOM  18471  CB  THR B 557      -14.258  14.412  59.000  1.00  9.00     0.146 C
ATOM  18473  CG2 THR B 557      -13.269  13.564  59.830  1.00  8.93     0.042 C
ATOM  18477  OG1 THR B 557      -14.039  14.004  57.634  1.00  9.67    -0.393 OA
ATOM  18478  HG1 THR B 557      -14.647  14.526  57.124  1.00  0.00     0.210 HD
ATOM  18479  N   GLY B 558      -16.659  16.112  58.327  1.00  8.11    -0.350 N
ATOM  18480  HN  GLY B 558      -16.288  16.598  59.144  1.00  0.00     0.163 HD
ATOM  18481  CA  GLY B 558      -17.265  16.900  57.268  1.00  8.11     0.225 C
ATOM  18484  C   GLY B 558      -18.569  16.389  56.721  1.00 11.30     0.236 C
ATOM  18485  O   GLY B 558      -19.435  16.033  57.515  1.00  9.60    -0.272 OA
ATOM  18486  N   SER B 559      -18.658  16.285  55.398  1.00  7.81    -0.344 N
ATOM  18487  HN  SER B 559      -17.852  16.507  54.813  1.00  0.00     0.163 HD
ATOM  18488  CA  SER B 559      -19.902  15.855  54.787  1.00 12.13     0.200 C
ATOM  18490  C   SER B 559      -20.303  14.424  55.130  1.00 12.14     0.243 C
ATOM  18491  O   SER B 559      -21.441  14.072  54.779  1.00 15.13    -0.271 OA
ATOM  18492  CB  SER B 559      -19.828  16.022  53.250  1.00 14.16     0.199 C
ATOM  18495  OG  SER B 559      -18.658  15.405  52.714  1.00 11.19    -0.398 OA
ATOM  18496  HG  SER B 559      -18.613  15.507  51.771  1.00  0.00     0.209 HD
ATOM  18497  N   GLU B 560      -19.461  13.537  55.619  1.00  6.95    -0.346 N
ATOM  18498  HN  GLU B 560      -18.511  13.848  55.820  1.00  0.00     0.163 HD
ATOM  18499  CA  GLU B 560      -19.784  12.156  55.891  1.00  9.96     0.177 C
ATOM  18501  C   GLU B 560      -20.359  11.927  57.295  1.00  8.99     0.241 C
ATOM  18502  O   GLU B 560      -20.764  10.810  57.630  1.00 13.00    -0.271 OA
ATOM  18503  CB  GLU B 560      -18.499  11.291  55.693  1.00  9.10     0.045 C
ATOM  18506  CG  GLU B 560      -18.298  11.013  54.173  1.00  9.24     0.116 C
ATOM  18509  CD  GLU B 560      -17.901  12.283  53.436  1.00 11.66     0.172 C
ATOM  18510  OE1 GLU B 560      -16.787  12.829  53.671  1.00 11.32    -0.648 OA
ATOM  18511  OE2 GLU B 560      -18.726  12.780  52.655  1.00  9.91    -0.648 OA
ATOM  18512  N   VAL B 561      -20.402  12.965  58.115  1.00  9.59    -0.346 N
ATOM  18513  HN  VAL B 561      -20.024  13.866  57.821  1.00  0.00     0.163 HD
ATOM  18514  CA  VAL B 561      -21.008  12.811  59.476  1.00 10.01     0.180 C
ATOM  18516  C   VAL B 561      -22.464  12.420  59.320  1.00 11.62     0.241 C
ATOM  18517  O   VAL B 561      -22.993  11.574  60.040  1.00 10.70    -0.271 OA
ATOM  18518  CB  VAL B 561      -20.855  14.090  60.296  1.00  8.72     0.009 C
ATOM  18520  CG1 VAL B 561      -21.722  14.070  61.575  1.00  9.37     0.012 C
ATOM  18524  CG2 VAL B 561      -19.372  14.245  60.709  1.00  9.31     0.012 C
ATOM  18528  N   GLU B 562      -23.163  13.007  58.356  1.00 13.53    -0.346 N
ATOM  18529  HN  GLU B 562      -22.699  13.699  57.768  1.00  0.00     0.163 HD
ATOM  18530  CA  GLU B 562      -24.562  12.705  58.103  1.00 13.03     0.177 C
ATOM  18532  C   GLU B 562      -24.808  11.229  57.815  1.00 15.32     0.241 C
ATOM  18533  O   GLU B 562      -25.794  10.648  58.261  1.00 14.61    -0.271 OA
ATOM  18534  CB  GLU B 562      -25.066  13.461  56.859  1.00 23.13     0.045 C
ATOM  18537  CG  GLU B 562      -25.409  14.910  57.147  1.00 39.83     0.116 C
ATOM  18540  CD  GLU B 562      -25.671  15.607  55.800  1.00 46.76     0.172 C
ATOM  18541  OE1 GLU B 562      -26.712  15.247  55.200  1.00 39.61    -0.648 OA
ATOM  18542  OE2 GLU B 562      -24.817  16.447  55.448  1.00 34.47    -0.648 OA
ATOM  18543  N   LEU B 563      -23.964  10.641  56.980  1.00 12.39    -0.346 N
ATOM  18544  HN  LEU B 563      -23.249  11.219  56.539  1.00  0.00     0.163 HD
ATOM  18545  CA  LEU B 563      -23.991   9.222  56.651  1.00 12.70     0.177 C
ATOM  18547  C   LEU B 563      -23.764   8.388  57.892  1.00 14.71     0.241 C
ATOM  18548  O   LEU B 563      -24.457   7.364  58.088  1.00 16.33    -0.271 OA
ATOM  18549  CB  LEU B 563      -22.837   8.977  55.685  1.00 16.64     0.038 C
ATOM  18552  CG  LEU B 563      -22.895   8.621  54.241  1.00 35.99    -0.020 C
ATOM  18554  CD1 LEU B 563      -21.521   8.152  53.753  1.00 21.42     0.009 C
ATOM  18558  CD2 LEU B 563      -23.940   7.522  54.036  1.00 35.61     0.009 C
ATOM  18562  N   ALA B 564      -22.795   8.769  58.747  1.00  9.87    -0.346 N
ATOM  18563  HN  ALA B 564      -22.244   9.612  58.586  1.00  0.00     0.163 HD
ATOM  18564  CA  ALA B 564      -22.567   7.914  59.923  1.00  8.66     0.172 C
ATOM  18566  C   ALA B 564      -23.737   8.028  60.923  1.00 12.57     0.240 C
ATOM  18567  O   ALA B 564      -24.015   7.074  61.659  1.00 12.50    -0.271 OA
ATOM  18568  CB  ALA B 564      -21.276   8.317  60.637  1.00 11.30     0.042 C
ATOM  18572  N   VAL B 565      -24.375   9.188  61.032  1.00 13.77    -0.346 N
ATOM  18573  HN  VAL B 565      -24.052   9.987  60.486  1.00  0.00     0.163 HD
ATOM  18574  CA  VAL B 565      -25.533   9.348  61.918  1.00 13.76     0.180 C
ATOM  18576  C   VAL B 565      -26.677   8.482  61.388  1.00 16.20     0.241 C
ATOM  18577  O   VAL B 565      -27.306   7.749  62.179  1.00 14.84    -0.271 OA
ATOM  18578  CB  VAL B 565      -25.955  10.810  62.051  1.00 14.95     0.009 C
ATOM  18580  CG1 VAL B 565      -27.307  10.983  62.751  1.00 20.10     0.012 C
ATOM  18584  CG2 VAL B 565      -24.897  11.633  62.808  1.00 15.14     0.012 C
ATOM  18588  N   ALA B 566      -26.865   8.477  60.055  1.00 12.63    -0.346 N
ATOM  18589  HN  ALA B 566      -26.286   9.041  59.433  1.00  0.00     0.163 HD
ATOM  18590  CA  ALA B 566      -27.945   7.620  59.533  1.00 17.48     0.172 C
ATOM  18592  C   ALA B 566      -27.641   6.154  59.778  1.00 18.97     0.240 C
ATOM  18593  O   ALA B 566      -28.572   5.376  60.065  1.00 18.64    -0.271 OA
ATOM  18594  CB  ALA B 566      -28.181   7.917  58.053  1.00 18.19     0.042 C
ATOM  18598  N   ALA B 567      -26.389   5.705  59.689  1.00 16.77    -0.346 N
ATOM  18599  HN  ALA B 567      -25.649   6.357  59.429  1.00  0.00     0.163 HD
ATOM  18600  CA  ALA B 567      -26.042   4.310  59.951  1.00 18.88     0.172 C
ATOM  18602  C   ALA B 567      -26.214   4.028  61.442  1.00 22.19     0.240 C
ATOM  18603  O   ALA B 567      -26.646   2.958  61.866  1.00 19.89    -0.271 OA
ATOM  18604  CB  ALA B 567      -24.616   3.980  59.526  1.00 15.90     0.042 C
ATOM  18608  N   TYR B 568      -25.867   5.008  62.278  1.00 18.23    -0.346 N
ATOM  18609  HN  TYR B 568      -25.467   5.871  61.910  1.00  0.00     0.163 HD
ATOM  18610  CA  TYR B 568      -26.059   4.849  63.728  1.00 19.49     0.180 C
ATOM  18612  C   TYR B 568      -27.555   4.635  63.993  1.00 21.89     0.241 C
ATOM  18613  O   TYR B 568      -27.911   3.769  64.802  1.00 19.29    -0.271 OA
ATOM  18614  CB  TYR B 568      -25.524   6.072  64.452  1.00 15.49     0.073 C
ATOM  18617  CG  TYR B 568      -26.075   6.324  65.828  1.00 18.60    -0.056 A
ATOM  18618  CD1 TYR B 568      -27.237   7.089  65.944  1.00 20.17     0.010 A
ATOM  18620  CD2 TYR B 568      -25.441   5.866  66.991  1.00 14.80     0.010 A
ATOM  18622  CE1 TYR B 568      -27.784   7.347  67.184  1.00 22.71     0.037 A
ATOM  18624  CE2 TYR B 568      -25.994   6.145  68.241  1.00 21.02     0.037 A
ATOM  18626  CZ  TYR B 568      -27.153   6.878  68.320  1.00 25.67     0.065 A
ATOM  18627  OH  TYR B 568      -27.745   7.191  69.538  1.00 25.76    -0.361 OA
ATOM  18628  HH  TYR B 568      -27.311   6.868  70.319  1.00  0.00     0.217 HD
ATOM  18629  N   GLU B 569      -28.407   5.397  63.320  1.00 17.20    -0.346 N
ATOM  18630  HN  GLU B 569      -28.063   6.086  62.651  1.00  0.00     0.163 HD
ATOM  18631  CA  GLU B 569      -29.848   5.241  63.545  1.00 23.30     0.177 C
ATOM  18633  C   GLU B 569      -30.361   3.860  63.159  1.00 25.14     0.241 C
ATOM  18634  O   GLU B 569      -31.107   3.257  63.930  1.00 25.71    -0.271 OA
ATOM  18635  CB  GLU B 569      -30.624   6.385  62.871  1.00 22.98     0.045 C
ATOM  18638  CG  GLU B 569      -30.523   7.536  63.862  1.00 38.49     0.116 C
ATOM  18641  CD  GLU B 569      -31.014   8.899  63.493  1.00 57.26     0.172 C
ATOM  18642  OE1 GLU B 569      -31.361   9.137  62.319  1.00 61.01    -0.648 OA
ATOM  18643  OE2 GLU B 569      -31.031   9.750  64.423  1.00 64.79    -0.648 OA
ATOM  18644  N   LYS B 570      -29.920   3.324  62.049  1.00 22.06    -0.346 N
ATOM  18645  HN  LYS B 570      -29.299   3.888  61.469  1.00  0.00     0.163 HD
ATOM  18646  CA  LYS B 570      -30.244   1.994  61.581  1.00 25.15     0.176 C
ATOM  18648  C   LYS B 570      -29.750   0.930  62.539  1.00 29.35     0.241 C
ATOM  18649  O   LYS B 570      -30.583   0.099  62.955  1.00 28.92    -0.271 OA
ATOM  18650  CB  LYS B 570      -29.728   1.832  60.157  1.00 27.34     0.035 C
ATOM  18653  CG  LYS B 570      -30.237   0.641  59.369  1.00 44.93     0.004 C
ATOM  18656  CD  LYS B 570      -30.302   0.950  57.875  1.00 63.89     0.027 C
ATOM  18659  CE  LYS B 570      -30.363  -0.324  57.054  1.00 72.14     0.229 C
ATOM  18662  NZ  LYS B 570      -29.624  -0.222  55.765  1.00 75.25    -0.079 N
ATOM  18663  HZ1 LYS B 570      -29.665  -1.079  55.213  1.00  0.00     0.274 HD
ATOM  18664  HZ2 LYS B 570      -28.658   0.065  55.921  1.00  0.00     0.274 HD
ATOM  18665  HZ3 LYS B 570      -29.949   0.577  55.221  1.00  0.00     0.274 HD
ATOM  18666  N   LEU B 571      -28.510   0.940  63.022  1.00 23.44    -0.346 N
ATOM  18667  HN  LEU B 571      -27.872   1.681  62.731  1.00  0.00     0.163 HD
ATOM  18668  CA  LEU B 571      -28.037  -0.071  63.950  1.00 25.97     0.177 C
ATOM  18670  C   LEU B 571      -28.609   0.018  65.357  1.00 28.06     0.241 C
ATOM  18671  O   LEU B 571      -28.865  -1.011  66.022  1.00 26.79    -0.271 OA
ATOM  18672  CB  LEU B 571      -26.492  -0.025  64.001  1.00 25.76     0.038 C
ATOM  18675  CG  LEU B 571      -25.852  -0.403  62.643  1.00 29.36    -0.020 C
ATOM  18677  CD1 LEU B 571      -24.359  -0.104  62.699  1.00 34.93     0.009 C
ATOM  18681  CD2 LEU B 571      -26.060  -1.875  62.318  1.00 35.57     0.009 C
ATOM  18685  N   THR B 572      -28.856   1.240  65.833  1.00 22.90    -0.344 N
ATOM  18686  HN  THR B 572      -28.648   2.065  65.270  1.00  0.00     0.163 HD
ATOM  18687  CA  THR B 572      -29.428   1.384  67.172  1.00 24.66     0.205 C
ATOM  18689  C   THR B 572      -30.844   0.772  67.168  1.00 30.60     0.243 C
ATOM  18690  O   THR B 572      -31.186   0.070  68.124  1.00 28.65    -0.271 OA
ATOM  18691  CB  THR B 572      -29.485   2.810  67.706  1.00 26.16     0.146 C
ATOM  18693  CG2 THR B 572      -28.113   3.478  67.789  1.00 25.19     0.042 C
ATOM  18697  OG1 THR B 572      -30.270   3.607  66.812  1.00 45.04    -0.393 OA
ATOM  18698  HG1 THR B 572      -30.306   4.496  67.145  1.00  0.00     0.210 HD
ATOM  18699  N   ALA B 573      -31.615   0.947  66.100  1.00 29.39    -0.346 N
ATOM  18700  HN  ALA B 573      -31.267   1.528  65.337  1.00  0.00     0.163 HD
ATOM  18701  CA  ALA B 573      -32.936   0.346  65.970  1.00 35.40     0.172 C
ATOM  18703  C   ALA B 573      -32.867  -1.180  66.043  1.00 36.42     0.240 C
ATOM  18704  O   ALA B 573      -33.787  -1.781  66.590  1.00 37.20    -0.271 OA
ATOM  18705  CB  ALA B 573      -33.703   0.747  64.713  1.00 27.77     0.042 C
ATOM  18709  N   GLU B 574      -31.822  -1.832  65.574  1.00 35.67    -0.346 N
ATOM  18710  HN  GLU B 574      -31.095  -1.295  65.102  1.00  0.00     0.163 HD
ATOM  18711  CA  GLU B 574      -31.644  -3.259  65.688  1.00 36.30     0.177 C
ATOM  18713  C   GLU B 574      -31.083  -3.693  67.033  1.00 35.79     0.240 C
ATOM  18714  O   GLU B 574      -30.689  -4.854  67.162  1.00 40.44    -0.271 OA
ATOM  18715  CB  GLU B 574      -30.674  -3.743  64.602  1.00 42.78     0.045 C
ATOM  18718  CG  GLU B 574      -31.155  -3.403  63.201  1.00 48.73     0.116 C
ATOM  18721  CD  GLU B 574      -30.223  -3.990  62.159  1.00 53.77     0.172 C
ATOM  18722  OE1 GLU B 574      -29.415  -4.878  62.497  1.00 60.05    -0.648 OA
ATOM  18723  OE2 GLU B 574      -30.304  -3.547  60.997  1.00 68.59    -0.648 OA
ATOM  18724  N   GLY B 575      -30.940  -2.796  67.995  1.00 32.73    -0.351 N
ATOM  18725  HN  GLY B 575      -31.220  -1.832  67.813  1.00  0.00     0.163 HD
ATOM  18726  CA  GLY B 575      -30.404  -3.130  69.290  1.00 31.63     0.225 C
ATOM  18729  C   GLY B 575      -28.901  -3.021  69.451  1.00 33.91     0.236 C
ATOM  18730  O   GLY B 575      -28.428  -3.360  70.546  1.00 32.85    -0.272 OA
ATOM  18731  N   VAL B 576      -28.134  -2.564  68.470  1.00 26.85    -0.346 N
ATOM  18732  HN  VAL B 576      -28.556  -2.310  67.577  1.00  0.00     0.163 HD
ATOM  18733  CA  VAL B 576      -26.692  -2.420  68.655  1.00 25.50     0.180 C
ATOM  18735  C   VAL B 576      -26.370  -1.182  69.482  1.00 19.35     0.241 C
ATOM  18736  O   VAL B 576      -26.968  -0.129  69.259  1.00 22.53    -0.271 OA
ATOM  18737  CB  VAL B 576      -25.987  -2.315  67.281  1.00 28.17     0.009 C
ATOM  18739  CG1 VAL B 576      -24.477  -2.199  67.421  1.00 22.29     0.012 C
ATOM  18743  CG2 VAL B 576      -26.319  -3.537  66.438  1.00 29.75     0.012 C
ATOM  18747  N   LYS B 577      -25.420  -1.231  70.391  1.00 18.10    -0.346 N
ATOM  18748  HN  LYS B 577      -24.992  -2.136  70.587  1.00  0.00     0.163 HD
ATOM  18749  CA  LYS B 577      -24.944  -0.082  71.130  1.00 20.82     0.176 C
ATOM  18751  C   LYS B 577      -23.832   0.625  70.312  1.00 16.38     0.241 C
ATOM  18752  O   LYS B 577      -22.698   0.168  70.296  1.00 20.51    -0.271 OA
ATOM  18753  CB  LYS B 577      -24.354  -0.552  72.463  1.00 18.99     0.035 C
ATOM  18756  CG  LYS B 577      -25.548  -0.912  73.399  1.00 23.90     0.004 C
ATOM  18759  CD  LYS B 577      -24.989  -0.972  74.821  1.00 37.17     0.027 C
ATOM  18762  CE  LYS B 577      -26.003  -1.591  75.772  1.00 44.89     0.229 C
ATOM  18765  NZ  LYS B 577      -27.229  -0.747  75.883  1.00 51.95    -0.079 N
ATOM  18766  HZ1 LYS B 577      -27.909  -1.162  76.520  1.00  0.00     0.274 HD
ATOM  18767  HZ2 LYS B 577      -27.639  -0.561  74.968  1.00  0.00     0.274 HD
ATOM  18768  HZ3 LYS B 577      -27.001   0.211  76.150  1.00  0.00     0.274 HD
ATOM  18769  N   ALA B 578      -24.222   1.680  69.619  1.00 16.18    -0.346 N
ATOM  18770  HN  ALA B 578      -25.186   2.006  69.691  1.00  0.00     0.163 HD
ATOM  18771  CA  ALA B 578      -23.281   2.381  68.751  1.00 15.93     0.172 C
ATOM  18773  C   ALA B 578      -23.118   3.834  69.204  1.00 13.87     0.240 C
ATOM  18774  O   ALA B 578      -23.882   4.414  69.980  1.00 16.63    -0.271 OA
ATOM  18775  CB  ALA B 578      -23.778   2.348  67.309  1.00 12.42     0.042 C
ATOM  18779  N   ARG B 579      -21.981   4.383  68.729  1.00 12.09    -0.346 N
ATOM  18780  HN  ARG B 579      -21.360   3.836  68.132  1.00  0.00     0.163 HD
ATOM  18781  CA  ARG B 579      -21.642   5.758  69.070  1.00  9.44     0.176 C
ATOM  18783  C   ARG B 579      -21.151   6.442  67.776  1.00 14.80     0.241 C
ATOM  18784  O   ARG B 579      -20.494   5.764  66.972  1.00 10.96    -0.271 OA
ATOM  18785  CB  ARG B 579      -20.500   5.747  70.107  1.00  9.97     0.036 C
ATOM  18788  CG  ARG B 579      -19.829   7.115  70.334  1.00 15.69     0.023 C
ATOM  18791  CD  ARG B 579      -18.666   7.032  71.301  1.00 13.64     0.138 C
ATOM  18794  NE  ARG B 579      -19.190   6.849  72.688  1.00 12.80    -0.227 N
ATOM  18795  HE  ARG B 579      -20.198   6.770  72.821  1.00  0.00     0.177 HD
ATOM  18796  CZ  ARG B 579      -18.405   6.785  73.754  1.00 23.16     0.665 C
ATOM  18797  NH1 ARG B 579      -17.087   6.896  73.644  1.00 18.31    -0.235 N
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ATOM  18798 1HH1 ARG B 579     -16.704   7.015  72.706  1.00  0.00     0.174 HD
ATOM  18799 2HH1 ARG B 579     -16.483   6.847  74.464  1.00  0.00     0.174 HD
ATOM  18800  NH2 ARG B 579     -18.909   6.628  74.988  1.00 21.81    -0.235 N
ATOM  18801 1HH2 ARG B 579     -19.922   6.543  75.073  1.00  0.00     0.174 HD
ATOM  18802 2HH2 ARG B 579     -18.305   6.579  75.808  1.00  0.00     0.174 HD
ATOM  18803  N   VAL B 580     -21.396   7.741  67.652  1.00  9.77    -0.346 N
ATOM  18804  HN  VAL B 580     -21.977   8.228  68.334  1.00  0.00     0.163 HD
ATOM  18805  CA  VAL B 580     -20.808   8.469  66.503  1.00  9.80     0.180 C
ATOM  18807  C   VAL B 580     -19.860   9.526  67.093  1.00 13.04     0.241 C
ATOM  18808  O   VAL B 580     -20.283  10.304  67.949  1.00 11.19    -0.271 OA
ATOM  18809  CB  VAL B 580     -21.863   9.167  65.643  1.00 11.16     0.009 C
ATOM  18811  CG1 VAL B 580     -21.199  10.022  64.537  1.00 13.78     0.012 C
ATOM  18815  CG2 VAL B 580     -22.748   8.065  65.015  1.00 11.14     0.012 C
ATOM  18819  N   VAL B 581     -18.624   9.567  66.598  1.00  7.94    -0.346 N
ATOM  18820  HN  VAL B 581     -18.327   8.862  65.924  1.00  0.00     0.163 HD
ATOM  18821  CA  VAL B 581     -17.688  10.612  67.011  1.00  7.60     0.180 C
ATOM  18823  C   VAL B 581     -17.478  11.512  65.779  1.00  8.53     0.241 C
ATOM  18824  O   VAL B 581     -17.162  11.002  64.697  1.00 11.03    -0.271 OA
ATOM  18825  CB  VAL B 581     -16.330   9.984  67.367  1.00  7.59     0.009 C
ATOM  18827  CG1 VAL B 581     -15.229  11.012  67.526  1.00  9.60     0.012 C
ATOM  18831  CG2 VAL B 581     -16.491   9.151  68.656  1.00 14.53     0.012 C
ATOM  18835  N   SER B 582     -17.673  12.810  65.951  1.00  7.95    -0.344 N
ATOM  18836  HN  SER B 582     -18.010  13.152  66.851  1.00  0.00     0.163 HD
ATOM  18837  CA  SER B 582     -17.415  13.751  64.882  1.00 10.19     0.200 C
ATOM  18839  C   SER B 582     -15.959  14.195  65.156  1.00  8.61     0.243 C
ATOM  18840  O   SER B 582     -15.661  14.586  66.303  1.00  9.31    -0.271 OA
ATOM  18841  CB  SER B 582     -18.329  14.978  64.988  1.00 10.24     0.199 C
ATOM  18844  OG  SER B 582     -18.054  15.926  63.926  1.00 10.02    -0.398 OA
ATOM  18845  HG  SER B 582     -18.620  16.686  63.992  1.00  0.00     0.209 HD
ATOM  18846  N   MET B 583     -15.107  14.202  64.152  1.00  6.17    -0.346 N
ATOM  18847  HN  MET B 583     -15.441  13.937  63.225  1.00  0.00     0.163 HD
ATOM  18848  CA  MET B 583     -13.712  14.571  64.311  1.00  5.00     0.177 C
ATOM  18850  C   MET B 583     -13.312  15.678  63.362  1.00  8.48     0.243 C
ATOM  18851  O   MET B 583     -12.540  15.475  62.392  1.00  8.65    -0.271 OA
ATOM  18852  CB  MET B 583     -12.814  13.305  64.092  1.00 13.13     0.045 C
ATOM  18855  CG AMET B 583     -11.487  13.540  64.836  0.50 21.88     0.076 C
ATOM  18858  SD AMET B 583     -10.305  12.203  64.743  0.50 19.22    -0.173 SA
ATOM  18859  CE AMET B 583     -10.714  11.154  66.125  0.50 17.86     0.089 C
ATOM  18863  N   PRO B 584     -13.782  16.911  63.579  1.00  7.43    -0.337 N
ATOM  18864  CA  PRO B 584     -13.446  18.010  62.682  1.00  7.92     0.179 C
ATOM  18866  C   PRO B 584     -11.937  18.285  62.663  1.00 10.57     0.241 C
ATOM  18867  O   PRO B 584     -11.477  18.730  61.615  1.00  9.17    -0.271 OA
ATOM  18868  CB  PRO B 584     -14.262  19.188  63.204  1.00  7.43     0.037 C
ATOM  18871  CG  PRO B 584     -14.569  18.857  64.658  1.00  8.53     0.022 C
ATOM  18874  CD  PRO B 584     -14.707  17.331  64.658  1.00 11.90     0.127 C
ATOM  18877  N   SER B 585     -11.207  18.059  63.787  1.00  6.14    -0.344 N
ATOM  18878  HN  SER B 585     -11.630  17.743  64.660  1.00  0.00     0.163 HD
ATOM  18879  CA  SER B 585      -9.760  18.303  63.654  1.00  9.58     0.200 C
ATOM  18881  C   SER B 585      -8.993  17.199  64.378  1.00 11.29     0.243 C
ATOM  18882  O   SER B 585      -9.027  17.186  65.614  1.00  7.62    -0.271 OA
ATOM  18883  CB  SER B 585      -9.371  19.676  64.262  1.00  9.26     0.199 C
ATOM  18886  OG  SER B 585      -7.951  19.804  64.383  1.00 10.69    -0.398 OA
ATOM  18887  HG  SER B 585      -7.713  20.645  64.755  1.00  0.00     0.209 HD
ATOM  18888  N   THR B 586      -8.203  16.427  63.633  1.00  6.01    -0.344 N
ATOM  18889  HN  THR B 586      -8.160  16.543  62.621  1.00  0.00     0.163 HD
ATOM  18890  CA  THR B 586      -7.384  15.390  64.319  1.00  7.03     0.205 C
ATOM  18892  C   THR B 586      -6.272  16.009  65.132  1.00 12.00     0.243 C
ATOM  18893  O   THR B 586      -5.913  15.476  66.207  1.00  8.05    -0.271 OA
ATOM  18894  CB  THR B 586      -6.799  14.453  63.221  1.00 11.41     0.146 C
ATOM  18896  CG2 THR B 586      -7.898  13.748  62.445  1.00  9.26     0.042 C
ATOM  18900  OG1 THR B 586      -6.044  15.262  62.325  1.00  8.79    -0.393 OA
ATOM  18901  HG1 THR B 586      -5.357  15.703  62.810  1.00  0.00     0.210 HD
ATOM  18902  N   ASP B 587      -5.654  17.135  64.689  1.00  9.58    -0.345 N
ATOM  18903  HN  ASP B 587      -5.921  17.558  63.800  1.00  0.00     0.163 HD
ATOM  18904  CA  ASP B 587      -4.606  17.727  65.503  1.00  8.26     0.186 C
ATOM  18906  C   ASP B 587      -5.082  18.315  66.828  1.00 10.99     0.241 C
ATOM  18907  O   ASP B 587      -4.379  18.148  67.857  1.00  9.24    -0.271 OA
ATOM  18908  CB  ASP B 587      -3.824  18.791  64.700  1.00 10.21     0.147 C
ATOM  18911  CG  ASP B 587      -4.758  19.834  64.137  1.00  8.24     0.175 C
ATOM  18912  OD1 ASP B 587      -5.359  19.560  63.085  1.00  9.84    -0.648 OA
ATOM  18913  OD2 ASP B 587      -4.881  20.925  64.743  1.00  9.53    -0.648 OA
ATOM  18914  N   ALA B 588      -6.267  18.921  66.883  1.00 11.41    -0.346 N
ATOM  18915  HN  ALA B 588      -6.821  19.009  66.031  1.00  0.00     0.163 HD
ATOM  18916  CA  ALA B 588      -6.793  19.462  68.134  1.00 12.49     0.172 C
ATOM  18918  C   ALA B 588      -7.167  18.296  69.038  1.00  9.17     0.240 C
ATOM  18919  O   ALA B 588      -6.839  18.306  70.226  1.00 12.16    -0.271 OA
ATOM  18920  CB  ALA B 588      -8.014  20.360  67.893  1.00  7.85     0.042 C
ATOM  18924  N   PHE B 589      -7.740  17.215  68.486  1.00  5.00    -0.346 N
ATOM  18925  HN  PHE B 589      -7.975  17.224  67.493  1.00  0.00     0.163 HD
ATOM  18926  CA  PHE B 589      -8.035  16.020  69.287  1.00  7.91     0.180 C
ATOM  18928  C   PHE B 589      -6.801  15.376  69.893  1.00 11.75     0.241 C
ATOM  18929  O   PHE B 589      -6.748  14.987  71.074  1.00 10.86    -0.271 OA
ATOM  18930  CB  PHE B 589      -8.736  14.946  68.396  1.00  9.13     0.073 C
ATOM  18933  CG  PHE B 589      -9.122  13.705  69.168  1.00  9.48    -0.056 A
ATOM  18934  CD1 PHE B 589     -10.174  13.764  70.078  1.00  9.59     0.007 A
ATOM  18936  CD2 PHE B 589      -8.407  12.522  69.019  1.00 12.87     0.007 A
ATOM  18938  CE1 PHE B 589     -10.522  12.612  70.802  1.00 12.94     0.001 A
ATOM  18940  CE2 PHE B 589      -8.747  11.382  69.747  1.00 12.49     0.001 A
ATOM  18942  CZ  PHE B 589      -9.823  11.443  70.638  1.00 10.44     0.000 A
ATOM  18944  N   ASP B 590      -5.720  15.186  69.101  1.00  9.00    -0.345 N
ATOM  18945  HN  ASP B 590      -5.758  15.488  68.128  1.00  0.00     0.163 HD
ATOM  18946  CA  ASP B 590      -4.495  14.557  69.606  1.00 12.47     0.186 C
ATOM  18948  C   ASP B 590      -3.838  15.333  70.759  1.00 15.21     0.241 C
ATOM  18949  O   ASP B 590      -3.154  14.734  71.589  1.00 12.68    -0.271 OA
ATOM  18950  CB  ASP B 590      -3.438  14.437  68.504  1.00 11.73     0.147 C
ATOM  18953  CG  ASP B 590      -3.766  13.375  67.473  1.00 18.41     0.175 C
ATOM  18954  OD1 ASP B 590      -4.726  12.574  67.632  1.00 11.89    -0.648 OA
ATOM  18955  OD2 ASP B 590      -3.058  13.385  66.432  1.00 15.43    -0.648 OA
ATOM  18956  N   LYS B 591      -4.064  16.630  70.825  1.00 12.20    -0.346 N
ATOM  18957  HN  LYS B 591      -4.633  17.067  70.100  1.00  0.00     0.163 HD
ATOM  18958  CA  LYS B 591      -3.533  17.458  71.892  1.00 12.36     0.176 C
ATOM  18960  C   LYS B 591      -4.335  17.385  73.180  1.00 17.09     0.241 C
ATOM  18961  O   LYS B 591      -3.815  17.910  74.191  1.00 15.83    -0.271 OA
ATOM  18962  CB  LYS B 591      -3.520  18.949  71.443  1.00 15.67     0.035 C
ATOM  18965  CG  LYS B 591      -2.494  19.111  70.335  1.00 26.56     0.004 C
ATOM  18968  CD  LYS B 591      -2.379  20.549  69.849  1.00 25.84     0.027 C
ATOM  18971  CE  LYS B 591      -1.182  20.641  68.905  1.00 30.62     0.229 C
ATOM  18974  NZ  LYS B 591      -1.498  21.506  67.731  1.00 36.65    -0.079 N
ATOM  18975  HZ1 LYS B 591      -0.699  21.567  67.101  1.00  0.00     0.274 HD
ATOM  18976  HZ2 LYS B 591      -1.823  22.429  68.019  1.00  0.00     0.274 HD
ATOM  18977  HZ3 LYS B 591      -2.338  21.191  67.246  1.00  0.00     0.274 HD
ATOM  18978  N   GLN B 592      -5.505  16.780  73.208  1.00 13.81    -0.346 N
ATOM  18979  HN  GLN B 592      -5.880  16.353  72.361  1.00  0.00     0.163 HD
ATOM  18980  CA  GLN B 592      -6.265  16.722  74.457  1.00  9.96     0.177 C
ATOM  18982  C   GLN B 592      -5.584  15.761  75.421  1.00 14.30     0.241 C
ATOM  18983  O   GLN B 592      -4.786  14.885  75.046  1.00 10.62    -0.271 OA
ATOM  18984  CB  GLN B 592      -7.707  16.249  74.186  1.00 10.66     0.044 C
ATOM  18987  CG  GLN B 592      -8.455  17.164  73.166  1.00 10.23     0.105 C
ATOM  18990  CD  GLN B 592      -8.489  18.609  73.586  1.00 18.25     0.215 C
ATOM  18991  NE2 GLN B 592      -8.056  19.545  72.751  1.00 15.71    -0.370 N
ATOM  18992 1HE2 GLN B 592      -8.079  20.524  73.036  1.00  0.00     0.159 HD
ATOM  18993 2HE2 GLN B 592      -7.699  19.292  71.830  1.00  0.00     0.159 HD
ATOM  18994  OE1 GLN B 592      -8.925  18.918  74.712  1.00 13.30    -0.274 OA
ATOM  18995  N   ASP B 593      -5.977  15.901  76.695  1.00 14.00    -0.346 N
ATOM  18996  HN  ASP B 593      -6.645  16.627  76.955  1.00  0.00     0.163 HD
ATOM  18997  CA  ASP B 593      -5.426  14.985  77.716  1.00 13.38     0.186 C
ATOM  18999  C   ASP B 593      -5.838  13.572  77.423  1.00 14.84     0.241 C
ATOM  19000  O   ASP B 593      -6.873  13.280  76.816  1.00 14.06    -0.271 OA
ATOM  19001  CB  ASP B 593      -5.858  15.426  79.122  1.00 18.70     0.147 C
ATOM  19004  CG  ASP B 593      -7.368  15.542  79.211  1.00 23.05     0.175 C
ATOM  19005  OD1 ASP B 593      -7.976  16.499  78.694  1.00 25.37    -0.648 OA
ATOM  19006  OD2 ASP B 593      -7.938  14.590  79.748  1.00 16.94    -0.648 OA
ATOM  19007  N   ALA B 594      -5.081  12.595  77.977  1.00 10.98    -0.346 N
ATOM  19008  HN  ALA B 594      -4.303  12.851  78.585  1.00  0.00     0.163 HD
ATOM  19009  CA  ALA B 594      -5.351  11.195  77.726  1.00 15.90     0.172 C
ATOM  19011  C   ALA B 594      -6.728  10.728  78.184  1.00 14.28     0.240 C
ATOM  19012  O   ALA B 594      -7.292   9.858  77.545  1.00 11.55    -0.271 OA
ATOM  19013  CB  ALA B 594      -4.287  10.355  78.464  1.00 22.60     0.042 C
ATOM  19017  N   ALA B 595      -7.201  11.200  79.344  1.00 13.56    -0.346 N
ATOM  19018  HN  ALA B 595      -6.648  11.871  79.877  1.00  0.00     0.163 HD
ATOM  19019  CA  ALA B 595      -8.500  10.767  79.858  1.00 13.82     0.172 C
ATOM  19021  C   ALA B 595      -9.597  11.291  78.941  1.00 13.65     0.240 C
ATOM  19022  O   ALA B 595     -10.575  10.544  78.725  1.00 11.39    -0.271 OA
ATOM  19023  CB  ALA B 595      -8.683  11.343  81.295  1.00 15.86     0.042 C
ATOM  19027  N   TYR B 596      -9.493  12.526  78.427  1.00 10.12    -0.346 N
ATOM  19028  HN  TYR B 596      -8.747  13.158  78.718  1.00  0.00     0.163 HD
ATOM  19029  CA  TYR B 596     -10.505  12.941  77.416  1.00 10.69     0.180 C
ATOM  19031  C   TYR B 596     -10.526  12.033  76.183  1.00  8.51     0.241 C
ATOM  19032  O   TYR B 596     -11.584  11.532  75.718  1.00 12.11    -0.271 OA
ATOM  19033  CB  TYR B 596     -10.294  14.412  76.982  1.00  9.46     0.073 C
ATOM  19036  CG  TYR B 596     -11.344  14.801  75.941  1.00 12.82    -0.056 A
ATOM  19037  CD1 TYR B 596     -12.657  15.048  76.338  1.00 11.38     0.010 A
ATOM  19039  CD2 TYR B 596     -11.030  14.854  74.581  1.00 12.85     0.010 A
ATOM  19041  CE1 TYR B 596     -13.648  15.346  75.425  1.00 16.79     0.037 A
ATOM  19043  CE2 TYR B 596     -12.027  15.186  73.672  1.00 12.83     0.037 A
ATOM  19045  CZ  TYR B 596     -13.315  15.426  74.074  1.00 14.95     0.065 A
ATOM  19046  OH  TYR B 596     -14.303  15.769  73.159  1.00  9.36    -0.361 OA
ATOM  19047  HH  TYR B 596     -15.196  15.935  73.438  1.00  0.00     0.217 HD
ATOM  19048  N   ARG B 597      -9.353  11.740  75.603  1.00 12.31    -0.346 N
ATOM  19049  HN  ARG B 597      -8.487  12.082  76.019  1.00  0.00     0.163 HD
ATOM  19050  CA  ARG B 597      -9.300  10.939  74.385  1.00 13.39     0.176 C
ATOM  19052  C   ARG B 597      -9.811   9.525  74.645  1.00 11.45     0.241 C
ATOM  19053  O   ARG B 597     -10.495   8.945  73.811  1.00 14.14    -0.271 OA
ATOM  19054  CB  ARG B 597      -7.905  10.874  73.770  1.00 14.26     0.036 C
ATOM  19057  CG  ARG B 597      -7.374  12.296  73.443  1.00 15.28     0.023 C
ATOM  19060  CD  ARG B 597      -6.077  12.083  72.633  1.00 16.68     0.138 C
ATOM  19063  NE  ARG B 597      -4.952  12.234  73.564  1.00 25.67    -0.227 N
ATOM  19064  HE  ARG B 597      -4.811  13.196  73.872  1.00  0.00     0.177 HD
ATOM  19065  CZ  ARG B 597      -4.093  11.395  74.081  1.00 22.94     0.665 C
ATOM  19066  NH1 ARG B 597      -4.057  10.096  73.811  1.00 29.23    -0.235 N
ATOM  19067 1HH1 ARG B 597      -3.387   9.441  74.214  1.00  0.00     0.174 HD
ATOM  19068 2HH1 ARG B 597      -4.761   9.754  73.157  1.00  0.00     0.174 HD
ATOM  19069  NH2 ARG B 597      -3.181  11.838  74.929  1.00 28.91    -0.235 N
ATOM  19070 1HH2 ARG B 597      -2.511  11.183  75.332  1.00  0.00     0.174 HD
ATOM  19071 2HH2 ARG B 597      -3.209  12.836  75.136  1.00  0.00     0.174 HD
ATOM  19072  N   GLU B 598      -9.505   8.981  75.825  1.00 11.19    -0.346 N
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ATOM  19073  HN  GLU B 598      -8.914   9.474  76.494  1.00  0.00     0.163 HD
ATOM  19074  CA  GLU B 598     -10.053   7.635  76.133  1.00 10.86     0.177 C
ATOM  19076  C   GLU B 598     -11.534   7.626  76.330  1.00 12.05     0.241 C
ATOM  19077  O   GLU B 598     -12.255   6.643  76.039  1.00 14.00    -0.271 OA
ATOM  19078  CB  GLU B 598      -9.316   7.158  77.405  1.00 15.97     0.045 C
ATOM  19081  CG  GLU B 598     -10.010   5.978  78.066  1.00 21.13     0.116 C
ATOM  19084  CD  GLU B 598      -9.798   4.627  77.396  1.00 26.70     0.172 C
ATOM  19085  OE1 GLU B 598      -8.904   4.396  76.544  1.00 21.70    -0.648 OA
ATOM  19086  OE2 GLU B 598     -10.572   3.694  77.723  1.00 27.37    -0.648 OA
ATOM  19087  N   SER B 599     -12.101   8.750  76.782  1.00 12.46    -0.344 N
ATOM  19088  HN  SER B 599     -11.528   9.567  76.995  1.00  0.00     0.163 HD
ATOM  19089  CA  SER B 599     -13.557   8.796  76.969  1.00 13.85     0.200 C
ATOM  19091  C   SER B 599     -14.283   8.944  75.636  1.00 19.01     0.243 C
ATOM  19092  O   SER B 599     -15.439   8.476  75.516  1.00 20.15    -0.271 OA
ATOM  19093  CB  SER B 599     -13.919   9.963  77.902  1.00 15.94     0.199 C
ATOM  19096  OG  SER B 599     -13.958  11.172  77.168  1.00 19.69    -0.398 OA
ATOM  19097  HG  SER B 599     -14.182  11.893  77.745  1.00  0.00     0.209 HD
ATOM  19098  N   VAL B 600     -13.598   9.363  74.580  1.00 13.32    -0.346 N
ATOM  19099  HN  VAL B 600     -12.619   9.626  74.691  1.00  0.00     0.163 HD
ATOM  19100  CA  VAL B 600     -14.222   9.455  73.257  1.00 11.50     0.180 C
ATOM  19102  C   VAL B 600     -14.021   8.169  72.476  1.00 11.83     0.241 C
ATOM  19103  O   VAL B 600     -14.941   7.666  71.828  1.00 12.58    -0.271 OA
ATOM  19104  CB  VAL B 600     -13.589  10.629  72.477  1.00 10.64     0.009 C
ATOM  19106  CG1 VAL B 600     -14.088  10.755  71.030  1.00 10.70     0.012 C
ATOM  19110  CG2 VAL B 600     -13.932  11.941  73.205  1.00 12.54     0.012 C
ATOM  19114  N   LEU B 601     -12.783   7.686  72.455  1.00 11.37    -0.346 N
ATOM  19115  HN  LEU B 601     -12.067   8.186  72.982  1.00  0.00     0.163 HD
ATOM  19116  CA  LEU B 601     -12.384   6.495  71.731  1.00 11.46     0.177 C
ATOM  19118  C   LEU B 601     -11.763   5.486  72.722  1.00 15.36     0.243 C
ATOM  19119  O   LEU B 601     -10.554   5.375  72.826  1.00 15.47    -0.271 OA
ATOM  19120  CB  LEU B 601     -11.349   6.817  70.633  1.00 13.49     0.038 C
ATOM  19123  CG  LEU B 601     -11.779   7.715  69.455  1.00 17.49    -0.020 C
ATOM  19125  CD1 LEU B 601     -10.618   7.971  68.489  1.00 18.49     0.009 C
ATOM  19129  CD2 LEU B 601     -12.959   7.046  68.759  1.00 14.81     0.009 C
ATOM  19133  N   PRO B 602     -12.565   4.782  73.497  1.00 14.42    -0.337 N
ATOM  19134  CA  PRO B 602     -12.073   3.849  74.507  1.00 13.97     0.179 C
ATOM  19136  C   PRO B 602     -11.239   2.741  73.871  1.00 18.36     0.241 C
ATOM  19137  O   PRO B 602     -11.600   2.066  72.899  1.00 15.01    -0.271 OA
ATOM  19138  CB  PRO B 602     -13.309   3.333  75.211  1.00 17.22     0.037 C
ATOM  19141  CG  PRO B 602     -14.431   3.599  74.268  1.00 18.97     0.022 C
ATOM  19144  CD  PRO B 602     -14.048   4.850  73.497  1.00 16.23     0.127 C
ATOM  19147  N   LYS B 603     -10.080   2.530  74.508  1.00 15.45    -0.346 N
ATOM  19148  HN  LYS B 603      -9.890   3.049  75.365  1.00  0.00     0.163 HD
ATOM  19149  CA  LYS B 603      -9.079   1.586  74.022  1.00 23.43     0.176 C
ATOM  19151  C   LYS B 603      -9.588   0.162  73.933  1.00 21.32     0.241 C
ATOM  19152  O   LYS B 603      -9.201  -0.609  73.036  1.00 20.78    -0.271 OA
ATOM  19153  CB  LYS B 603      -7.908   1.761  74.997  1.00 29.82     0.035 C
ATOM  19156  CG  LYS B 603      -6.866   0.665  74.954  1.00 54.92     0.004 C
ATOM  19159  CD  LYS B 603      -5.806   0.900  76.022  1.00 64.35     0.027 C
ATOM  19162  CE  LYS B 603      -5.164  -0.399  76.473  1.00 74.11     0.229 C
ATOM  19165  NZ  LYS B 603      -4.466  -1.132  75.385  1.00 72.13    -0.079 N
ATOM  19166  HZ1 LYS B 603      -4.034  -2.005  75.688  1.00  0.00     0.274 HD
ATOM  19167  HZ2 LYS B 603      -3.779  -0.531  74.930  1.00  0.00     0.274 HD
ATOM  19168  HZ3 LYS B 603      -5.097  -1.296  74.600  1.00  0.00     0.274 HD
ATOM  19169  N   ALA B 604     -10.545  -0.204  74.777  1.00 17.95    -0.346 N
ATOM  19170  HN  ALA B 604     -10.850   0.468  75.481  1.00  0.00     0.163 HD
ATOM  19171  CA  ALA B 604     -11.185  -1.515  74.752  1.00 23.48     0.172 C
ATOM  19173  C   ALA B 604     -12.105  -1.729  73.562  1.00 22.45     0.240 C
ATOM  19174  O   ALA B 604     -12.408  -2.887  73.269  1.00 23.59    -0.271 OA
ATOM  19175  CB  ALA B 604     -12.066  -1.704  76.009  1.00 22.58     0.042 C
ATOM  19179  N   VAL B 605     -12.628  -0.673  72.923  1.00 18.34    -0.346 N
ATOM  19180  HN  VAL B 605     -12.387   0.271  73.226  1.00  0.00     0.163 HD
ATOM  19181  CA  VAL B 605     -13.538  -0.860  71.800  1.00 15.36     0.180 C
ATOM  19183  C   VAL B 605     -12.747  -0.876  70.512  1.00 20.26     0.241 C
ATOM  19184  O   VAL B 605     -12.241   0.155  70.053  1.00 19.10    -0.271 OA
ATOM  19185  CB  VAL B 605     -14.618   0.234  71.777  1.00 25.04     0.009 C
ATOM  19187  CG1 VAL B 605     -15.605   0.034  70.636  1.00 15.51     0.012 C
ATOM  19191  CG2 VAL B 605     -15.343   0.237  73.130  1.00 20.44     0.012 C
ATOM  19195  N   THR B 606     -12.604  -2.049  69.894  1.00 17.79    -0.344 N
ATOM  19196  HN  THR B 606     -13.048  -2.899  70.242  1.00  0.00     0.163 HD
ATOM  19197  CA  THR B 606     -11.763  -2.050  68.672  1.00 18.33     0.205 C
ATOM  19199  C   THR B 606     -12.648  -2.111  67.446  1.00 17.98     0.243 C
ATOM  19200  O   THR B 606     -12.115  -2.017  66.328  1.00 17.30    -0.271 OA
ATOM  19201  CB  THR B 606     -10.825  -3.272  68.684  1.00 27.53     0.146 C
ATOM  19203  CG2 THR B 606      -9.926  -3.291  69.913  1.00 34.27     0.042 C
ATOM  19207  OG1 THR B 606     -11.648  -4.444  68.754  1.00 22.23    -0.393 OA
ATOM  19208  HG1 THR B 606     -11.070  -5.198  68.761  1.00  0.00     0.210 HD
ATOM  19209  N   ALA B 607     -13.948  -2.303  67.588  1.00 14.49    -0.346 N
ATOM  19210  HN  ALA B 607     -14.348  -2.429  68.518  1.00  0.00     0.163 HD
ATOM  19211  CA  ALA B 607     -14.821  -2.335  66.396  1.00 12.34     0.172 C
ATOM  19213  C   ALA B 607     -15.062  -0.863  66.002  1.00 15.22     0.240 C
ATOM  19214  O   ALA B 607     -15.943  -0.182  66.573  1.00 13.63    -0.271 OA
ATOM  19215  CB  ALA B 607     -16.174  -2.970  66.686  1.00 15.64     0.042 C
ATOM  19219  N   ARG B 608     -14.208  -0.324  65.131  1.00 14.36    -0.346 N
ATOM  19220  HN  ARG B 608     -13.491  -0.912  64.706  1.00  0.00     0.163 HD
ATOM  19221  CA  ARG B 608     -14.278   1.083  64.775  1.00 10.98     0.176 C
ATOM  19223  C   ARG B 608     -14.328   1.254  63.249  1.00 12.21     0.241 C
ATOM  19224  O   ARG B 608     -13.713   0.469  62.536  1.00 13.74    -0.271 OA
ATOM  19225  CB  ARG B 608     -13.074   1.910  65.217  1.00 12.77     0.036 C
ATOM  19228  CG  ARG B 608     -12.838   1.914  66.715  1.00 17.71     0.023 C
ATOM  19231  CD  ARG B 608     -11.449   2.374  67.092  1.00 13.67     0.138 C
ATOM  19234  NE  ARG B 608     -11.251   2.309  68.574  1.00 11.42    -0.227 N
ATOM  19235  HE  ARG B 608     -11.878   1.716  69.118  1.00  0.00     0.177 HD
ATOM  19236  CZ  ARG B 608     -10.316   2.972  69.211  1.00 14.72     0.665 C
ATOM  19237  NH1 ARG B 608      -9.495   3.795  68.540  1.00 13.45    -0.235 N
ATOM  19238 1HH1 ARG B 608      -8.768   4.311  69.035  1.00  0.00     0.174 HD
ATOM  19239 2HH1 ARG B 608      -9.614   3.871  67.530  1.00  0.00     0.174 HD
ATOM  19240  NH2 ARG B 608     -10.160   2.872  70.536  1.00 13.51    -0.235 N
ATOM  19241 1HH2 ARG B 608      -9.433   3.388  71.031  1.00  0.00     0.174 HD
ATOM  19242 2HH2 ARG B 608     -10.784   2.247  71.046  1.00  0.00     0.174 HD
ATOM  19243  N   VAL B 609     -15.226   2.153  62.841  1.00  8.87    -0.346 N
ATOM  19244  HN  VAL B 609     -15.772   2.672  63.528  1.00  0.00     0.163 HD
ATOM  19245  CA  VAL B 609     -15.432   2.398  61.413  1.00  7.95     0.180 C
ATOM  19247  C   VAL B 609     -15.208   3.867  61.090  1.00  7.12     0.241 C
ATOM  19248  O   VAL B 609     -15.940   4.700  61.623  1.00 12.83    -0.271 OA
ATOM  19249  CB  VAL B 609     -16.862   2.023  60.976  1.00 13.47     0.009 C
ATOM  19251  CG1 VAL B 609     -17.043   2.283  59.488  1.00 14.16     0.012 C
ATOM  19255  CG2 VAL B 609     -17.169   0.554  61.252  1.00 15.14     0.012 C
ATOM  19259  N   ALA B 610     -14.287   4.212  60.227  1.00  6.27    -0.346 N
ATOM  19260  HN  ALA B 610     -13.705   3.495  59.793  1.00  0.00     0.163 HD
ATOM  19261  CA  ALA B 610     -14.085   5.630  59.878  1.00  7.08     0.172 C
ATOM  19263  C   ALA B 610     -14.770   5.883  58.539  1.00 10.71     0.240 C
ATOM  19264  O   ALA B 610     -14.826   4.964  57.668  1.00 11.30    -0.271 OA
ATOM  19265  CB  ALA B 610     -12.570   5.860  59.750  1.00 12.17     0.042 C
ATOM  19269  N   VAL B 611     -15.368   7.045  58.415  1.00  8.01    -0.346 N
ATOM  19270  HN  VAL B 611     -15.301   7.731  59.166  1.00  0.00     0.163 HD
ATOM  19271  CA  VAL B 611     -16.134   7.365  57.202  1.00  7.58     0.180 C
ATOM  19273  C   VAL B 611     -15.663   8.752  56.708  1.00  9.07     0.241 C
ATOM  19274  O   VAL B 611     -15.893   9.709  57.432  1.00  8.90    -0.271 OA
ATOM  19275  CB  VAL B 611     -17.652   7.373  57.421  1.00 11.80     0.009 C
ATOM  19277  CG1 VAL B 611     -18.362   7.480  56.040  1.00  9.62     0.012 C
ATOM  19281  CG2 VAL B 611     -18.123   6.060  58.084  1.00 14.12     0.012 C
ATOM  19285  N   GLU B 612     -15.008   8.847  55.561  1.00  9.12    -0.346 N
ATOM  19286  HN  GLU B 612     -14.834   8.006  55.011  1.00  0.00     0.163 HD
ATOM  19287  CA  GLU B 612     -14.529  10.146  55.070  1.00  8.19     0.177 C
ATOM  19289  C   GLU B 612     -14.256   9.979  53.578  1.00  7.60     0.241 C
ATOM  19290  O   GLU B 612     -13.652   8.998  53.096  1.00  8.50    -0.271 OA
ATOM  19291  CB  GLU B 612     -13.265  10.639  55.785  1.00  9.00     0.045 C
ATOM  19294  CG  GLU B 612     -12.602  11.825  55.039  1.00  8.93     0.116 C
ATOM  19297  CD  GLU B 612     -11.442  12.338  55.877  1.00  9.37     0.172 C
ATOM  19298  OE1 GLU B 612     -11.666  13.219  56.726  1.00  8.37    -0.648 OA
ATOM  19299  OE2 GLU B 612     -10.305  11.886  55.696  1.00  8.65    -0.648 OA
ATOM  19300  N   ALA B 613     -14.741  10.988  52.829  1.00  6.68    -0.346 N
ATOM  19301  HN  ALA B 613     -15.263  11.755  53.253  1.00  0.00     0.163 HD
ATOM  19302  CA  ALA B 613     -14.491  10.948  51.370  1.00  6.55     0.172 C
ATOM  19304  C   ALA B 613     -13.092  11.466  51.061  1.00 10.81     0.240 C
ATOM  19305  O   ALA B 613     -12.903  12.546  50.445  1.00  9.74    -0.271 OA
ATOM  19306  CB  ALA B 613     -15.534  11.803  50.633  1.00 14.29     0.042 C
ATOM  19310  N   GLY B 614     -12.098  10.721  51.460  1.00  8.57    -0.351 N
ATOM  19311  HN  GLY B 614     -12.337   9.837  51.909  1.00  0.00     0.163 HD
ATOM  19312  CA  GLY B 614     -10.680  11.028  51.327  1.00 10.29     0.225 C
ATOM  19315  C   GLY B 614      -9.908   9.682  51.381  1.00 11.90     0.236 C
ATOM  19316  O   GLY B 614     -10.487   8.618  51.641  1.00  8.97    -0.272 OA
ATOM  19317  N   ILE B 615      -8.605   9.744  51.112  1.00  8.56    -0.346 N
ATOM  19318  HN  ILE B 615      -8.155  10.650  50.984  1.00  0.00     0.163 HD
ATOM  19319  CA  ILE B 615      -7.819   8.518  51.000  1.00  7.16     0.180 C
ATOM  19321  C   ILE B 615      -7.930   7.690  52.285  1.00  9.17     0.241 C
ATOM  19322  O   ILE B 615      -7.861   8.171  53.441  1.00  9.27    -0.271 OA
ATOM  19323  CB  ILE B 615      -6.353   8.812  50.638  1.00  9.17     0.013 C
ATOM  19325  CG1 ILE B 615      -5.666   7.530  50.161  1.00 12.30     0.002 C
ATOM  19328  CG2 ILE B 615      -5.622   9.437  51.856  1.00  6.05     0.012 C
ATOM  19332  CD1 ILE B 615      -6.067   7.155  48.720  1.00 13.35     0.005 C
ATOM  19336  N   ALA B 616      -8.186   6.405  52.076  1.00  6.66    -0.346 N
ATOM  19337  HN  ALA B 616      -8.180   6.022  51.130  1.00  0.00     0.163 HD
ATOM  19338  CA  ALA B 616      -8.480   5.536  53.237  1.00 11.66     0.172 C
ATOM  19340  C   ALA B 616      -7.319   5.325  54.173  1.00 10.41     0.240 C
ATOM  19341  O   ALA B 616      -7.475   5.247  55.405  1.00 11.13    -0.271 OA
ATOM  19342  CB  ALA B 616      -8.966   4.155  52.744  1.00 15.88     0.042 C
ATOM  19346  N   ASP B 617      -6.086   5.239  53.690  1.00  7.57    -0.346 N
ATOM  19347  HN  ASP B 617      -5.947   5.468  52.706  1.00  0.00     0.163 HD
ATOM  19348  CA  ASP B 617      -4.928   4.845  54.454  1.00 10.11     0.186 C
ATOM  19350  C   ASP B 617      -4.637   5.748  55.656  1.00 10.90     0.241 C
ATOM  19351  O   ASP B 617      -4.042   5.251  56.599  1.00 11.20    -0.271 OA
ATOM  19352  CB  ASP B 617      -3.676   4.837  53.562  1.00 13.69     0.147 C
ATOM  19355  CG  ASP B 617      -3.702   3.618  52.642  1.00 28.33     0.175 C
ATOM  19356  OD1 ASP B 617      -4.620   2.785  52.703  1.00 34.83    -0.648 OA
ATOM  19357  OD2 ASP B 617      -2.723   3.514  51.902  1.00 25.65    -0.648 OA
ATOM  19358  N   TYR B 618      -5.063   7.004  55.615  1.00 10.72    -0.346 N
ATOM  19359  HN  TYR B 618      -5.531   7.372  54.787  1.00  0.00     0.163 HD
ATOM  19360  CA  TYR B 618      -4.840   7.853  56.802  1.00  9.17     0.180 C
ATOM  19362  C   TYR B 618      -5.476   7.262  58.048  1.00 10.03     0.241 C
ATOM  19363  O   TYR B 618      -4.919   7.368  59.148  1.00  8.59    -0.271 OA
ATOM  19364  CB  TYR B 618      -5.474   9.246  56.510  1.00  9.88     0.073 C
ATOM  19367  CG  TYR B 618      -5.237  10.103  57.775  1.00 10.98    -0.056 A
ATOM  19368  CD1 TYR B 618      -3.978  10.627  58.052  1.00 13.98     0.010 A
ATOM  19370  CD2 TYR B 618      -6.291  10.287  58.656  1.00 10.38     0.010 A
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ATOM  19372  CE1 TYR B 618      -3.787  11.344  59.239  1.00 15.27     0.037 A
ATOM  19374  CE2 TYR B 618      -6.092  10.981  59.844  1.00  8.89     0.037 A
ATOM  19376  CZ  TYR B 618      -4.858  11.514  60.101  1.00 10.77     0.065 A
ATOM  19377  OH  TYR B 618      -4.661  12.195  61.304  1.00 12.43    -0.361 OA
ATOM  19378  HH  TYR B 618      -5.395  12.312  61.895  1.00  0.00     0.217 HD
ATOM  19379  N   TRP B 619      -6.684   6.721  57.953  1.00  9.72    -0.346 N
ATOM  19380  HN  TRP B 619      -7.053   6.552  57.017  1.00  0.00     0.163 HD
ATOM  19381  CA  TRP B 619      -7.512   6.355  59.070  1.00 10.78     0.181 C
ATOM  19383  C   TRP B 619      -7.096   5.152  59.897  1.00 11.04     0.241 C
ATOM  19384  O   TRP B 619      -7.626   5.072  61.024  1.00 10.35    -0.271 OA
ATOM  19385  CB  TRP B 619      -9.012   6.201  58.652  1.00  6.37     0.075 C
ATOM  19388  CG  TRP B 619      -9.486   7.614  58.382  1.00  6.75    -0.028 A
ATOM  19389  CD1 TRP B 619      -9.626   8.162  57.150  1.00  9.64     0.096 A
ATOM  19391  CD2 TRP B 619      -9.823   8.608  59.367  1.00  5.68    -0.002 A
ATOM  19392  CE2 TRP B 619     -10.173   9.779  58.661  1.00 11.54     0.042 A
ATOM  19393  CE3 TRP B 619      -9.873   8.590  60.776  1.00 11.30     0.014 A
ATOM  19395  NE1 TRP B 619     -10.044   9.478  57.351  1.00  9.94    -0.365 N
ATOM  19396  HE1 TRP B 619     -10.231  10.137  56.595  1.00  0.00     0.165 HD
ATOM  19397  CZ2 TRP B 619     -10.559  10.960  59.313  1.00 11.00     0.030 A
ATOM  19399  CZ3 TRP B 619     -10.259   9.752  61.421  1.00 12.98     0.001 A
ATOM  19401  CH2 TRP B 619     -10.563  10.942  60.698  1.00 12.89     0.002 A
ATOM  19403  N   TYR B 620      -6.056   4.410  59.508  1.00  9.65    -0.346 N
ATOM  19404  HN  TYR B 620      -5.619   4.582  58.602  1.00  0.00     0.163 HD
ATOM  19405  CA  TYR B 620      -5.541   3.352  60.377  1.00  9.05     0.180 C
ATOM  19407  C   TYR B 620      -4.985   3.928  61.681  1.00 10.40     0.241 C
ATOM  19408  O   TYR B 620      -4.991   3.251  62.697  1.00  9.14    -0.271 OA
ATOM  19409  CB  TYR B 620      -4.407   2.549  59.743  1.00  9.43     0.073 C
ATOM  19412  CG  TYR B 620      -4.942   1.671  58.615  1.00 13.24    -0.056 A
ATOM  19413  CD1 TYR B 620      -5.581   0.489  58.886  1.00 13.17     0.010 A
ATOM  19415  CD2 TYR B 620      -4.727   2.054  57.286  1.00  9.02     0.010 A
ATOM  19417  CE1 TYR B 620      -6.066  -0.313  57.848  1.00 19.19     0.037 A
ATOM  19419  CE2 TYR B 620      -5.219   1.256  56.267  1.00 15.53     0.037 A
ATOM  19421  CZ  TYR B 620      -5.852   0.079  56.545  1.00 22.77     0.065 A
ATOM  19422  OH  TYR B 620      -6.330  -0.699  55.509  1.00 23.56    -0.361 OA
ATOM  19423  HH  TYR B 620      -6.771  -1.518  55.702  1.00  0.00     0.217 HD
ATOM  19424  N   LYS B 621      -4.608   5.199  61.724  1.00  7.38    -0.346 N
ATOM  19425  HN  LYS B 621      -4.615   5.752  60.867  1.00  0.00     0.163 HD
ATOM  19426  CA  LYS B 621      -4.183   5.824  62.976  1.00  8.72     0.176 C
ATOM  19428  C   LYS B 621      -5.253   5.749  64.057  1.00 11.58     0.241 C
ATOM  19429  O   LYS B 621      -4.918   5.645  65.257  1.00 10.01    -0.271 OA
ATOM  19430  CB  LYS B 621      -3.932   7.308  62.666  1.00  9.85     0.035 C
ATOM  19433  CG  LYS B 621      -3.568   8.059  63.952  1.00 11.27     0.004 C
ATOM  19436  CD  LYS B 621      -3.075   9.479  63.509  1.00 13.52     0.027 C
ATOM  19439  CE  LYS B 621      -2.773  10.222  64.829  1.00 17.49     0.229 C
ATOM  19442  NZ  LYS B 621      -2.381  11.619  64.659  1.00 26.11    -0.079 N
ATOM  19443  HZ1 LYS B 621      -2.182  12.110  65.531  1.00  0.00     0.274 HD
ATOM  19444  HZ2 LYS B 621      -3.085  12.123  64.120  1.00  0.00     0.274 HD
ATOM  19445  HZ3 LYS B 621      -1.588  11.691  64.021  1.00  0.00     0.274 HD
ATOM  19446  N   TYR B 622      -6.538   5.821  63.731  1.00  8.68    -0.346 N
ATOM  19447  HN  TYR B 622      -6.777   5.885  62.741  1.00  0.00     0.163 HD
ATOM  19448  CA  TYR B 622      -7.625   5.815  64.694  1.00  9.56     0.180 C
ATOM  19450  C   TYR B 622      -8.434   4.511  64.634  1.00 11.81     0.241 C
ATOM  19451  O   TYR B 622      -9.177   4.317  65.610  1.00 14.63    -0.271 OA
ATOM  19452  CB  TYR B 622      -8.620   7.004  64.488  1.00  7.76     0.073 C
ATOM  19455  CG  TYR B 622      -7.871   8.304  64.731  1.00 12.24    -0.056 A
ATOM  19456  CD1 TYR B 622      -7.579   8.744  66.012  1.00  9.53     0.010 A
ATOM  19458  CD2 TYR B 622      -7.442   9.067  63.660  1.00 12.52     0.010 A
ATOM  19460  CE1 TYR B 622      -6.858   9.909  66.216  1.00  8.70     0.037 A
ATOM  19462  CE2 TYR B 622      -6.751  10.254  63.851  1.00 10.13     0.037 A
ATOM  19464  CZ  TYR B 622      -6.482  10.672  65.145  1.00 13.36     0.065 A
ATOM  19465  OH  TYR B 622      -5.792  11.856  65.325  1.00 13.68    -0.361 OA
ATOM  19466  HH  TYR B 622      -5.608  12.142  66.212  1.00  0.00     0.217 HD
ATOM  19467  N   VAL B 623      -8.368   3.679  63.595  1.00 10.16    -0.346 N
ATOM  19468  HN  VAL B 623      -7.750   3.866  62.805  1.00  0.00     0.163 HD
ATOM  19469  CA  VAL B 623      -9.226   2.472  63.631  1.00 11.59     0.180 C
ATOM  19471  C   VAL B 623      -8.419   1.196  63.814  1.00 13.49     0.241 C
ATOM  19472  O   VAL B 623      -9.013   0.159  64.143  1.00 17.60    -0.271 OA
ATOM  19473  CB  VAL B 623     -10.168   2.287  62.424  1.00 14.40     0.009 C
ATOM  19475  CG1 VAL B 623     -10.929   3.592  62.113  1.00 14.55     0.012 C
ATOM  19479  CG2 VAL B 623      -9.397   1.942  61.163  1.00 15.29     0.012 C
ATOM  19483  N   GLY B 624      -7.130   1.228  63.616  1.00 14.08    -0.351 N
ATOM  19484  HN  GLY B 624      -6.724   2.100  63.278  1.00  0.00     0.163 HD
ATOM  19485  CA  GLY B 624      -6.232   0.107  63.843  1.00 12.01     0.225 C
ATOM  19488  C   GLY B 624      -6.391  -0.958  62.757  1.00 17.52     0.236 C
ATOM  19489  O   GLY B 624      -6.976  -0.700  61.716  1.00 15.04    -0.272 OA
ATOM  19490  N   LEU B 625      -5.842  -2.157  63.011  1.00 14.43    -0.346 N
ATOM  19491  HN  LEU B 625      -5.367  -2.328  63.897  1.00  0.00     0.163 HD
ATOM  19492  CA  LEU B 625      -5.930  -3.208  62.013  1.00 17.38     0.177 C
ATOM  19494  C   LEU B 625      -7.210  -4.008  62.118  1.00 19.34     0.241 C
ATOM  19495  O   LEU B 625      -7.456  -4.834  61.236  1.00 23.56    -0.271 OA
ATOM  19496  CB  LEU B 625      -4.726  -4.165  62.171  1.00 15.93     0.038 C
ATOM  19499  CG  LEU B 625      -3.359  -3.476  62.020  1.00 23.89    -0.020 C
ATOM  19501  CD1 LEU B 625      -2.251  -4.410  62.456  1.00 24.81     0.009 C
ATOM  19505  CD2 LEU B 625      -3.195  -3.056  60.558  1.00 30.23     0.009 C
ATOM  19509  N   ASN B 626      -8.019  -3.835  63.132  1.00 14.78    -0.346 N
ATOM  19510  HN  ASN B 626      -7.800  -3.126  63.832  1.00  0.00     0.163 HD
ATOM  19511  CA  ASN B 626      -9.232  -4.639  63.281  1.00 20.37     0.185 C
ATOM  19513  C   ASN B 626     -10.469  -3.799  62.997  1.00 23.90     0.241 C
ATOM  19514  O   ASN B 626     -11.545  -4.227  63.426  1.00 25.59    -0.271 OA
ATOM  19515  CB  ASN B 626      -9.318  -5.254  64.694  1.00 25.89     0.137 C
ATOM  19518  CG  ASN B 626      -8.110  -6.139  64.970  1.00 33.05     0.217 C
ATOM  19519  ND2 ASN B 626      -7.286  -5.734  65.920  1.00 42.22    -0.370 N
ATOM  19520 1HD2 ASN B 626      -7.439  -4.896  66.481  1.00  0.00     0.159 HD
ATOM  19521 2HD2 ASN B 626      -6.477  -6.327  66.105  1.00  0.00     0.159 HD
ATOM  19522  OD1 ASN B 626      -7.926  -7.150  64.294  1.00 41.40    -0.274 OA
ATOM  19523  N   GLY B 627     -10.305  -2.617  62.388  1.00 20.79    -0.351 N
ATOM  19524  HN  GLY B 627      -9.380  -2.293  62.105  1.00  0.00     0.163 HD
ATOM  19525  CA  GLY B 627     -11.506  -1.802  62.142  1.00 18.49     0.225 C
ATOM  19528  C   GLY B 627     -11.873  -1.856  60.669  1.00 23.21     0.236 C
ATOM  19529  O   GLY B 627     -11.385  -2.744  59.966  1.00 19.89    -0.272 OA
ATOM  19530  N   ALA B 628     -12.673  -0.888  60.216  1.00 14.65    -0.347 N
ATOM  19531  HN  ALA B 628     -13.048  -0.186  60.854  1.00  0.00     0.163 HD
ATOM  19532  CA  ALA B 628     -13.006  -0.848  58.781  1.00 15.30     0.172 C
ATOM  19534  C   ALA B 628     -12.980   0.618  58.351  1.00 16.29     0.240 C
ATOM  19535  O   ALA B 628     -13.197   1.501  59.206  1.00 11.80    -0.271 OA
ATOM  19536  CB  ALA B 628     -14.441  -1.343  58.610  1.00 14.84     0.042 C
ATOM  19540  N   ILE B 629     -12.736   0.907  57.081  1.00 10.96    -0.346 N
ATOM  19541  HN  ILE B 629     -12.605   0.156  56.404  1.00  0.00     0.163 HD
ATOM  19542  CA  ILE B 629     -12.655   2.294  56.652  1.00  9.70     0.180 C
ATOM  19544  C   ILE B 629     -13.488   2.446  55.386  1.00 14.73     0.241 C
ATOM  19545  O   ILE B 629     -13.288   1.633  54.490  1.00 12.20    -0.271 OA
ATOM  19546  CB  ILE B 629     -11.209   2.721  56.287  1.00 14.23     0.013 C
ATOM  19548  CG1 ILE B 629     -10.271   2.537  57.485  1.00 12.55     0.002 C
ATOM  19551  CG2 ILE B 629     -11.216   4.180  55.777  1.00 11.04     0.012 C
ATOM  19555  CD1 ILE B 629      -8.789   2.489  57.222  1.00 12.96     0.005 C
ATOM  19559  N   VAL B 630     -14.446   3.336  55.400  1.00 11.44    -0.346 N
ATOM  19560  HN  VAL B 630     -14.657   3.812  56.277  1.00  0.00     0.163 HD
ATOM  19561  CA  VAL B 630     -15.228   3.678  54.211  1.00  6.78     0.180 C
ATOM  19563  C   VAL B 630     -14.623   4.996  53.661  1.00 12.06     0.241 C
ATOM  19564  O   VAL B 630     -14.923   6.070  54.128  1.00 11.53    -0.271 OA
ATOM  19565  CB  VAL B 630     -16.709   3.864  54.516  1.00 14.66     0.009 C
ATOM  19567  CG1 VAL B 630     -17.488   4.185  53.248  1.00 14.17     0.012 C
ATOM  19571  CG2 VAL B 630     -17.207   2.534  55.090  1.00 16.47     0.012 C
ATOM  19575  N   GLY B 631     -13.694   4.815  52.739  1.00 10.55    -0.351 N
ATOM  19576  HN  GLY B 631     -13.480   3.876  52.404  1.00  0.00     0.163 HD
ATOM  19577  CA  GLY B 631     -12.960   5.991  52.192  1.00 11.83     0.225 C
ATOM  19580  C   GLY B 631     -12.704   5.782  50.705  1.00 13.86     0.236 C
ATOM  19581  O   GLY B 631     -13.301   4.875  50.127  1.00 13.86    -0.272 OA
ATOM  19582  N   MET B 632     -11.879   6.638  50.102  1.00 13.58    -0.346 N
ATOM  19583  HN  MET B 632     -11.449   7.383  50.650  1.00  0.00     0.163 HD
ATOM  19584  CA  MET B 632     -11.573   6.537  48.669  1.00 13.39     0.177 C
ATOM  19586  C   MET B 632     -10.250   5.809  48.509  1.00 12.52     0.241 C
ATOM  19587  O   MET B 632      -9.335   5.921  49.345  1.00 14.65    -0.271 OA
ATOM  19588  CB  MET B 632     -11.406   7.951  48.077  1.00 11.33     0.045 C
ATOM  19591  CG  MET B 632     -12.659   8.836  47.973  1.00 15.84     0.076 C
ATOM  19594  SD  MET B 632     -13.702   8.177  46.659  1.00 21.78    -0.173 SA
ATOM  19595  CE  MET B 632     -12.778   8.701  45.190  1.00 19.22     0.089 C
ATOM  19599  N   THR B 633     -10.060   5.001  47.460  1.00  7.22    -0.344 N
ATOM  19600  HN  THR B 633     -10.822   4.847  46.800  1.00  0.00     0.163 HD
ATOM  19601  CA  THR B 633      -8.794   4.345  47.249  1.00  8.17     0.205 C
ATOM  19603  C   THR B 633      -8.282   4.656  45.847  1.00 12.56     0.243 C
ATOM  19604  O   THR B 633      -7.259   4.119  45.396  1.00 13.97    -0.271 OA
ATOM  19605  CB  THR B 633      -8.894   2.801  47.418  1.00 14.37     0.146 C
ATOM  19607  CG2 THR B 633      -9.161   2.393  48.877  1.00 21.26     0.042 C
ATOM  19611  OG1 THR B 633      -9.974   2.311  46.626  1.00 16.56    -0.393 OA
ATOM  19612  HG1 THR B 633     -10.035   1.369  46.729  1.00  0.00     0.210 HD
ATOM  19613  N   THR B 634      -9.018   5.463  45.087  1.00 12.66    -0.344 N
ATOM  19614  HN  THR B 634      -9.834   5.905  45.510  1.00  0.00     0.163 HD
ATOM  19615  CA  THR B 634      -8.735   5.752  43.702  1.00 12.69     0.205 C
ATOM  19617  C   THR B 634      -9.004   7.232  43.433  1.00 10.71     0.243 C
ATOM  19618  O   THR B 634      -9.466   7.994  44.279  1.00 12.08    -0.271 OA
ATOM  19619  CB  THR B 634      -9.693   4.969  42.742  1.00 15.51     0.146 C
ATOM  19621  CG2 THR B 634      -9.815   3.479  42.998  1.00 22.96     0.042 C
ATOM  19625  OG1 THR B 634     -11.058   5.435  42.988  1.00 18.92    -0.393 OA
ATOM  19626  HG1 THR B 634     -10.982   6.368  42.828  1.00  0.00     0.210 HD
ATOM  19627  N   PHE B 635      -8.696   7.652  42.198  1.00 10.28    -0.346 N
ATOM  19628  HN  PHE B 635      -8.230   7.023  41.544  1.00  0.00     0.163 HD
ATOM  19629  CA  PHE B 635      -9.036   9.035  41.788  1.00 11.08     0.180 C
ATOM  19631  C   PHE B 635     -10.551   9.065  41.568  1.00 13.68     0.241 C
ATOM  19632  O   PHE B 635     -11.205   8.011  41.454  1.00 11.77    -0.271 OA
ATOM  19633  CB  PHE B 635      -8.299   9.366  40.453  1.00 11.40     0.073 C
ATOM  19636  CG  PHE B 635      -6.807   9.522  40.637  1.00 11.01    -0.056 A
ATOM  19637  CD1 PHE B 635      -6.276  10.575  41.321  1.00 15.65     0.007 A
ATOM  19639  CD2 PHE B 635      -5.941   8.594  40.031  1.00  8.84     0.007 A
ATOM  19641  CE1 PHE B 635      -4.913  10.746  41.499  1.00 16.43     0.001 A
ATOM  19643  CE2 PHE B 635      -4.574   8.769  40.188  1.00 12.62     0.001 A
ATOM  19645  CZ  PHE B 635      -4.062   9.818  40.890  1.00 12.37     0.000 A
ATOM  19647  N   GLY B 636     -11.107  10.263  41.442  1.00 11.39    -0.351 N
ATOM  19648  HN  GLY B 636     -10.525  11.099  41.504  1.00  0.00     0.163 HD
ATOM  19649  CA  GLY B 636     -12.525  10.396  41.218  1.00 10.50     0.225 C
ATOM  19652  C   GLY B 636     -12.931  10.271  39.754  1.00 12.17     0.236 C
ATOM  19653  O   GLY B 636     -12.219   9.698  38.912  1.00 13.06    -0.272 OA
ATOM  19654  N   GLU B 637     -14.113  10.780  39.434  1.00 13.79    -0.346 N
ATOM  19655  HN  GLU B 637     -14.620  11.293  40.155  1.00  0.00     0.163 HD
ATOM  19656  CA  GLU B 637     -14.736  10.658  38.126  1.00 13.01     0.177 C
ATOM  19658  C   GLU B 637     -15.624  11.871  37.891  1.00 13.79     0.241 C
ATOM  19659  O   GLU B 637     -16.195  12.460  38.808  1.00 11.62    -0.271 OA
ATOM  19660  CB  GLU B 637     -15.702   9.471  37.991  1.00 18.97     0.045 C
ATOM  19663  CG  GLU B 637     -15.092   8.086  38.007  1.00 25.57     0.116 C
ATOM  19666  CD  GLU B 637     -14.251   7.790  36.783  1.00 45.66     0.172 C
ATOM  19667  OE1 GLU B 637     -14.528   8.368  35.700  1.00 40.70    -0.648 OA
ATOM  19668  OE2 GLU B 637     -13.287   6.991  36.886  1.00 47.79    -0.648 OA
ATOM  19669  N   SER B 638     -15.807  12.217  36.610  1.00 11.97    -0.344 N
ATOM  19670  HN  SER B 638     -15.334  11.711  35.861  1.00  0.00     0.163 HD
ATOM  19671  CA  SER B 638     -16.698  13.334  36.307  1.00 11.44     0.200 C
ATOM  19673  C   SER B 638     -18.171  12.875  36.230  1.00 13.39     0.243 C
ATOM  19674  O   SER B 638     -18.597  12.191  35.290  1.00 16.36    -0.271 OA
ATOM  19675  CB  SER B 638     -16.233  13.851  34.922  1.00 12.14     0.199 C
ATOM  19678  OG  SER B 638     -17.033  14.949  34.549  1.00 15.05    -0.398 OA
ATOM  19679  HG  SER B 638     -16.748  15.266  33.700  1.00  0.00     0.209 HD
ATOM  19680  N   ALA B 639     -19.019  13.330  37.140  1.00 11.40    -0.346 N
ATOM  19681  HN  ALA B 639     -18.639  13.927  37.875  1.00  0.00     0.163 HD
ATOM  19682  CA  ALA B 639     -20.445  13.051  37.180  1.00 11.98     0.172 C
ATOM  19684  C   ALA B 639     -21.093  13.875  38.267  1.00 16.16     0.243 C
ATOM  19685  O   ALA B 639     -20.374  14.419  39.094  1.00 14.17    -0.271 OA
ATOM  19686  CB  ALA B 639     -20.682  11.554  37.491  1.00 17.18     0.042 C
ATOM  19690  N   PRO B 640     -22.405  13.943  38.326  1.00 16.32    -0.337 N
ATOM  19691  CA  PRO B 640     -23.125  14.659  39.365  1.00 15.75     0.179 C
ATOM  19693  C   PRO B 640     -22.740  14.008  40.692  1.00 12.40     0.241 C
ATOM  19694  O   PRO B 640     -22.575  12.784  40.821  1.00 13.89    -0.271 OA
ATOM  19695  CB  PRO B 640     -24.589  14.433  39.015  1.00 20.18     0.037 C
ATOM  19698  CG  PRO B 640     -24.583  14.209  37.526  1.00 21.05     0.022 C
ATOM  19701  CD  PRO B 640     -23.331  13.385  37.280  1.00 22.54     0.127 C
ATOM  19704  N   ALA B 641     -22.612  14.835  41.706  1.00 16.71    -0.346 N
ATOM  19705  HN  ALA B 641     -22.866  15.815  41.580  1.00  0.00     0.163 HD
ATOM  19706  CA  ALA B 641     -22.117  14.394  43.006  1.00 15.91     0.172 C
ATOM  19708  C   ALA B 641     -22.902  13.241  43.588  1.00 16.51     0.240 C
ATOM  19709  O   ALA B 641     -22.360  12.293  44.170  1.00 17.36    -0.271 OA
ATOM  19710  CB  ALA B 641     -22.179  15.592  43.965  1.00 16.95     0.042 C
ATOM  19714  N   GLU B 642     -24.227  13.288  43.499  1.00 14.97    -0.346 N
ATOM  19715  HN  GLU B 642     -24.681  14.056  43.004  1.00  0.00     0.163 HD
ATOM  19716  CA  GLU B 642     -25.039  12.220  44.122  1.00 23.20     0.177 C
ATOM  19718  C   GLU B 642     -24.699  10.868  43.539  1.00 20.79     0.241 C
ATOM  19719  O   GLU B 642     -24.656   9.873  44.280  1.00 20.53    -0.271 OA
ATOM  19720  CB  GLU B 642     -26.549  12.484  44.022  1.00 34.06     0.045 C
ATOM  19723  CG  GLU B 642     -26.844  13.207  42.714  1.00 67.23     0.116 C
ATOM  19726  CD  GLU B 642     -28.232  13.000  42.149  1.00 85.60     0.172 C
ATOM  19727  OE1 GLU B 642     -29.183  12.794  42.937  1.00 92.45    -0.648 OA
ATOM  19728  OE2 GLU B 642     -28.355  13.061  40.899  1.00 92.40    -0.648 OA
ATOM  19729  N   LEU B 643     -24.466  10.772  42.230  1.00 16.50    -0.346 N
ATOM  19730  HN  LEU B 643     -24.563  11.600  41.642  1.00  0.00     0.163 HD
ATOM  19731  CA  LEU B 643     -24.079   9.520  41.629  1.00 14.41     0.177 C
ATOM  19733  C   LEU B 643     -22.700   9.048  42.063  1.00 13.36     0.241 C
ATOM  19734  O   LEU B 643     -22.447   7.845  42.121  1.00 14.38    -0.271 OA
ATOM  19735  CB  LEU B 643     -24.082   9.624  40.088  1.00 25.47     0.038 C
ATOM  19738  CG  LEU B 643     -25.385  10.114  39.462  1.00 38.42    -0.020 C
ATOM  19740  CD1 LEU B 643     -25.361   9.943  37.941  1.00 32.28     0.009 C
ATOM  19744  CD2 LEU B 643     -26.619   9.417  40.011  1.00 36.43     0.009 C
ATOM  19748  N   LEU B 644     -21.780  10.002  42.293  1.00 10.95    -0.346 N
ATOM  19749  HN  LEU B 644     -22.018  10.987  42.175  1.00  0.00     0.163 HD
ATOM  19750  CA  LEU B 644     -20.428   9.611  42.716  1.00 14.20     0.177 C
ATOM  19752  C   LEU B 644     -20.423   9.052  44.128  1.00 12.82     0.241 C
ATOM  19753  O   LEU B 644     -19.726   8.065  44.385  1.00 14.14    -0.271 OA
ATOM  19754  CB  LEU B 644     -19.503  10.846  42.684  1.00 15.78     0.038 C
ATOM  19757  CG  LEU B 644     -19.263  11.420  41.280  1.00 18.06    -0.020 C
ATOM  19759  CD1 LEU B 644     -18.481  12.722  41.388  1.00 14.99     0.009 C
ATOM  19763  CD2 LEU B 644     -18.498  10.377  40.445  1.00 15.13     0.009 C
ATOM  19767  N   PHE B 645     -21.213   9.674  45.020  1.00 14.47    -0.346 N
ATOM  19768  HN  PHE B 645     -21.770  10.489  44.763  1.00  0.00     0.163 HD
ATOM  19769  CA  PHE B 645     -21.237   9.119  46.395  1.00 14.34     0.180 C
ATOM  19771  C   PHE B 645     -21.770   7.692  46.321  1.00 18.08     0.241 C
ATOM  19772  O   PHE B 645     -21.248   6.779  46.952  1.00 20.29    -0.271 OA
ATOM  19773  CB  PHE B 645     -22.105   9.962  47.368  1.00 17.71     0.073 C
ATOM  19776  CG  PHE B 645     -21.431  11.245  47.808  1.00 17.67    -0.056 A
ATOM  19777  CD1 PHE B 645     -20.222  11.179  48.503  1.00 21.22     0.007 A
ATOM  19779  CD2 PHE B 645     -21.956  12.479  47.538  1.00 20.18     0.007 A
ATOM  19781  CE1 PHE B 645     -19.565  12.333  48.918  1.00 18.52     0.001 A
ATOM  19783  CE2 PHE B 645     -21.306  13.644  47.939  1.00 19.16     0.001 A
ATOM  19785  CZ  PHE B 645     -20.121  13.576  48.637  1.00 17.79     0.000 A
ATOM  19787  N   GLU B 646     -22.774   7.416  45.457  1.00 17.55    -0.346 N
ATOM  19788  HN  GLU B 646     -23.201   8.157  44.901  1.00  0.00     0.163 HD
ATOM  19789  CA  GLU B 646     -23.232   6.041  45.338  1.00 19.64     0.177 C
ATOM  19791  C   GLU B 646     -22.181   5.140  44.745  1.00 19.92     0.241 C
ATOM  19792  O   GLU B 646     -21.930   4.028  45.228  1.00 19.11    -0.271 OA
ATOM  19793  CB  GLU B 646     -24.482   5.884  44.471  1.00 23.76     0.045 C
ATOM  19796  CG  GLU B 646     -25.647   6.756  44.894  1.00 39.43     0.116 C
ATOM  19799  CD  GLU B 646     -26.805   6.541  43.903  1.00 58.93     0.172 C
ATOM  19800  OE1 GLU B 646     -27.049   5.365  43.527  1.00 56.74    -0.648 OA
ATOM  19801  OE2 GLU B 646     -27.436   7.549  43.518  1.00 58.58    -0.648 OA
ATOM  19802  N   GLU B 647     -21.543   5.555  43.647  1.00 19.12    -0.346 N
ATOM  19803  HN  GLU B 647     -21.778   6.468  43.258  1.00  0.00     0.163 HD
ATOM  19804  CA  GLU B 647     -20.526   4.753  42.986  1.00 20.97     0.177 C
ATOM  19806  C   GLU B 647     -19.357   4.369  43.889  1.00 20.63     0.241 C
ATOM  19807  O   GLU B 647     -18.797   3.286  43.791  1.00 17.05    -0.271 OA
ATOM  19808  CB  GLU B 647     -19.964   5.620  41.831  1.00 19.19     0.045 C
ATOM  19811  CG  GLU B 647     -18.915   4.960  40.975  1.00 35.89     0.116 C
ATOM  19814  CD  GLU B 647     -19.575   4.294  39.768  1.00 50.18     0.172 C
ATOM  19815  OE1 GLU B 647     -20.742   3.846  39.886  1.00 45.32    -0.648 OA
ATOM  19816  OE2 GLU B 647     -18.852   4.282  38.747  1.00 53.79    -0.648 OA
ATOM  19817  N   PHE B 648     -18.936   5.288  44.773  1.00 13.42    -0.346 N
ATOM  19818  HN  PHE B 648     -19.435   6.173  44.863  1.00  0.00     0.163 HD
ATOM  19819  CA  PHE B 648     -17.769   5.025  45.603  1.00 17.93     0.180 C
ATOM  19821  C   PHE B 648     -18.122   4.477  46.978  1.00 19.59     0.241 C
ATOM  19822  O   PHE B 648     -17.252   4.355  47.859  1.00 17.40    -0.271 OA
ATOM  19823  CB  PHE B 648     -16.938   6.318  45.663  1.00 16.15     0.073 C
ATOM  19826  CG  PHE B 648     -16.216   6.584  44.356  1.00 12.56    -0.056 A
ATOM  19827  CD1 PHE B 648     -15.246   5.707  43.913  1.00 15.19     0.007 A
ATOM  19829  CD2 PHE B 648     -16.493   7.712  43.610  1.00 18.56     0.007 A
ATOM  19831  CE1 PHE B 648     -14.556   5.949  42.730  1.00 20.87     0.001 A
ATOM  19833  CE2 PHE B 648     -15.840   7.950  42.426  1.00 14.62     0.001 A
ATOM  19835  CZ  PHE B 648     -14.872   7.061  41.973  1.00 15.24     0.000 A
ATOM  19837  N   GLY B 649     -19.372   4.091  47.213  1.00 18.66    -0.351 N
ATOM  19838  HN  GLY B 649     -20.103   4.282  46.527  1.00  0.00     0.163 HD
ATOM  19839  CA  GLY B 649     -19.699   3.391  48.459  1.00 17.57     0.225 C
ATOM  19842  C   GLY B 649     -20.073   4.304  49.605  1.00 14.14     0.236 C
ATOM  19843  O   GLY B 649     -20.206   3.805  50.746  1.00 17.69    -0.272 OA
ATOM  19844  N   PHE B 650     -20.394   5.575  49.363  1.00 12.95    -0.346 N
ATOM  19845  HN  PHE B 650     -20.366   5.941  48.411  1.00  0.00     0.163 HD
ATOM  19846  CA  PHE B 650     -20.789   6.445  50.482  1.00 10.42     0.180 C
ATOM  19848  C   PHE B 650     -22.310   6.410  50.586  1.00 13.43     0.241 C
ATOM  19849  O   PHE B 650     -23.008   7.352  50.212  1.00 15.21    -0.271 OA
ATOM  19850  CB  PHE B 650     -20.289   7.896  50.323  1.00 13.37     0.073 C
ATOM  19853  CG  PHE B 650     -18.776   7.869  50.385  1.00 16.98    -0.056 A
ATOM  19854  CD1 PHE B 650     -18.127   7.913  51.611  1.00 16.43     0.007 A
ATOM  19856  CD2 PHE B 650     -18.019   7.758  49.232  1.00 14.61     0.007 A
ATOM  19858  CE1 PHE B 650     -16.755   7.843  51.724  1.00 13.93     0.001 A
ATOM  19860  CE2 PHE B 650     -16.637   7.714  49.309  1.00 16.56     0.001 A
ATOM  19862  CZ  PHE B 650     -16.003   7.755  50.548  1.00 14.01     0.000 A
ATOM  19864  N   THR B 651     -22.850   5.268  50.998  1.00 19.58    -0.344 N
ATOM  19865  HN  THR B 651     -22.239   4.482  51.221  1.00  0.00     0.163 HD
ATOM  19866  CA  THR B 651     -24.294   5.109  51.140  1.00 18.42     0.205 C
ATOM  19868  C   THR B 651     -24.559   4.496  52.535  1.00 19.77     0.243 C
ATOM  19869  O   THR B 651     -23.682   3.818  53.033  1.00 14.32    -0.271 OA
ATOM  19870  CB  THR B 651     -24.916   4.130  50.130  1.00 16.25     0.146 C
ATOM  19872  CG2 THR B 651     -24.661   4.642  48.711  1.00 18.69     0.042 C
ATOM  19876  OG1 THR B 651     -24.287   2.859  50.324  1.00 24.61    -0.393 OA
ATOM  19877  HG1 THR B 651     -24.445   2.541  51.205  1.00  0.00     0.210 HD
ATOM  19878  N   VAL B 652     -25.774   4.695  53.038  1.00 17.34    -0.346 N
ATOM  19879  HN  VAL B 652     -26.467   5.230  52.514  1.00  0.00     0.163 HD
ATOM  19880  CA  VAL B 652     -26.109   4.139  54.353  1.00 17.86     0.180 C
ATOM  19882  C   VAL B 652     -25.981   2.637  54.358  1.00 18.62     0.241 C
ATOM  19883  O   VAL B 652     -25.420   2.063  55.292  1.00 18.11    -0.271 OA
ATOM  19884  CB  VAL B 652     -27.530   4.555  54.784  1.00 27.79     0.009 C
ATOM  19886  CG1 VAL B 652     -27.795   4.116  56.220  1.00 32.35     0.012 C
ATOM  19890  CG2 VAL B 652     -27.660   6.059  54.655  1.00 27.52     0.012 C
ATOM  19894  N   ASP B 653     -26.397   1.987  53.261  1.00 22.18    -0.345 N
ATOM  19895  HN  ASP B 653     -26.758   2.499  52.456  1.00  0.00     0.163 HD
ATOM  19896  CA  ASP B 653     -26.320   0.523  53.247  1.00 22.20     0.186 C
ATOM  19898  C   ASP B 653     -24.913  -0.008  53.310  1.00 21.26     0.241 C
ATOM  19899  O   ASP B 653     -24.679  -1.011  53.991  1.00 23.76    -0.271 OA
ATOM  19900  CB  ASP B 653     -27.035  -0.104  52.047  1.00 33.96     0.147 C
ATOM  19903  CG  ASP B 653     -28.536   0.126  52.124  1.00 39.91     0.175 C
ATOM  19904  OD1 ASP B 653     -29.061   0.323  53.237  1.00 44.77    -0.648 OA
ATOM  19905  OD2 ASP B 653     -29.168   0.142  51.046  1.00 58.37    -0.648 OA
ATOM  19906  N   ASN B 654     -23.973   0.601  52.585  1.00 19.24    -0.346 N
ATOM  19907  HN  ASN B 654     -24.210   1.413  52.016  1.00  0.00     0.163 HD
ATOM  19908  CA  ASN B 654     -22.611   0.101  52.611  1.00 14.01     0.185 C
ATOM  19910  C   ASN B 654     -21.980   0.403  53.972  1.00 14.10     0.241 C
ATOM  19911  O   ASN B 654     -21.184  -0.429  54.430  1.00 17.58    -0.271 OA
ATOM  19912  CB  ASN B 654     -21.778   0.746  51.478  1.00 21.15     0.137 C
ATOM  19915  CG  ASN B 654     -20.364   0.242  51.401  1.00 28.16     0.217 C
ATOM  19916  ND2 ASN B 654     -19.318   1.078  51.384  1.00 21.78    -0.370 N
ATOM  19917 1HD2 ASN B 654     -19.477   2.085  51.427  1.00  0.00     0.159 HD
ATOM  19918 2HD2 ASN B 654     -18.358   0.736  51.332  1.00  0.00     0.159 HD
ATOM  19919  OD1 ASN B 654     -20.172  -0.975  51.349  1.00 28.11    -0.274 OA
ATOM  19920  N   VAL B 655     -22.300   1.554  54.561  1.00 15.18    -0.346 N
ATOM  19921  HN  VAL B 655     -22.937   2.214  54.116  1.00  0.00     0.163 HD
ATOM  19922  CA  VAL B 655     -21.702   1.843  55.879  1.00 17.21     0.180 C
ATOM  19924  C   VAL B 655     -22.173   0.838  56.933  1.00 16.48     0.241 C
ATOM  19925  O   VAL B 655     -21.372   0.290  57.706  1.00 15.60    -0.271 OA
ATOM  19926  CB  VAL B 655     -21.971   3.295  56.283  1.00 14.82     0.009 C
ATOM  19928  CG1 VAL B 655     -21.509   3.642  57.688  1.00 14.97     0.012 C
ATOM  19932  CG2 VAL B 655     -21.174   4.185  55.307  1.00 11.12     0.012 C
ATOM  19936  N   VAL B 656     -23.477   0.578  56.959  1.00 20.17    -0.346 N
ATOM  19937  HN  VAL B 656     -24.102   1.063  56.315  1.00  0.00     0.163 HD
ATOM  19938  CA  VAL B 656     -24.029  -0.406  57.912  1.00 16.02     0.180 C
ATOM  19940  C   VAL B 656     -23.427  -1.776  57.694  1.00 17.96     0.241 C
ATOM  19941  O   VAL B 656     -23.041  -2.503  58.592  1.00 20.03    -0.271 OA
ATOM  19942  CB  VAL B 656     -25.565  -0.468  57.682  1.00 21.06     0.009 C
ATOM  19944  CG1 VAL B 656     -26.155  -1.702  58.353  1.00 24.79     0.012 C
ATOM  19948  CG2 VAL B 656     -26.156   0.828  58.198  1.00 15.38     0.012 C
ATOM  19952  N   ALA B 657     -23.335  -2.200  56.425  1.00 20.61    -0.346 N
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ATOM  19953  HN  ALA B 657     -23.657  -1.586  55.677  1.00  0.00      0.163 HD
ATOM  19954  CA  ALA B 657     -22.789  -3.513  56.076  1.00 22.39      0.172 C
ATOM  19956  C   ALA B 657     -21.362  -3.692  56.539  1.00 21.74      0.240 C
ATOM  19957  O   ALA B 657     -20.986  -4.688  57.181  1.00 20.89     -0.271 OA
ATOM  19958  CB  ALA B 657     -22.892  -3.717  54.559  1.00 27.87      0.042 C
ATOM  19962  N   LYS B 658     -20.506  -2.688  56.302  1.00 21.36     -0.346 N
ATOM  19963  HN  LYS B 658     -20.805  -1.884  55.751  1.00  0.00      0.163 HD
ATOM  19964  CA  LYS B 658     -19.149  -2.743  56.830  1.00 16.66      0.176 C
ATOM  19966  C   LYS B 658     -19.129  -2.819  58.358  1.00 16.93      0.241 C
ATOM  19967  O   LYS B 658     -18.272  -3.484  58.926  1.00 18.74     -0.271 OA
ATOM  19968  CB  LYS B 658     -18.397  -1.440  56.529  1.00 22.21      0.035 C
ATOM  19971  CG  LYS B 658     -17.583  -1.284  55.303  1.00 32.54      0.004 C
ATOM  19974  CD  LYS B 658     -17.312  -2.489  54.459  1.00 36.82      0.027 C
ATOM  19977  CE  LYS B 658     -18.082  -2.393  53.151  1.00 50.03      0.229 C
ATOM  19980  NZ  LYS B 658     -17.393  -3.154  52.075  1.00 57.14     -0.079 N
ATOM  19981  HZ1 LYS B 658     -17.909  -3.090  51.198  1.00  0.00      0.274 HD
ATOM  19982  HZ2 LYS B 658     -17.228  -4.124  52.345  1.00  0.00      0.274 HD
ATOM  19983  HZ3 LYS B 658     -16.423  -2.857  51.965  1.00  0.00      0.274 HD
ATOM  19984  N   ALA B 659     -19.980  -2.046  59.040  1.00 15.19     -0.346 N
ATOM  19985  HN  ALA B 659     -20.615  -1.430  58.533  1.00  0.00      0.163 HD
ATOM  19986  CA  ALA B 659     -20.013  -2.071  60.492  1.00 19.10      0.172 C
ATOM  19988  C   ALA B 659     -20.416  -3.467  61.014  1.00 22.57      0.240 C
ATOM  19989  O   ALA B 659     -19.841  -4.048  61.940  1.00 20.85     -0.271 OA
ATOM  19990  CB  ALA B 659     -21.047  -1.062  61.025  1.00 19.39      0.042 C
ATOM  19994  N   LYS B 660     -21.449  -4.023  60.381  1.00 21.45     -0.346 N
ATOM  19995  HN  LYS B 660     -21.913  -3.509  59.632  1.00  0.00      0.163 HD
ATOM  19996  CA  LYS B 660     -21.933  -5.365  60.742  1.00 26.24      0.176 C
ATOM  19998  C   LYS B 660     -20.903  -6.465  60.591  1.00 27.01      0.241 C
ATOM  19999  O   LYS B 660     -20.903  -7.439  61.360  1.00 26.97     -0.271 OA
ATOM  20000  CB  LYS B 660     -23.180  -5.732  59.946  1.00 25.27      0.035 C
ATOM  20003  CG  LYS B 660     -24.464  -5.146  60.521  1.00 34.80      0.004 C
ATOM  20006  CD  LYS B 660     -25.612  -5.475  59.565  1.00 42.36      0.027 C
ATOM  20009  CE  LYS B 660     -26.953  -5.509  60.274  1.00 42.35      0.229 C
ATOM  20012  NZ  LYS B 660     -28.076  -5.609  59.286  1.00 54.92     -0.079 N
ATOM  20013  HZ1 LYS B 660     -28.977  -5.632  59.763  1.00  0.00      0.274 HD
ATOM  20014  HZ2 LYS B 660     -27.959  -6.407  58.662  1.00  0.00      0.274 HD
ATOM  20015  HZ3 LYS B 660     -28.035  -4.863  58.592  1.00  0.00      0.274 HD
ATOM  20016  N   GLU B 661     -19.955  -6.360  59.678  1.00 26.91     -0.346 N
ATOM  20017  HN  GLU B 661     -19.972  -5.556  59.051  1.00  0.00      0.163 HD
ATOM  20018  CA  GLU B 661     -18.884  -7.338  59.523  1.00 26.27      0.177 C
ATOM  20020  C   GLU B 661     -17.974  -7.371  60.737  1.00 29.08      0.241 C
ATOM  20021  O   GLU B 661     -17.232  -8.344  60.962  1.00 30.19     -0.271 OA
ATOM  20022  CB  GLU B 661     -18.105  -7.074  58.243  1.00 33.00      0.045 C
ATOM  20025  CG  GLU B 661     -18.798  -7.423  56.937  1.00 46.16      0.116 C
ATOM  20028  CD  GLU B 661     -18.157  -6.746  55.734  1.00 57.89      0.172 C
ATOM  20029  OE1 GLU B 661     -16.954  -6.406  55.820  1.00 51.49     -0.648 OA
ATOM  20030  OE2 GLU B 661     -18.831  -6.538  54.696  1.00 60.71     -0.648 OA
ATOM  20031  N   LEU B 662     -17.957  -6.343  61.592  1.00 19.78     -0.346 N
ATOM  20032  HN  LEU B 662     -18.561  -5.542  61.406  1.00  0.00      0.163 HD
ATOM  20033  CA  LEU B 662     -17.122  -6.320  62.764  1.00 21.60      0.177 C
ATOM  20035  C   LEU B 662     -17.847  -6.901  63.987  1.00 28.52      0.241 C
ATOM  20036  O   LEU B 662     -17.242  -7.021  65.054  1.00 31.15     -0.271 OA
ATOM  20037  CB  LEU B 662     -16.726  -4.859  63.096  1.00 20.33      0.038 C
ATOM  20040  CG  LEU B 662     -16.026  -4.105  61.937  1.00 18.64     -0.020 C
ATOM  20042  CD1 LEU B 662     -15.685  -2.666  62.328  1.00 16.83      0.009 C
ATOM  20046  CD2 LEU B 662     -14.758  -4.813  61.507  1.00 22.60      0.009 C
ATOM  20050  N   LEU B 663     -19.153  -7.075  63.882  1.00 30.45     -0.345 N
ATOM  20051  HN  LEU B 663     -19.604  -6.909  62.982  1.00  0.00      0.163 HD
ATOM  20052  CA  LEU B 663     -19.967  -7.497  65.015  1.00 33.60      0.186 C
ATOM  20054  C   LEU B 663     -20.122  -9.017  65.120  1.00 40.57      0.196 C
ATOM  20055  O   LEU B 663     -20.203  -9.431  66.299  1.00 47.25     -0.646 OA
ATOM  20056  CB  LEU B 663     -21.338  -6.842  64.947  1.00 27.35      0.040 C
ATOM  20059  CG  LEU B 663     -21.392  -5.310  65.031  1.00 40.25     -0.020 C
ATOM  20061  CD1 LEU B 663     -22.825  -4.831  64.874  1.00 40.03      0.009 C
ATOM  20065  CD2 LEU B 663     -20.797  -4.842  66.354  1.00 38.68      0.009 C
ATOM  20069  OXT LEU B 663     -19.647  -9.796  64.263  1.00 40.12     -0.646 OA
ATOM      4  H1' TPP A 670      -5.600  27.610  40.336  1.00  0.00      0.166 HD
ATOM     15  H3' TPP A 670      -6.093  24.915  37.319  1.00  0.00      0.168 HD
ATOM     20 1H4' TPP A 670      -9.487  25.521  36.862  1.00  0.00      0.157 HD
ATOM     21 2H4' TPP A 670      -8.083  24.575  36.312  1.00  0.00      0.157 HD
TER      22      TPP A 670
HETATM    1  CM2 TPP A 670      -4.284  25.837  38.892  1.00 12.30      0.089 C
HETATM    2  CM4 TPP A 670      -9.185  30.397  38.331  1.00 13.51      0.069 C
HETATM    3  N1' TPP A 670      -6.215  27.154  39.661  1.00 11.68     -0.355 N
HETATM    5  S1  TPP A 670     -10.712  28.618  35.038  1.00 30.38     -0.087 SA
HETATM    6  C2  TPP A 670     -10.608  27.569  36.364  1.00 26.93      0.141 A
HETATM    7  N3  TPP A 670     -10.107  28.153  37.465  1.00 14.24     -0.349 N
HETATM    8  C4  TPP A 670      -9.768  29.477  37.318  1.00 11.95      0.021 A
HETATM    9  C5  TPP A 670     -10.041  29.900  36.035  1.00 24.73      0.008 A
HETATM   10  C6  TPP A 670      -9.745  31.317  35.653  1.00 26.35      0.075 C
HETATM   11  C7  TPP A 670     -10.442  31.600  34.338  1.00 31.82      0.186 C
HETATM   12  O7  TPP A 670      -9.507  32.396  33.647  1.00 31.26     -0.289 OA
HETATM   13  C2' TPP A 670      -5.727  26.214  38.824  1.00 16.98      0.078 A
HETATM   14  N3' TPP A 670      -6.486  25.622  37.940  1.00 10.00     -0.332 N
HETATM   16  O1A TPP A 670      -8.853  33.580  31.697  1.00 16.83     -0.624 OA
HETATM   17  O1B TPP A 670     -12.764  32.684  31.687  1.00 21.70     -0.616 OA
HETATM   18  C4' TPP A 670      -7.833  25.960  37.850  1.00 13.02      0.109 A
HETATM   19  N4' TPP A 670      -8.500  25.273  36.928  1.00 11.07     -0.385 N
HETATM   22  O2A TPP A 670      -8.105  31.185  31.990  1.00 26.35     -0.624 OA
HETATM   23  O2B TPP A 670     -11.189  33.334  29.876  1.00 14.28     -0.616 OA
HETATM   24  C5' TPP A 670      -8.419  26.941  38.715  1.00 13.90      0.019 A
HETATM   25  O3A TPP A 670     -10.518  31.603  31.476  1.00 18.42     -0.173 OA
HETATM   26  O3B TPP A 670     -12.271  31.028  29.842  1.00 18.52     -0.616 OA
HETATM   27  C6' TPP A 670      -7.550  27.494  39.598  1.00 12.25      0.102 A
HETATM   28  C7' TPP A 670      -9.885  27.369  38.723  1.00 13.72      0.172 C
HETATM   29  PA  TPP A 670      -9.198  32.182  32.091  1.00 19.03      0.418 P
HETATM   30  PB  TPP A 670     -11.770  32.192  30.618  1.00 18.84      0.431 P
ATOM     34  H1' TPP B 670      14.558  24.087  43.661  1.00  0.00      0.166 HD
ATOM     45  H3' TPP B 670      15.022  26.390  47.008  1.00  0.00      0.168 HD
ATOM     50 1H4' TPP B 670      18.336  25.661  47.594  1.00  0.00      0.157 HD
ATOM     51 2H4' TPP B 670      16.948  26.552  48.201  1.00  0.00      0.157 HD
TER      52      TPP B 670
HETATM   31  CM2 TPP B 670      13.263  25.676  45.343  1.00 12.39      0.089 C
HETATM   32  CM4 TPP B 670      19.449  24.862  42.708  1.00 16.57      0.069 C
HETATM   33  N1' TPP B 670      15.159  24.422  44.414  1.00 11.86     -0.355 N
HETATM   35  S1  TPP B 670      20.992  27.390  45.462  1.00 30.40     -0.087 SA
HETATM   36  C2  TPP B 670      20.126  26.072  46.130  1.00 37.83      0.141 A
HETATM   37  N3  TPP B 670      19.619  25.216  45.225  1.00 15.93     -0.349 N
HETATM   38  C4  TPP B 670      19.904  25.620  43.919  1.00 15.83      0.021 A
HETATM   39  C5  TPP B 670      20.631  26.767  43.911  1.00 23.52      0.008 A
HETATM   40  C6  TPP B 670      21.049  27.380  42.601  1.00 29.24      0.075 C
HETATM   41  C7  TPP B 670      22.155  28.390  42.779  1.00 37.00      0.186 C
HETATM   42  O7  TPP B 670      21.759  29.438  41.934  1.00 26.78     -0.289 OA
HETATM   43  C2' TPP B 670      14.693  25.261  45.362  1.00 17.34      0.078 A
HETATM   44  N3' TPP B 670      15.431  25.740  46.336  1.00 10.49     -0.332 N
HETATM   46  O1A TPP B 670      22.099  31.530  40.915  1.00 13.93     -0.624 OA
HETATM   47  O1B TPP B 670      25.165  30.190  42.941  1.00 19.65     -0.616 OA
HETATM   48  C4' TPP B 670      16.745  25.376  46.459  1.00 12.70      0.109 A
HETATM   49  N4' TPP B 670      17.357  25.932  47.502  1.00  9.64     -0.385 N
HETATM   52  O2A TPP B 670      20.458  31.401  42.855  1.00 25.34     -0.624 OA
HETATM   53  O2B TPP B 670      24.714  32.540  42.249  1.00 12.95     -0.616 OA
HETATM   54  C5' TPP B 670      17.318  24.508  45.479  1.00 12.05      0.019 A
HETATM   55  O3A TPP B 670      22.884  31.215  43.312  1.00 18.45     -0.173 OA
HETATM   56  O3B TPP B 670      24.810  31.986  44.671  1.00 16.68     -0.616 OA
HETATM   57  C6' TPP B 670      16.490  24.032  44.503  1.00 13.53      0.102 A
HETATM   58  C7' TPP B 670      18.782  24.055  45.557  1.00 12.87      0.172 C
HETATM   59  PA  TPP B 670      21.727  30.991  42.244  1.00 21.10      0.418 P
HETATM   60  PB  TPP B 670      24.453  31.508  43.301  1.00 18.88      0.431 P
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