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3-(1-Naphthyl)-*N*-phenyloxirane-2-carboxamide

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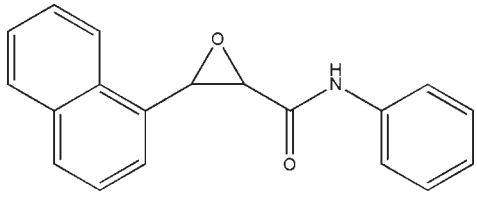
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.093; data-to-parameter ratio = 8.8.

In the title compound, $C_{19}H_{15}NO_2$, the molecule adopts a *syn* configuration with the naphthalene and *N*-phenylformamide units located on the same side of the epoxy ring. The epoxy ring makes dihedral angles of 58.73 (9) and 65.18 (9)°, respectively, with the naphthalene ring system and the benzene ring. Intermolecular N—H···O and C—H···O hydrogen bonding is present in the crystal structure.

Related literature

For background to the use of epoxide-containing compounds as building blocks in the synthesis of biologically active compounds, see: Porter & Skidmore (2000); Shing *et al.* (2006); Watanabe *et al.* (1998). For related structures, see: He (2009); He & Chen (2009); He *et al.* (2009).



Experimental

Crystal data

$C_{19}H_{15}NO_2$
M_r = 289.32
Orthorhombic, $P2_12_12_1$
a = 6.62890 (10) Å
b = 10.03500 (10) Å
c = 23.2033 (3) Å
V = 1543.51 (3) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.65 mm^{-1}
T = 290 K
0.40 × 0.36 × 0.30 mm

Data collection

Oxford Diffraction Gemini S Ultra diffractometer
Absorption correction: multi-scan (*CrysAlis Pro*; Oxford Diffraction, 2009)
T_{min} = 0.782, T_{max} = 0.829
13761 measured reflections
1783 independent reflections
1641 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.093
S = 1.08
1783 reflections
203 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.08 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H4···O2^{i}	0.84 (2)	2.17 (2)	2.954 (1)	155.7 (18)
C5—H5···O1^{ii}	0.93	2.58	3.431 (2)	153 (1)

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

Data collection: *CrysAlis Pro* (Oxford Diffraction, 2009); cell refinement: *CrysAlis Pro*; data reduction: *CrysAlis Pro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The diffraction data were collected at the Centre for Testing and Analysis, Sichuan University. We are grateful for financial support from China West Normal University (No 412374).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2678).

References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
He, L. (2009). *Acta Cryst.* E**65**, o2052.
He, L. & Chen, L.-M. (2009). *Acta Cryst.* E**65**, o2976.
He, L., Qin, H.-M. & Chen, L.-M. (2009). *Acta Cryst.* E**65**, o2999.
Oxford Diffraction (2009). *CrysAlis Pro*. Oxford Diffraction Ltd, Yarnton, England.
Porter, M. J. & Skidmore, J. (2000). *Chem. Commun.* pp. 1215–1225.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shing, T. K. M., Luk, T. & Lee, C. M. (2006). *Tetrahedron*, **62**, 6621–6629.
Watanabe, S., Arai, T., Sasai, H., Bougauchi, M. & Shibasaki, M. (1998). *J. Org. Chem.* **63**, 8090–8091.

supporting information

Acta Cryst. (2009). E**65**, o3137 [doi:10.1107/S1600536809048752]

3-(1-Naphthyl)-*N*-phenyloxirane-2-carboxamide

Lian-Mei Chen and Tai-Ran Kang

S1. Comment

α,*β*-Epoxides are very important building blocks for the synthesis of complex molecules, in particular, of biologically active compounds (Porter & Skidmore, 2000; Shing *et al.*, 2006; Watanabe *et al.*, 1998). Various effective systems have been developed over the years for the preparation of *α*,*β*-epoxides. The most common approach to access these molecules is the epoxidation of *α*,*β*-unsaturatd carbonyl compound. As a part of our interest in the synthsis of epoxides ring systems, we synthesis the title compound by using Darzens reaction. We report herein the crystal structure of the title compound.

The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles in (I) are normal. In the molecular, the 1-naphthyl ring with the phenyl ring adopts a *cis* configuration about the epoxides ring. The dihedral angle between the phenyl ring and the 1-naphthyl ring is 77.79 (4)°, O1/C8/C9 epoxide ring makes dihedral angles of 58.73 (9)° and 65.18 (9)° with the 1-naphthyl ring and phenyl ring, respectively. These values are very similar to those observed in related structures (He, 2009; He & Chen, 2009; He *et al.*, 2009). The crystal packing is stabilized by N—H···0 and C—H···0 hydrogen bonding (Table 1).

S2. Experimental

2-Chloro-*N*-phenylacetamide (0.085 g, 0.5 mmol) and potassium hydroxide (0.056 g, 1.0 mmol) were dissolved in chloroform (4 ml). To the solution was added 1-naphthaldehyde (0.094 g, 0.6 mmol) at 298 K, the solution was stirred for 6 h and removal of solvent under reduced pressure, the residue was purified through column chromatography. Colourless single crystals of (I) were obtained by recrystallization from an ethyl acetate solution.

S3. Refinement

Imine H atom was located in a difference Fourier map and refined isotropically, with restrains of N—H = 0.84±1 Å. The carbon-bound hydrogen atoms were placed in calculated positions with C—H = 0.93–0.98 Å, and refined using a riding model with U_{iso}(H) =1.2U_{eq}(C). In the absence of significant anomalous scattering effects, Friedel pairs were merged.

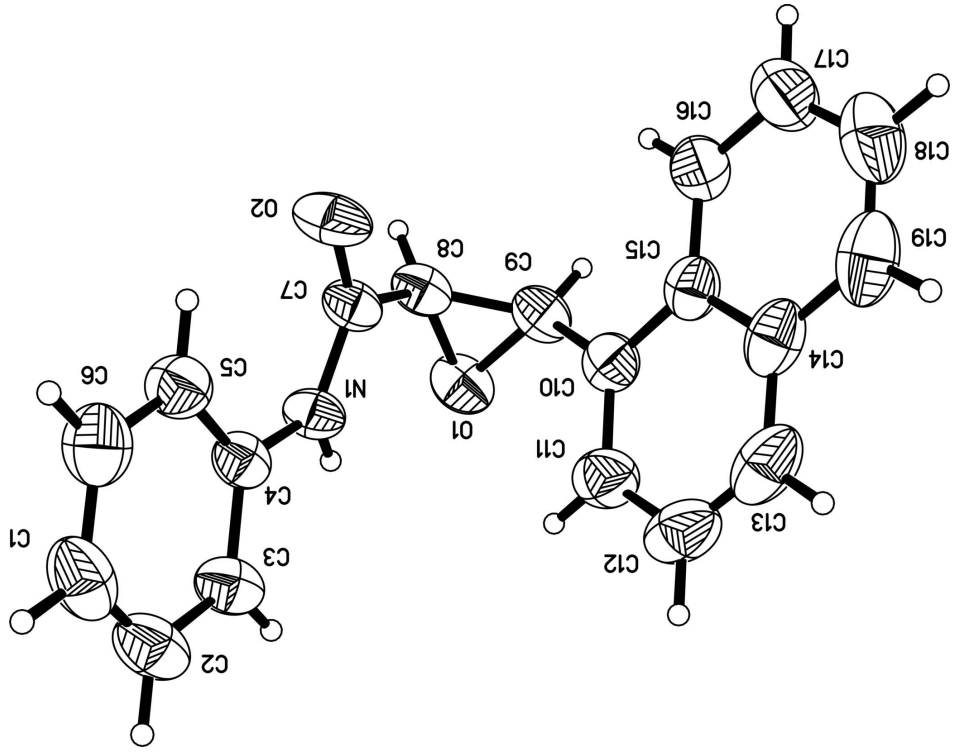


Figure 1

The molecular structure of (I) with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

3-(1-Naphthyl)-*N*-phenyloxirane-2-carboxamide

Crystal data

$C_{19}H_{15}NO_2$
$M_r = 289.32$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 6.6289$ (1) Å
$b = 10.0350$ (1) Å
$c = 23.2033$ (3) Å
$V = 1543.51$ (3) Å^3
$Z = 4$
$F(000) = 608$
$D_x = 1.245$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 9381 reflections
$\theta = 3.8$–$72.1°$
$\mu = 0.65$ mm^{-1}
$T = 290$ K
Block, colorless
0.40 × 0.36 × 0.30 mm

Data collection

Oxford Diffraction Gemini S Ultra diffractometer
Radiation source: Enhance Ultra (Cu) X-ray Source
Mirror monochromator
Detector resolution: 15.9149 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
$T_{min} = 0.782$, $T_{max} = 0.829$
13761 measured reflections
1783 independent reflections
1641 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 72.3°$, $\theta_{min} = 3.8°$
$h = -6 \rightarrow 8$
$k = -12 \rightarrow 12$
$l = -26 \rightarrow 28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.093$
$S = 1.08$
1783 reflections
203 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 0.0314P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.08$ e Å^{-3}
$\Delta\rho_{min} = -0.13$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.
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	1.20270 (19)	0.10810 (12)	0.82723 (5)	0.0681 (3)
O2	1.0096 (2)	0.38001 (11)	0.74225 (7)	0.0738 (4)
N1	0.8951 (2)	0.16688 (13)	0.74912 (6)	0.0534 (3)
H4	0.926 (3)	0.092 (2)	0.7622 (8)	0.065 (5)*
C1	0.3564 (3)	0.1625 (3)	0.65510 (8)	0.0820 (6)
H1	0.2376	0.1592	0.6339	0.098*
C2	0.4104 (3)	0.0578 (2)	0.68938 (9)	0.0750 (5)
H2	0.3275	−0.0168	0.6917	0.090*
C3	0.5874 (3)	0.06219 (17)	0.72067 (8)	0.0619 (4)
H3	0.6224	−0.0090	0.7443	0.074*
C4	0.7135 (2)	0.17226 (15)	0.71700 (6)	0.0521 (3)
C5	0.6590 (3)	0.27941 (19)	0.68282 (8)	0.0659 (4)
H5	0.7411	0.3543	0.6804	0.079*
C6	0.4786 (3)	0.2728 (2)	0.65216 (9)	0.0806 (6)
H6	0.4402	0.3445	0.6292	0.097*
C7	1.0258 (2)	0.26612 (14)	0.75961 (7)	0.0523 (3)
C8	1.2046 (2)	0.23071 (15)	0.79612 (7)	0.0558 (4)
H8	1.3359	0.2573	0.7805	0.067*
C9	1.1896 (2)	0.23005 (17)	0.85940 (8)	0.0597 (4)
H9	1.3135	0.2555	0.8797	0.072*
C10	0.9999 (3)	0.25565 (18)	0.89182 (7)	0.0588 (4)
C11	0.8539 (3)	0.1600 (2)	0.89662 (8)	0.0738 (5)
H11	0.8689	0.0791	0.8776	0.089*
C12	0.6808 (3)	0.1835 (3)	0.93030 (9)	0.0855 (7)

H12	0.5819	0.1181	0.9330	0.103*
C13	0.6567 (3)	0.2994 (3)	0.95855 (9)	0.0854 (7)
H13	0.5414	0.3127	0.9807	0.103*
C14	0.8028 (3)	0.4013 (2)	0.95534 (7)	0.0718 (5)
C15	0.9780 (3)	0.38002 (19)	0.92061 (7)	0.0587 (4)
C16	1.1212 (3)	0.4825 (2)	0.91701 (8)	0.0690 (4)
H16	1.2345	0.4710	0.8939	0.083*
C17	1.0979 (4)	0.5988 (3)	0.94673 (10)	0.0880 (6)
H17	1.1938	0.6659	0.9432	0.106*
C18	0.9322 (5)	0.6176 (3)	0.98222 (11)	0.1012 (8)
H18	0.9205	0.6956	1.0036	0.121*
C19	0.7874 (4)	0.5231 (3)	0.98595 (9)	0.0927 (7)
H19	0.6752	0.5383	1.0091	0.111*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0674 (7)	0.0523 (6)	0.0846 (7)	0.0119 (6)	−0.0146 (6)	−0.0057 (5)
O2	0.0694 (7)	0.0412 (6)	0.1109 (10)	−0.0041 (6)	−0.0195 (7)	0.0016 (6)
N1	0.0506 (7)	0.0396 (6)	0.0700 (7)	−0.0001 (5)	−0.0054 (6)	−0.0003 (6)
C1	0.0604 (10)	0.1084 (17)	0.0771 (11)	0.0011 (11)	−0.0134 (9)	−0.0229 (12)
C2	0.0523 (9)	0.0768 (12)	0.0960 (13)	−0.0071 (9)	0.0031 (9)	−0.0250 (11)
C3	0.0518 (8)	0.0524 (8)	0.0814 (10)	−0.0007 (7)	0.0049 (7)	−0.0099 (8)
C4	0.0486 (8)	0.0488 (7)	0.0590 (8)	0.0025 (7)	0.0020 (6)	−0.0085 (6)
C5	0.0660 (10)	0.0609 (9)	0.0707 (9)	−0.0014 (8)	−0.0075 (8)	0.0042 (8)
C6	0.0768 (12)	0.0928 (14)	0.0722 (11)	0.0095 (12)	−0.0161 (10)	0.0058 (10)
C7	0.0491 (8)	0.0411 (7)	0.0666 (8)	0.0019 (6)	−0.0003 (7)	−0.0092 (6)
C8	0.0455 (7)	0.0464 (7)	0.0754 (9)	0.0041 (7)	−0.0016 (7)	−0.0099 (7)
C9	0.0476 (8)	0.0591 (8)	0.0725 (9)	0.0031 (7)	−0.0106 (7)	−0.0094 (7)
C10	0.0505 (8)	0.0687 (9)	0.0571 (8)	0.0000 (8)	−0.0086 (7)	0.0031 (7)
C11	0.0653 (10)	0.0803 (12)	0.0757 (10)	−0.0129 (10)	−0.0124 (9)	0.0083 (10)
C12	0.0612 (11)	0.1093 (17)	0.0859 (13)	−0.0194 (13)	−0.0057 (10)	0.0263 (13)
C13	0.0564 (11)	0.131 (2)	0.0693 (10)	0.0054 (12)	0.0082 (9)	0.0238 (12)
C14	0.0595 (10)	0.1020 (14)	0.0539 (8)	0.0149 (11)	0.0018 (7)	0.0095 (9)
C15	0.0531 (8)	0.0723 (10)	0.0505 (7)	0.0054 (8)	−0.0034 (6)	0.0030 (7)
C16	0.0660 (10)	0.0751 (11)	0.0658 (9)	−0.0003 (9)	−0.0002 (8)	−0.0080 (9)
C17	0.0988 (16)	0.0799 (13)	0.0853 (12)	−0.0038 (13)	−0.0017 (12)	−0.0181 (11)
C18	0.120 (2)	0.1003 (17)	0.0831 (13)	0.0244 (18)	0.0033 (14)	−0.0278 (13)
C19	0.0897 (15)	0.1226 (19)	0.0658 (10)	0.0355 (16)	0.0118 (11)	−0.0050 (12)

Geometric parameters (Å, º)

O1—C8	1.4266 (19)	C9—C10	1.488 (2)
O1—C9	1.436 (2)	C9—H9	0.9800
O2—C7	1.217 (2)	C10—C11	1.367 (3)
N1—C7	1.342 (2)	C10—C15	1.423 (2)
N1—C4	1.417 (2)	C11—C12	1.408 (3)
N1—H4	0.84 (2)	C11—H11	0.9300

C1—C2	1.365 (3)	C12—C13	1.345 (4)
C1—C6	1.373 (3)	C12—H12	0.9300
C1—H1	0.9300	C13—C14	1.410 (3)
C2—C3	1.381 (3)	C13—H13	0.9300
C2—H2	0.9300	C14—C19	1.417 (4)
C3—C4	1.388 (2)	C14—C15	1.429 (2)
C3—H3	0.9300	C15—C16	1.402 (3)
C4—C5	1.384 (2)	C16—C17	1.364 (3)
C5—C6	1.393 (3)	C16—H16	0.9300
C5—H5	0.9300	C17—C18	1.386 (4)
C6—H6	0.9300	C17—H17	0.9300
C7—C8	1.499 (2)	C18—C19	1.352 (4)
C8—C9	1.472 (2)	C18—H18	0.9300
C8—H8	0.9800	C19—H19	0.9300

C8—O1—C9	61.87 (10)	O1—C9—H9	114.9
C7—N1—C4	127.99 (14)	C8—C9—H9	114.9
C7—N1—H4	116.1 (15)	C10—C9—H9	114.9
C4—N1—H4	115.8 (15)	C11—C10—C15	120.32 (16)
C2—C1—C6	119.65 (18)	C11—C10—C9	121.23 (17)
C2—C1—H1	120.2	C15—C10—C9	118.36 (15)
C6—C1—H1	120.2	C10—C11—C12	120.3 (2)
C1—C2—C3	120.29 (19)	C10—C11—H11	119.8
C1—C2—H2	119.9	C12—C11—H11	119.8
C3—C2—H2	119.9	C13—C12—C11	120.8 (2)
C2—C3—C4	120.33 (18)	C13—C12—H12	119.6
C2—C3—H3	119.8	C11—C12—H12	119.6
C4—C3—H3	119.8	C12—C13—C14	121.31 (19)
C5—C4—C3	119.75 (15)	C12—C13—H13	119.3
C5—C4—N1	123.56 (15)	C14—C13—H13	119.3
C3—C4—N1	116.68 (14)	C13—C14—C19	123.3 (2)
C4—C5—C6	118.67 (18)	C13—C14—C15	118.65 (19)
C4—C5—H5	120.7	C19—C14—C15	118.0 (2)
C6—C5—H5	120.7	C16—C15—C10	123.11 (16)
C1—C6—C5	121.3 (2)	C16—C15—C14	118.30 (18)
C1—C6—H6	119.4	C10—C15—C14	118.59 (17)
C5—C6—H6	119.4	C17—C16—C15	121.4 (2)
O2—C7—N1	125.45 (15)	C17—C16—H16	119.3
O2—C7—C8	118.66 (14)	C15—C16—H16	119.3
N1—C7—C8	115.89 (13)	C16—C17—C18	120.5 (2)
O1—C8—C9	59.38 (10)	C16—C17—H17	119.8
O1—C8—C7	118.91 (13)	C18—C17—H17	119.8
C9—C8—C7	120.76 (13)	C19—C18—C17	120.4 (2)
O1—C8—H8	115.4	C19—C18—H18	119.8
C9—C8—H8	115.4	C17—C18—H18	119.8
C7—C8—H8	115.4	C18—C19—C14	121.4 (2)
O1—C9—C8	58.75 (10)	C18—C19—H19	119.3
O1—C9—C10	117.46 (15)	C14—C19—H19	119.3

C8—C9—C10	124.10 (14)		
C6—C1—C2—C3	−0.4 (3)	O1—C9—C10—C15	−175.59 (13)
C1—C2—C3—C4	−0.8 (3)	C8—C9—C10—C15	−106.34 (18)
C2—C3—C4—C5	1.5 (2)	C15—C10—C11—C12	−0.3 (3)
C2—C3—C4—N1	−178.11 (15)	C9—C10—C11—C12	176.26 (16)
C7—N1—C4—C5	11.2 (2)	C10—C11—C12—C13	−0.5 (3)
C7—N1—C4—C3	−169.22 (16)	C11—C12—C13—C14	0.2 (3)
C3—C4—C5—C6	−0.9 (3)	C12—C13—C14—C19	−177.7 (2)
N1—C4—C5—C6	178.69 (16)	C12—C13—C14—C15	0.8 (3)
C2—C1—C6—C5	1.0 (3)	C11—C10—C15—C16	−179.42 (17)
C4—C5—C6—C1	−0.4 (3)	C9—C10—C15—C16	4.0 (2)
C4—N1—C7—O2	−0.7 (3)	C11—C10—C15—C14	1.2 (2)
C4—N1—C7—C8	179.01 (13)	C9—C10—C15—C14	−175.40 (14)
C9—O1—C8—C7	−110.62 (15)	C13—C14—C15—C16	179.15 (17)
O2—C7—C8—O1	165.96 (15)	C19—C14—C15—C16	−2.3 (2)
N1—C7—C8—O1	−13.7 (2)	C13—C14—C15—C10	−1.5 (2)
O2—C7—C8—C9	96.3 (2)	C19—C14—C15—C10	177.07 (16)
N1—C7—C8—C9	−83.36 (18)	C10—C15—C16—C17	−177.89 (18)
C8—O1—C9—C10	115.07 (16)	C14—C15—C16—C17	1.5 (3)
C7—C8—C9—O1	107.55 (15)	C15—C16—C17—C18	1.1 (4)
O1—C8—C9—C10	−103.91 (18)	C16—C17—C18—C19	−2.7 (4)
C7—C8—C9—C10	3.6 (2)	C17—C18—C19—C14	1.8 (4)
O1—C9—C10—C11	7.8 (2)	C13—C14—C19—C18	179.2 (2)
C8—C9—C10—C11	77.1 (2)	C15—C14—C19—C18	0.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H4···O2^{i}	0.84 (2)	2.17 (2)	2.954 (1)	155.7 (18)
C5—H5···O1^{ii}	0.93	2.58	3.431 (2)	153 (1)

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