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3-Benzyl-5-methyl-1,2-benzoxazole 2-oxide

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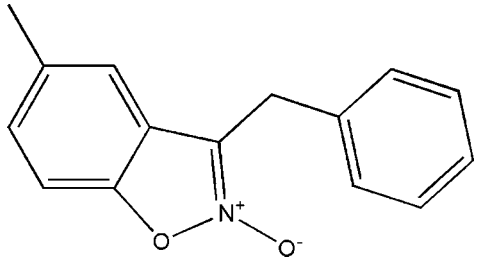
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.050; wR factor = 0.172; data-to-parameter ratio = 21.5.

In the title compound, $C_{15}H_{13}NO_2$, the isoxazole unit and the attached benzene ring are almost coplanar, making a dihedral angle of 1.42 (8)°. The benzyl ring is inclined to the isoxazole ring by 74.19 (8)° and is in a *+sc* conformation with respect to the benzisoxazole unit. In the crystal, C—H···O hydrogen bonds link the molecules, forming zigzag chains propagating along the *b* axis. There are also π–π interactions present involving the isoxazole and benzyl rings [centroid–centroid distance = 3.5209 (10) Å], and C—H···π interactions involving the benzene ring of the benzoisoxazole unit and the methylene bridging group.

Related literature

For the anti-epileptic, antispasmodic and antifungal properties of benzoxazole derivatives, see: Jian *et al.* (2007). For their antituberculer activity, see: Vinšová *et al.* (2007). For other biological activties of isoxazoles and benzisoxazole derivatives, see: Veera Reddy *et al.* (2011). For details of the synthesis, see: Veera Reddy *et al.* (2011). For the related structure 5-chloro-3-methyl-1,2-benzisoxazole-2-oxide, see: Ghari & Viterbo (1982).



Experimental

Crystal data

$C_{15}H_{13}NO_2$
M_r = 239.26
Monoclinic, $P2_1/n$
a = 6.4527 (2) Å
b = 11.2213 (4) Å
c = 16.9371 (7) Å
β = 100.002 (2)°
V = 1207.74 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.974, T_{max} = 0.983
13491 measured reflections
3512 independent reflections
2113 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.172
S = 1.06
3512 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*2 is the centroid of the C2–C7 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O2^{i}	0.93	2.49	3.154 (2)	128
C8—H8*B*···*Cg*2^{ii}	0.97	3.00	3.6800 (16)	129

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

The authors thank the Sophisticated Analytical Instrument Facility, IIT-Madras, Chennai-36, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2493).

References

Bruker (1999). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Ghari, G. & Viterbo, D. (1982). *Acta Cryst.* B**38**, 323–325.
Jian, F.-F., Yi, W., Wang, L.-M. & Wang, J. (2007). *Acta Cryst.* E**63**, o3887.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Veera Reddy, A., Laxminarasimhulu, G., Uday, B. R. S. & Pramod, K. (2011). *Indian J. Chem. Sect. B*, **50**, 119–125.
Vinšová, J., Marek, J., Vančo, J. & Csöllei, J. (2007). *Acta Cryst.* E**63**, o2802–o2803.

supplementary materials

Acta Cryst. (2012). E**68**, o2957 [doi:10.1107/S160053681203838X]

3-Benzyl-5-methyl-1,2-benzoxazole 2-oxide

G. Anuradha, Vasuki Gopalsamy, A. Veera Reddy and G. Laxminarasimhulu

Comment

Isoxazoles and benzisoxazoles are important classes of nitrogen-oxygen containing heterocycles. They have extensive biological applications and are useful intermediates in medicinal chemistry (Veera Reddy *et al.*, 2011). The benzoxazole skeleton is an essential structural unit of several antibacterial, anticancer and anti-HIV-1 agents. The antituberculotic activity of several benzoxazole derivatives have been reported (Vinšová *et al.*, 2007). Some benzoxazoles exhibit high fluorescence and are used as optical whitening agents, photoluminesents and active components in dye lasers. Benzoxazole derivatives show antiepileptic, antispasmodic and antifungal properties (Jian *et al.*, 2007). 3-substituted 1,2-benzisoxazole derivatives are emerging as potential antipsychotic compounds, antiseizure agents and are also used to block the repetitive firing of voltage-sensitive sodium channels and so reduce voltage-sensitive T-type calcium currents (Veera Reddy *et al.*, 2011).

The molecular structure of the title functionalized 1,2-benzisoxazole compound is illustrated in Fig. 1. It contains three planar rings, namely, a methyl substituted benzene ring A = C2—C7, an isoxazole ring B =C1/C7/C6/O1/N1 and the benzyl ring C = C9—C14. The dihedral angles between rings A/B and B/C are 1.42 (8)° and 74.19 (8)°, respectively.

The bond lengths and angles in the title compound are in good agreement with the expected values and are comparable with the corresponding values reported for 5-chloro-3-methyl-1,2-benzisoxazole-2-oxide (Ghari & Viterbo, 1982).

In the crystal, molecules are linked *via* C—H···O hydrogen bonds leading to the formation of zigzag chains propagating along the *a* axis direction (Tabel 1 and Fig. 2). Molecules are also linked *via* C—H···π (Table 1) and π···π interactions. The latter involve the isoxazole (B = *Cg*1) and benzyl rings (C = *Cg*3) [*Cg*1···*Cg*3^{i} = 3.5209 (10) Å; symmetry code: (i) -*x* + 1.5, *y* - 1/2, -*z* + 1/2].

Experimental

The compound was synthesized by the published method (Veera Reddy *et al.*, 2011)

Refinement

All the H atoms were positioned geometrically and treated as riding atoms: C—H = 0.93, 0.96 and 0.97 Å for CH, CH_3 and CH_2 H atoms, respectively, with U_{iso}(H) = k × U_{eq}(C), where k = 1.5 for CH_3 H atoms and = 1.2 for other H atoms.

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

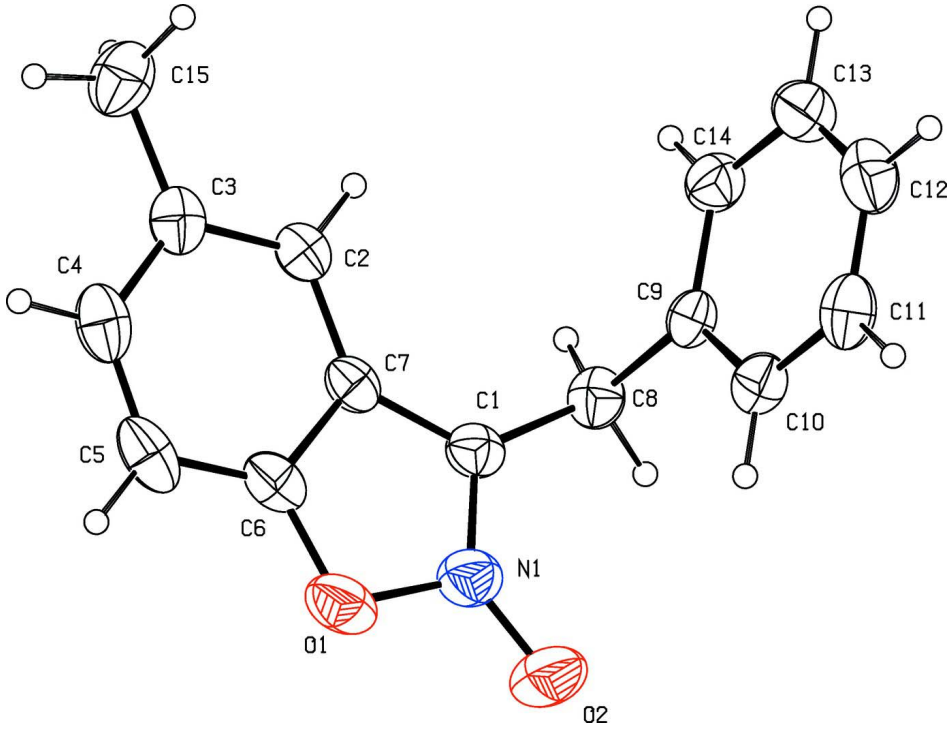


Figure 1

The molecular structure of the title molecule, with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

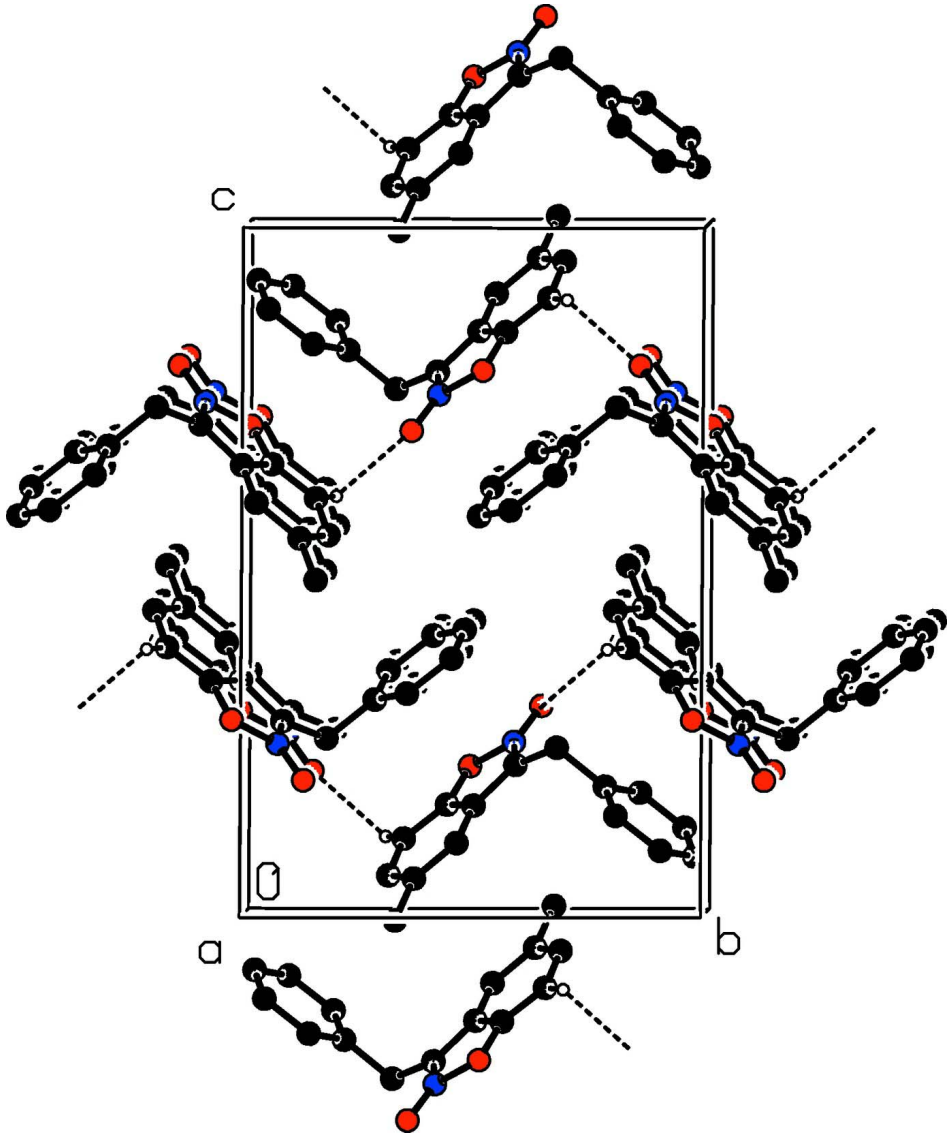


Figure 2

A view along the *a* axis of the crystal packing of the title compound. The intermolecular C—H···O hydrogen bonds are shown as dashed lines (see Table 1 for details; H atoms not involved in these interactions have been omitted for clarity).

3-Benzyl-5-methyl-1,2-benzoxazole 2-oxide

Crystal data

$C_{15}H_{13}NO_2$
$M_r = 239.26$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 6.4527$ (2) Å
$b = 11.2213$ (4) Å
$c = 16.9371$ (7) Å
$\beta = 100.002$ (2)°
$V = 1207.74$ (8) Å^3
$Z = 4$
$F(000) = 504$
$D_x = 1.316$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 13955 reflections
$\theta = 1.2$–$30.1°$
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.974, T_{max} = 0.983
13491 measured reflections
3512 independent reflections
2113 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 30.1°, θ_{min} = 2.2°
h = −9→8
k = −15→13
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.172
S = 1.06
3512 reflections
163 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0836P)^2 + 0.1125P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.28937 (17)	0.48425 (11)	0.21034 (8)	0.0760 (5)
O2	0.3491 (2)	0.63946 (12)	0.29866 (9)	0.0979 (6)
N1	0.4211 (2)	0.58198 (13)	0.24703 (9)	0.0682 (5)
C1	0.5941 (2)	0.58880 (13)	0.21630 (9)	0.0532 (5)
C2	0.7187 (2)	0.46425 (12)	0.10447 (8)	0.0508 (4)
C3	0.6602 (3)	0.37116 (13)	0.05213 (9)	0.0577 (5)
C4	0.4707 (3)	0.31228 (14)	0.05425 (11)	0.0688 (6)
C5	0.3391 (3)	0.34234 (15)	0.10596 (12)	0.0728 (6)
C6	0.3994 (2)	0.43709 (14)	0.15601 (10)	0.0590 (5)
C7	0.5868 (2)	0.49807 (12)	0.15712 (9)	0.0485 (4)
C8	0.7549 (2)	0.68132 (13)	0.24347 (9)	0.0574 (5)
C9	0.7396 (2)	0.78613 (12)	0.18692 (8)	0.0492 (4)
C10	0.5636 (2)	0.85898 (13)	0.17589 (9)	0.0578 (5)
C11	0.5506 (3)	0.95583 (15)	0.12500 (11)	0.0685 (6)
C12	0.7117 (3)	0.98059 (16)	0.08532 (11)	0.0753 (7)
C13	0.8872 (3)	0.90974 (17)	0.09595 (11)	0.0747 (7)
C14	0.9005 (2)	0.81256 (15)	0.14674 (10)	0.0615 (5)
C15	0.7953 (3)	0.33322 (18)	−0.00672 (11)	0.0800 (7)

H2	0.84520	0.50400	0.10450	0.0610*
H4	0.43230	0.24970	0.01870	0.0830*
H5	0.21500	0.30080	0.10730	0.0870*
H8A	0.89380	0.64610	0.24820	0.0690*
H8B	0.73800	0.70920	0.29620	0.0690*
H10	0.45330	0.84250	0.20300	0.0690*
H11	0.43170	1.00420	0.11780	0.0820*
H12	0.70270	1.04570	0.05090	0.0900*
H13	0.99740	0.92700	0.06900	0.0900*
H14	1.02000	0.76470	0.15370	0.0740*
H15A	0.72950	0.26790	−0.03810	0.1200*
H15B	0.93050	0.30870	0.02160	0.1200*
H15C	0.81250	0.39870	−0.04150	0.1200*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0529 (6)	0.0788 (8)	0.1006 (10)	−0.0032 (6)	0.0250 (6)	0.0178 (7)
O2	0.0986 (10)	0.0965 (10)	0.1127 (11)	0.0202 (8)	0.0581 (9)	−0.0021 (9)
N1	0.0641 (8)	0.0666 (9)	0.0788 (9)	0.0092 (7)	0.0262 (7)	0.0079 (7)
C1	0.0519 (8)	0.0538 (8)	0.0546 (8)	0.0049 (6)	0.0116 (6)	0.0101 (6)
C2	0.0481 (7)	0.0505 (8)	0.0512 (8)	−0.0029 (6)	0.0018 (6)	0.0074 (6)
C3	0.0650 (9)	0.0501 (8)	0.0521 (8)	0.0031 (7)	−0.0065 (7)	0.0055 (6)
C4	0.0748 (11)	0.0507 (9)	0.0710 (11)	−0.0063 (8)	−0.0148 (9)	0.0047 (8)
C5	0.0573 (9)	0.0597 (10)	0.0930 (13)	−0.0181 (8)	−0.0100 (9)	0.0202 (9)
C6	0.0467 (7)	0.0582 (9)	0.0708 (10)	−0.0024 (7)	0.0062 (7)	0.0187 (7)
C7	0.0439 (7)	0.0472 (7)	0.0524 (8)	−0.0022 (6)	0.0025 (6)	0.0115 (6)
C8	0.0628 (8)	0.0557 (8)	0.0516 (8)	0.0011 (7)	0.0040 (6)	−0.0009 (6)
C9	0.0541 (7)	0.0468 (7)	0.0451 (7)	−0.0011 (6)	0.0041 (6)	−0.0098 (6)
C10	0.0552 (8)	0.0563 (9)	0.0607 (9)	0.0023 (7)	0.0065 (7)	−0.0086 (7)
C11	0.0730 (10)	0.0533 (9)	0.0724 (11)	0.0085 (8)	−0.0059 (9)	−0.0047 (8)
C12	0.0993 (14)	0.0570 (10)	0.0650 (11)	−0.0094 (10)	0.0017 (10)	0.0035 (8)
C13	0.0853 (12)	0.0712 (11)	0.0713 (11)	−0.0149 (10)	0.0242 (9)	−0.0008 (9)
C14	0.0574 (8)	0.0609 (9)	0.0676 (10)	0.0022 (7)	0.0149 (7)	−0.0056 (7)
C15	0.0952 (13)	0.0782 (11)	0.0626 (11)	0.0089 (10)	0.0024 (9)	−0.0121 (9)

Geometric parameters (Å, º)

O1—N1	1.4587 (19)	C11—C12	1.361 (3)
O1—C6	1.363 (2)	C12—C13	1.370 (3)
O2—N1	1.240 (2)	C13—C14	1.382 (3)
N1—C1	1.3133 (19)	C2—H2	0.9300
C1—C7	1.424 (2)	C4—H4	0.9300
C1—C8	1.483 (2)	C5—H5	0.9300
C2—C3	1.380 (2)	C8—H8A	0.9700
C2—C7	1.3883 (19)	C8—H8B	0.9700
C3—C4	1.396 (3)	C10—H10	0.9300
C3—C15	1.496 (3)	C11—H11	0.9300
C4—C5	1.364 (3)	C12—H12	0.9300
C5—C6	1.373 (2)	C13—H13	0.9300

C6—C7	1.3867 (19)	C14—H14	0.9300
C8—C9	1.509 (2)	C15—H15A	0.9600
C9—C10	1.3854 (19)	C15—H15B	0.9600
C9—C14	1.3691 (19)	C15—H15C	0.9600
C10—C11	1.381 (2)		

N1—O1—C6	104.25 (11)	C3—C2—H2	120.00
O1—N1—O2	115.44 (12)	C7—C2—H2	120.00
O1—N1—C1	110.34 (13)	C3—C4—H4	118.00
O2—N1—C1	134.23 (15)	C5—C4—H4	118.00
N1—C1—C7	108.11 (13)	C4—C5—H5	122.00
N1—C1—C8	120.98 (13)	C6—C5—H5	122.00
C7—C1—C8	130.90 (12)	C1—C8—H8A	109.00
C3—C2—C7	119.33 (14)	C1—C8—H8B	109.00
C2—C3—C4	119.02 (15)	C9—C8—H8A	109.00
C2—C3—C15	121.18 (16)	C9—C8—H8B	109.00
C4—C3—C15	119.81 (15)	H8A—C8—H8B	108.00
C3—C4—C5	123.05 (16)	C9—C10—H10	120.00
C4—C5—C6	116.53 (16)	C11—C10—H10	120.00
O1—C6—C5	126.33 (14)	C10—C11—H11	120.00
O1—C6—C7	110.76 (13)	C12—C11—H11	120.00
C5—C6—C7	122.91 (15)	C11—C12—H12	120.00
C1—C7—C2	134.32 (13)	C13—C12—H12	120.00
C1—C7—C6	106.53 (12)	C12—C13—H13	120.00
C2—C7—C6	119.13 (13)	C14—C13—H13	120.00
C1—C8—C9	112.55 (12)	C9—C14—H14	120.00
C8—C9—C10	120.48 (12)	C13—C14—H14	120.00
C8—C9—C14	120.84 (12)	C3—C15—H15A	109.00
C10—C9—C14	118.67 (13)	C3—C15—H15B	109.00
C9—C10—C11	120.54 (14)	C3—C15—H15C	110.00
C10—C11—C12	120.02 (17)	H15A—C15—H15B	110.00
C11—C12—C13	120.11 (17)	H15A—C15—H15C	109.00
C12—C13—C14	120.02 (17)	H15B—C15—H15C	110.00
C9—C14—C13	120.65 (14)		

C6—O1—N1—O2	179.19 (14)	C2—C3—C4—C5	0.0 (3)
C6—O1—N1—C1	−0.63 (17)	C3—C4—C5—C6	1.5 (3)
N1—O1—C6—C5	−179.86 (16)	C4—C5—C6—C7	−2.1 (3)
N1—O1—C6—C7	0.19 (16)	C4—C5—C6—O1	177.92 (16)
O1—N1—C1—C7	0.80 (17)	O1—C6—C7—C1	0.26 (17)
O2—N1—C1—C8	0.1 (3)	O1—C6—C7—C2	−178.71 (13)
O2—N1—C1—C7	−178.98 (18)	C5—C6—C7—C1	−179.69 (16)
O1—N1—C1—C8	179.89 (12)	C5—C6—C7—C2	1.3 (2)
C8—C1—C7—C2	−0.9 (3)	C1—C8—C9—C10	65.02 (17)
C8—C1—C7—C6	−179.63 (15)	C1—C8—C9—C14	−116.26 (15)
N1—C1—C8—C9	−99.68 (17)	C8—C9—C10—C11	179.13 (14)
C7—C1—C8—C9	79.18 (19)	C14—C9—C10—C11	0.4 (2)
N1—C1—C7—C6	−0.66 (17)	C8—C9—C14—C13	−178.99 (15)
N1—C1—C7—C2	178.08 (16)	C10—C9—C14—C13	−0.2 (2)

C7—C2—C3—C15	178.79 (14)	C9—C10—C11—C12	−0.2 (3)
C7—C2—C3—C4	−0.8 (2)	C10—C11—C12—C13	−0.2 (3)
C3—C2—C7—C6	0.2 (2)	C11—C12—C13—C14	0.3 (3)
C3—C2—C7—C1	−178.40 (16)	C12—C13—C14—C9	−0.1 (3)
C15—C3—C4—C5	−179.66 (17)		

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C2–C7 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O2^{i}	0.93	2.49	3.154 (2)	128
C8—H8*B*···*Cg*2^{ii}	0.97	3.00	3.6800 (16)	129

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+1/2; (ii) −*x*+3/2, *y*+1/2, −*z*+1/2.