Appendix

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Table 1. Crystal data and structure refinement.

Identification code	**2007src1588 (Motherwell – LJ)**	
Empirical formula	$C_{17}H_{21}NO_4$	
Formula weight	303.35	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$C222_1$	
Unit cell dimensions	a = 7.4019(2) Å	α = 90°
	b = 15.8155(3) Å	β = 90°
	c = 26.8034(4) Å	γ = 90°
Volume	3137.73(11) Å^3	
Z	8	
Density (calculated)	1.284 Mg / m^3	
Absorption coefficient	0.091 mm^{-1}	
$F(000)$	1296	
Crystal	Block; colourless	
Crystal size	0.40 × 0.35 × 0.20 mm^3	
θ range for data collection	2.99 – 27.50°	
Index ranges	$-9 \le h \le 9$, $-20 \le k \le 20$, $-34 \le l \le 34$	
Reflections collected	28149	
Independent reflections	3609 [R_{int} = 0.0493]	
Completeness to θ = 27.50°	99.2 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.9820 and 0.9644	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3609 / 0 / 201	
Goodness-of-fit on F^2	1.039	
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.0339, $wR2$ = 0.0763	
R indices (all data)	$R1$ = 0.0375, $wR2$ = 0.0784	
Absolute structure parameter	–0.2(7)	
Largest diff. peak and hole	0.146 and –0.153 e Å^{-3}	

Diffractometer: *Nonius KappaCCD* area detector (ϕ scans and ω scans to fill *asymmetric unit* sphere). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography*, part A, pp. 307–326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: *SADABS Version 2.10.* (G. M. Sheldrick (2003)) Bruker AXS Inc., Madison, Wisconsin, USA. S**tructure solution**: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467–473). S**tructure refinement**: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** *PLATON* (A.L. Spek, J. Appl. Crystallogr. 2003, 36, 7).

Special details:

C3 = S, C7 = R, C9 = R

Table 2. Atomic coordinates [$\times 10^4$], equivalent isotropic displacement parameters [$Å^2 \times 10^3$] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

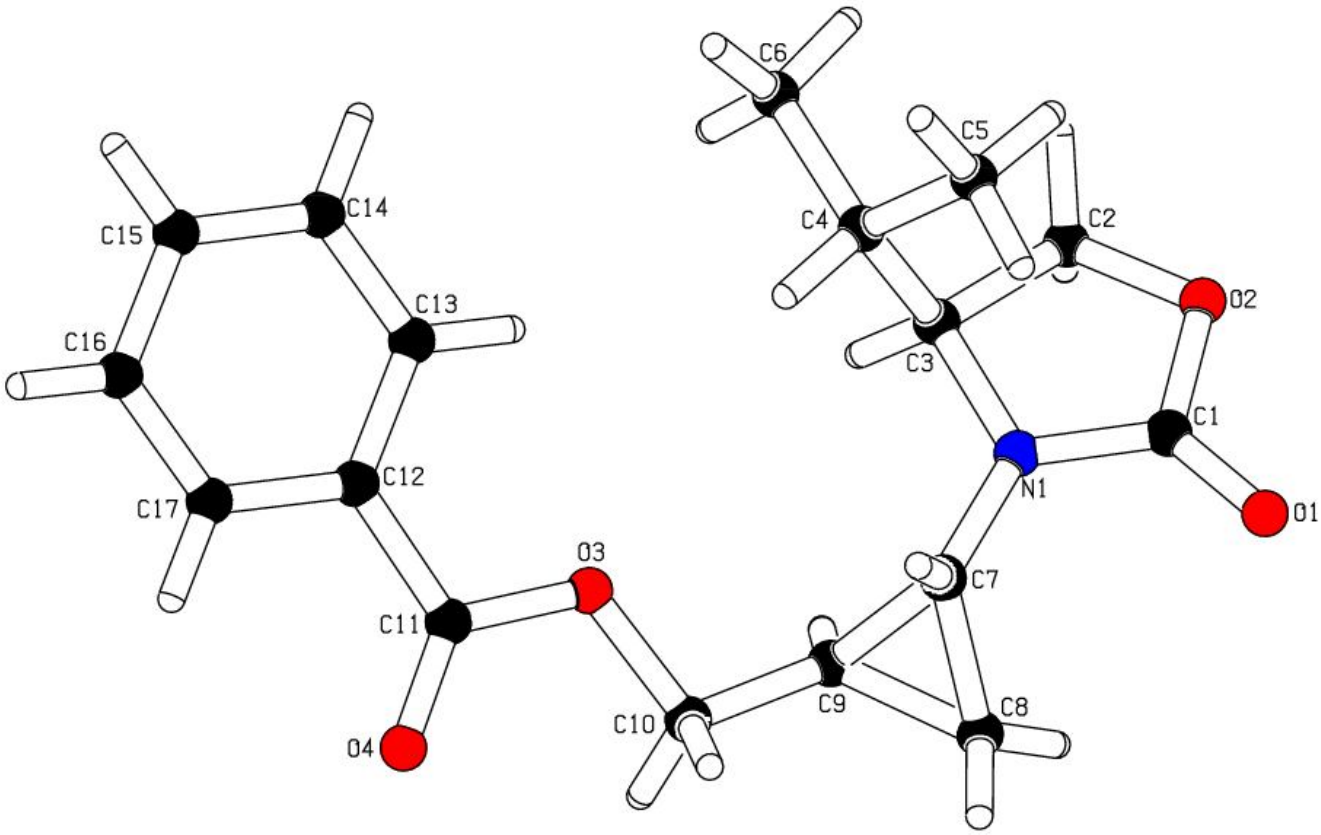
Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
C1	681(2)	3000(1)	24(1)	24(1)	1
C2	–787(2)	4089(1)	412(1)	28(1)	1
C3	224(2)	3592(1)	815(1)	20(1)	1
C4	1851(2)	4046(1)	1051(1)	21(1)	1
C5	3255(2)	4312(1)	663(1)	29(1)	1
C6	1222(2)	4802(1)	1364(1)	33(1)	1
C7	1542(2)	2112(1)	737(1)	20(1)	1
C8	756(2)	1269(1)	606(1)	26(1)	1
C9	416(2)	1644(1)	1116(1)	22(1)	1
C10	1299(2)	1270(1)	1566(1)	28(1)	1
C11	2312(2)	1736(1)	2358(1)	28(1)	1
C12	2745(2)	2479(1)	2677(1)	22(1)	1
C13	2439(2)	3304(1)	2516(1)	23(1)	1
C14	2882(2)	3978(1)	2825(1)	28(1)	1
C15	3620(2)	3821(1)	3293(1)	30(1)	1
C16	3917(2)	3001(1)	3456(1)	27(1)	1
C17	3483(2)	2326(1)	3148(1)	25(1)	1
N1	745(2)	2851(1)	522(1)	20(1)	1
O1	1191(1)	2552(1)	–315(1)	33(1)	1
O2	–88(1)	3774(1)	–59(1)	29(1)	1
O3	1699(1)	1960(1)	1905(1)	25(1)	1
O4	2486(2)	1013(1)	2487(1)	58(1)	1

Table 3. Bond lengths [Å] and angles [°].

C1–O1	1.2120(16)
C1–N1	1.3548(16)
C1–O2	1.3675(16)
C2–O2	1.4527(16)
C2–C3	1.5312(17)
C3–N1	1.4632(14)
C3–C4	1.5380(16)
C4–C5	1.5286(18)
C4–C6	1.5332(17)
C7–N1	1.4313(15)
C7–C8	1.4969(16)
C7–C9	1.5074(16)
C8–C9	1.5099(16)
C9–C10	1.4943(18)
C10–O3	1.4506(15)
C11–O4	1.2026(15)
C11–O3	1.3429(15)
C11–C12	1.4876(17)
C12–C13	1.3923(16)
C12–C17	1.3972(17)
C13–C14	1.3904(18)
C14–C15	1.3894(18)
C15–C16	1.387(2)
C16–C17	1.3874(19)
O1–C1–N1	128.68(13)
O1–C1–O2	122.05(12)
N1–C1–O2	109.28(11)
O2–C2–C3	105.24(10)
N1–C3–C2	99.23(9)
N1–C3–C4	112.86(10)
C2–C3–C4	115.61(10)
C5–C4–C6	111.36(11)
C5–C4–C3	112.43(10)
C6–C4–C3	110.56(11)
N1–C7–C8	118.17(10)
N1–C7–C9	116.45(10)
C8–C7–C9	60.34(8)
C7–C8–C9	60.18(8)
C10–C9–C7	119.71(12)
C10–C9–C8	120.16(11)
C7–C9–C8	59.48(8)
O3–C10–C9	107.32(10)
O4–C11–O3	123.20(13)
O4–C11–C12	124.22(12)
O3–C11–C12	112.57(10)
C13–C12–C17	120.43(12)
C13–C12–C11	121.74(11)
C17–C12–C11	117.83(11)
C14–C13–C12	119.67(12)
C15–C14–C13	119.60(13)
C16–C15–C14	120.94(13)
C15–C16–C17	119.67(12)
C16–C17–C12	119.69(12)
C1–N1–C7	123.68(10)
C1–N1–C3	112.39(10)
C7–N1–C3	123.00(9)
C1–O2–C2	108.30(9)
C11–O3–C10	115.87(10)

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	26(1)	23(1)	24(1)	–2(1)	–4(1)	–4(1)
C2	29(1)	25(1)	29(1)	–2(1)	–4(1)	3(1)
C3	23(1)	16(1)	23(1)	–1(1)	2(1)	1(1)
C4	28(1)	19(1)	18(1)	1(1)	–1(1)	–3(1)
C5	31(1)	30(1)	25(1)	4(1)	–2(1)	–10(1)
C6	43(1)	24(1)	32(1)	–9(1)	–2(1)	–1(1)
C7	21(1)	17(1)	22(1)	–1(1)	1(1)	–2(1)
C8	34(1)	19(1)	25(1)	–4(1)	2(1)	–4(1)
C9	24(1)	19(1)	23(1)	–1(1)	3(1)	–3(1)
C10	39(1)	18(1)	26(1)	–1(1)	–1(1)	–1(1)
C11	36(1)	22(1)	26(1)	4(1)	–2(1)	–1(1)
C12	21(1)	22(1)	21(1)	3(1)	3(1)	–1(1)
C13	25(1)	25(1)	21(1)	3(1)	2(1)	1(1)
C14	36(1)	22(1)	27(1)	2(1)	1(1)	1(1)
C15	31(1)	34(1)	24(1)	–4(1)	1(1)	–3(1)
C16	23(1)	38(1)	19(1)	2(1)	0(1)	–2(1)
C17	23(1)	28(1)	24(1)	7(1)	4(1)	0(1)
N1	26(1)	16(1)	19(1)	–2(1)	0(1)	–1(1)
O1	46(1)	34(1)	21(1)	–6(1)	–1(1)	1(1)
O2	36(1)	26(1)	24(1)	1(1)	–7(1)	1(1)
O3	34(1)	19(1)	22(1)	1(1)	–2(1)	–1(1)
O4	112(1)	20(1)	43(1)	7(1)	–30(1)	–1(1)


C6
C5
C4
C2
O2
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N1
O1
C7
C8
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O3
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C12
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