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Synthesis and crystal structure of *tert*-butyl 1-(2-iodobenzoyl)cyclopent-3-ene-1-carboxylate

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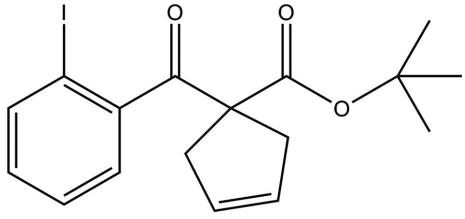
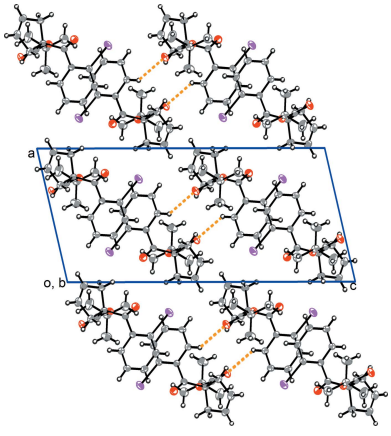
1-(2-Iodobenzoyl)-cyclopent-3-ene-1-carboxylates are novel substrates to construct bicyclo[3.2.1]octanes with antibacterial and antithrombotic activities. In this context, *tert*-butyl 1-(2-iodobenzoyl)-cyclopent-3-ene-1-carboxylate, $C_{17}H_{19}IO_3$, was synthesized and structurally characterized. The 2-iodobenzoyl group is attached to the tertiary C atom of the cyclopent-3-ene ring. The dihedral angle between the benzene ring and the mean plane of the envelope-type cyclopent-3-ene ring is 26.0 (3)°. In the crystal, pairs of C-H···O hydrogen bonds link the molecules to form inversion dimers.

1. Chemical context

1-(2-Iodobenzoyl)cyclopent-3-ene-1-carboxylates were recently employed as novel substrates to construct bicyclo[3.2.1]octanes that are widely found in natural products and bioactive molecules with antibacterial and antithrombotic activities (Yuan *et al.*, 2019). Although the authors carried out some control experiments to reveal the reaction mechanism, crystal structures of the substrates have not been reported yet. Moreover, 1-(2-iodobenzoyl)cyclopent-3-ene is crucial to the reductive Heck reaction and thus may provide more direct information on this reaction mechanism if more detailed structural data are available. Herein, the synthesis and crystal structure of *tert*-butyl 1-(2-iodobenzoyl)cyclopent-3-ene-1-carboxylate are reported.





2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The 2-iodobenzoyl group is attached to the tertiary C atom (C8) of the cyclopent-3-ene ring, with the *tert*-butyl carboxylate group as the other substituent. The five-membered C8–C12 ring adopts an envelope conformation, with atom C8 as the flap, and with puckering parameters (Cremer & Pople, 1975) Q = 0.1526 Å and φ = 0.5354°, and pseudo-rotation parameters (Rao *et al.*, 1981) P = 162.5 (1)° and τ(M) = 15.2 (3)°. The deviation of C8 from the mean plane defined by atoms C9–C12 is 0.097 (4) Å. The dihedral angle between the benzene ring and the alkene plane (C9–C12) of the cyclopent-3-ene ring is 26.51 (19)°.

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O3^{i}	0.93	2.48	3.219 (5)	136

Symmetry code: (i) $-x+1, -y+1, -z+1$.

3. Supramolecular features

In the crystal, molecules are linked by a pair of C—H···O hydrogen bonds forming inversion dimers (Table 1 and Fig. 2). They stack up the *b* axis and form layers parallel to the *bc* plane. There are no other significant intermolecular interactions present in the crystal.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.39, update of August 2018; Groom *et al.*, 2016) for entities containing (1-methylcyclopent-3-en-1-yl)(phenyl)methanone yielded 27 hits. Only two of these compounds involve no other substituents at the cyclopent-3-ene ring as in the title compound, *viz*. methyl 4-[(1-methylcyclopent-3-en-1-yl)carbonyl]benzoate in the space group *Pnma* (CSD refcode CIQHAM; Yang *et al.*, 2007), and 4-benzoyl-4-(methoxycarbonyl)cyclopentene in the space group $P2_1/c$, with four independent molecules in the asymmetric unit (CSD refcode KOGSIJ; Jiang *et al.*, 2008). In the structures of these two compounds, the folding angles of the cyclopent-3-ene ring are 17.00 (13) and 11.91 (12)°, respectively, while in the title compound it is 15.0 (3)°. The benzene ring in each structure is inclined to the alkene plane of the cyclopent-3-ene ring by 90.00 (8) and 61.40 (6)°, respectively, while the corresponding dihedral angle in the title compound is 26.51 (19)°. Apparently, different kinds of intermolecular C—H···O hydrogen bonds and the presence or not of weak π–π contacts in the three structures lead to different molecular packing and dihedral angles between the benzene ring and the cyclopent-3-ene ring.

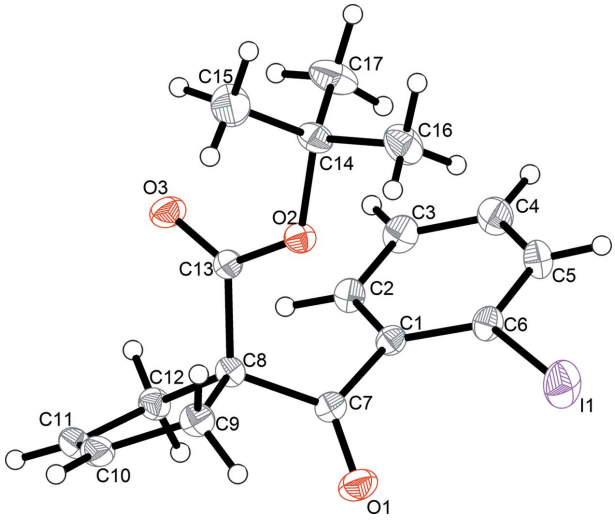


Figure 1
The molecular structure of title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 20% probability level.

5. Synthesis and crystallization

The title compound was prepared according to a general literature protocol (Yuan *et al.*, 2019). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.0 (*dd*, J = 7.9, 1.2 Hz, 1H), 7.4 (*dd*, J = 7.8, 1.8 Hz, 1H), 7.3 (*td*, J = 7.5, 1.2 Hz, 1H), 7.1 (*td*, J = 7.8, 1.8 Hz, 1H), 5.6 (*s*, 2H), 3.1 (*s*, 4H), 1.2 (*s*, 9H). HRMS (ESI) calcd for $[C_{17}H_{19}IO_3{}^{+}Na]^{+}$ 421.0271, found 421.0272. Crystallization from a 5:1 mixture (*v*/*v*) of dichloromethane and *n*-hexane by slow evaporation at room temperature for about 7 d gave block-shaped crystals of the title compound.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms attached to C atoms were included in calculated positions and refined using a riding model: C—H = 0.93-0.97 Å with U_{iso}(H) = 1.5U_{eq}(C-methyl) and 1.2U_{eq}(C) for other H atoms.

Acknowledgements

Generous financial support from the National Natural Science Foundation of China (21602084) is greatly acknowledged.

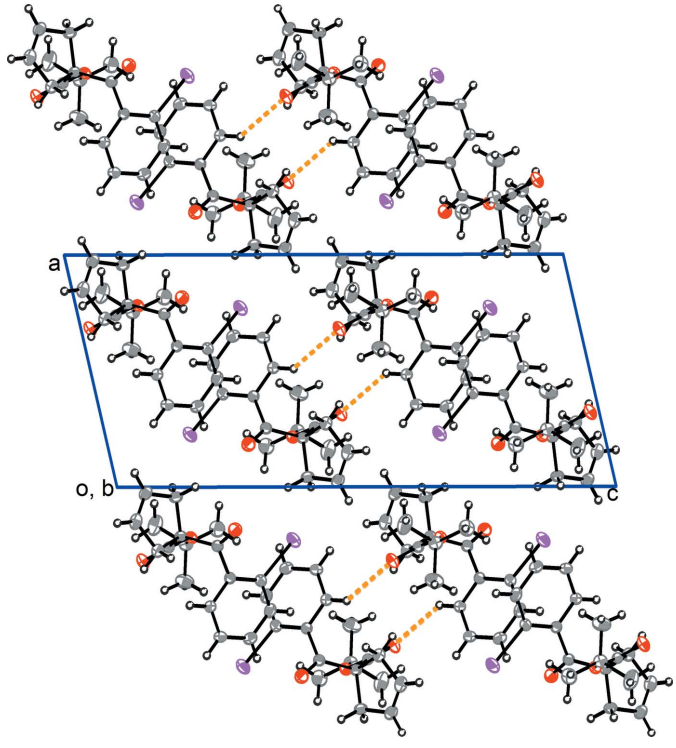


Figure 2
A view along [010] of the crystal packing of the title compound. The intermolecular C—H···O hydrogen bonds are shown as orange dashed lines (Table 1).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{19}IO_3$
M_r	398.22
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	299
a, b, c (Å)	9.4977 (2), 9.3635 (2), 19.8978 (4)
β (°)	102.752 (1)
V (Å^3)	1725.90 (6)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	14.64
Crystal size (mm)	0.3 × 0.2 × 0.1
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.262, 0.753
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16056, 3278, 2612
R_{int}	0.066
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.131, 1.06
No. of reflections	3278
No. of parameters	193
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.61, −1.22

Computer programs: *APEX3* and *SAINT* (Bruker, 2014), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg, 2006) and *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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References

Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.

Bruker (2014). *APEX3*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

Jiang, X. F., Ma, X. J., Zheng, Z. L. & Ma, S. M. (2008). *Chem. Eur. J.* **14**, 8572–8578.

Rao, S. T., Westhof, E. & Sundaralingam, M. (1981). *Acta Cryst.* A**37**, 421–425.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

Yang, C., Xia, W., Zhang, X., Li, B. & Gou, B. (2007). *Acta Cryst.* E**63**, o4729.

Yuan, Z. B., Feng, Z. W., Zeng, Y. Y., Zhao, X. B., Lin, A. J. & Yao, H. Q. (2019). *Angew. Chem. Int. Ed.* **58**, 2884–2888.

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Synthesis and crystal structure of *tert*-butyl 1-(2-iodobenzoyl)cyclopent-3-ene-1-carboxylate

Dejing Yin

Computing details

Data collection: *APEX3* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: SHELXT2014 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015b), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

tert-Butyl 1-(2-iodobenzoyl)-cyclopent-3-ene-1-carboxylate

Crystal data

$C_{17}H_{19}IO_3$
$M_r = 398.22$
Monoclinic, $P2_1/c$
$a = 9.4977$ (2) Å
$b = 9.3635$ (2) Å
$c = 19.8978$ (4) Å
$\beta = 102.752$ (1)°
$V = 1725.90$ (6) Å^3
$Z = 4$
$F(000) = 792$
$D_x = 1.533$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 5961 reflections
$\theta = 4.6$–$69.9°$
$\mu = 14.64$ mm^{-1}
$T = 299$ K
Block, colourless
0.3 × 0.2 × 0.1 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
$T_{min} = 0.262$, $T_{max} = 0.753$
16056 measured reflections
3278 independent reflections
2612 reflections with $I > 2\sigma(I)$
$R_{int} = 0.066$
$\theta_{max} = 70.1°$, $\theta_{min} = 4.6°$
$h = -10 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -24 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.131$
$S = 1.06$
3278 reflections
193 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 2.0895P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.61$ e Å^{-3}
$\Delta\rho_{min} = -1.22$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.22879 (4)	0.41049 (5)	0.17053 (2)	0.0858 (2)
O1	0.1852 (4)	0.6510 (4)	0.28314 (19)	0.0681 (9)
C1	0.3928 (4)	0.5060 (4)	0.3155 (2)	0.0425 (8)
O2	0.2177 (3)	0.3021 (3)	0.37481 (14)	0.0444 (6)
C2	0.5151 (4)	0.5150 (5)	0.3679 (2)	0.0489 (9)
H2	0.509986	0.562449	0.408373	0.059*
O3	0.3190 (4)	0.3762 (3)	0.48200 (17)	0.0596 (8)
C3	0.6447 (5)	0.4554 (6)	0.3617 (3)	0.0581 (12)
H3	0.726078	0.463818	0.397392	0.07*
C4	0.6522 (5)	0.3836 (6)	0.3024 (3)	0.0647 (13)
H4	0.738876	0.34243	0.298079	0.078*
C7	0.2544 (4)	0.5741 (4)	0.3257 (2)	0.0442 (9)
C6	0.4034 (5)	0.4366 (5)	0.2548 (2)	0.0496 (10)
C5	0.5325 (5)	0.3725 (6)	0.2497 (3)	0.0613 (12)
H5	0.537768	0.321576	0.21015	0.074*
C8	0.2122 (4)	0.5470 (4)	0.3950 (2)	0.0407 (8)
C9	0.0444 (4)	0.5578 (5)	0.3866 (3)	0.0528 (11)
H9A	−0.000447	0.601873	0.342983	0.063*
H9B	0.002167	0.464174	0.389089	0.063*
C10	0.0274 (5)	0.6489 (5)	0.4456 (3)	0.0600 (12)
H10	−0.060286	0.663186	0.458092	0.072*
C11	0.1492 (6)	0.7068 (5)	0.4781 (3)	0.0612 (12)
H11	0.156817	0.766726	0.515951	0.073*
C12	0.2749 (5)	0.6666 (5)	0.4479 (2)	0.0506 (10)
H12A	0.354422	0.630768	0.483133	0.061*
H12B	0.307966	0.747473	0.425131	0.061*
C13	0.2590 (4)	0.4002 (4)	0.4236 (2)	0.0397 (8)
C14	0.2441 (5)	0.1481 (5)	0.3876 (3)	0.0530 (10)
C15	0.1631 (9)	0.0987 (6)	0.4407 (4)	0.091 (2)
H15A	0.070819	0.145176	0.432802	0.137*
H15B	0.217624	0.122419	0.485973	0.137*
H15C	0.149492	−0.002829	0.437233	0.137*
C16	0.1791 (7)	0.0833 (6)	0.3183 (3)	0.0763 (16)
H16A	0.079978	0.112254	0.304044	0.114*
H16B	0.184221	−0.018889	0.321627	0.114*
H16C	0.231621	0.115416	0.285077	0.114*
C17	0.4050 (6)	0.1218 (6)	0.4074 (4)	0.0851 (19)
H17A	0.450457	0.165224	0.373923	0.128*
H17B	0.423246	0.020849	0.408884	0.128*

H17C	0.443561	0.16255	0.451908	0.128*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0721 (3)	0.1182 (4)	0.0569 (2)	−0.0009 (2)	−0.00751 (17)	−0.0218 (2)
O1	0.0613 (19)	0.078 (2)	0.065 (2)	0.0208 (17)	0.0140 (17)	0.0253 (18)
C1	0.0403 (19)	0.045 (2)	0.042 (2)	−0.0023 (16)	0.0093 (16)	0.0044 (17)
O2	0.0465 (14)	0.0380 (14)	0.0462 (15)	−0.0051 (11)	0.0046 (12)	−0.0032 (12)
C2	0.041 (2)	0.059 (3)	0.046 (2)	−0.0017 (18)	0.0091 (17)	−0.002 (2)
O3	0.074 (2)	0.0489 (17)	0.0468 (18)	0.0025 (14)	−0.0058 (15)	0.0017 (14)
C3	0.036 (2)	0.079 (3)	0.058 (3)	−0.002 (2)	0.0082 (19)	0.004 (2)
C4	0.046 (2)	0.083 (4)	0.068 (3)	0.010 (2)	0.019 (2)	0.002 (3)
C7	0.040 (2)	0.046 (2)	0.045 (2)	−0.0018 (17)	0.0072 (17)	0.0028 (18)
C6	0.045 (2)	0.058 (3)	0.043 (2)	−0.0054 (18)	0.0062 (17)	−0.0026 (19)
C5	0.067 (3)	0.069 (3)	0.053 (3)	0.003 (2)	0.024 (2)	−0.010 (2)
C8	0.0350 (18)	0.043 (2)	0.045 (2)	−0.0019 (15)	0.0090 (15)	−0.0025 (17)
C9	0.0351 (19)	0.063 (3)	0.062 (3)	0.0045 (18)	0.0126 (18)	0.005 (2)
C10	0.059 (3)	0.061 (3)	0.066 (3)	0.020 (2)	0.028 (2)	0.014 (2)
C11	0.084 (3)	0.044 (2)	0.062 (3)	0.012 (2)	0.029 (3)	0.001 (2)
C12	0.057 (2)	0.043 (2)	0.053 (2)	−0.0029 (18)	0.015 (2)	−0.0033 (19)
C13	0.0361 (18)	0.042 (2)	0.041 (2)	−0.0002 (15)	0.0096 (16)	0.0013 (16)
C14	0.057 (2)	0.035 (2)	0.068 (3)	−0.0008 (18)	0.016 (2)	−0.004 (2)
C15	0.143 (6)	0.051 (3)	0.096 (5)	−0.019 (3)	0.061 (5)	0.000 (3)
C16	0.087 (4)	0.057 (3)	0.082 (4)	−0.007 (3)	0.013 (3)	−0.024 (3)
C17	0.067 (3)	0.063 (3)	0.117 (5)	0.021 (3)	0.002 (3)	−0.008 (3)

Geometric parameters (Å, º)

I1—C6	2.096 (4)	C9—H9A	0.97
O1—C7	1.193 (5)	C9—H9B	0.97
C1—C2	1.382 (6)	C10—C11	1.312 (8)
C1—C6	1.395 (6)	C10—H10	0.93
C1—C7	1.514 (5)	C11—C12	1.497 (6)
O2—C13	1.331 (5)	C11—H11	0.93
O2—C14	1.476 (5)	C12—H12A	0.97
C2—C3	1.382 (6)	C12—H12B	0.97
C2—H2	0.93	C14—C16	1.508 (8)
O3—C13	1.197 (5)	C14—C15	1.511 (8)
C3—C4	1.373 (7)	C14—C17	1.512 (7)
C3—H3	0.93	C15—H15A	0.96
C4—C5	1.371 (7)	C15—H15B	0.96
C4—H4	0.93	C15—H15C	0.96
C7—C8	1.540 (6)	C16—H16A	0.96
C6—C5	1.389 (7)	C16—H16B	0.96
C5—H5	0.93	C16—H16C	0.96
C8—C13	1.516 (5)	C17—H17A	0.96
C8—C12	1.561 (6)	C17—H17B	0.96

C8—C9	1.568 (5)	C17—H17C	0.96
C9—C10	1.489 (7)		

C2—C1—C6	118.2 (4)	C10—C11—C12	113.1 (4)
C2—C1—C7	118.9 (4)	C10—C11—H11	123.4
C6—C1—C7	122.9 (4)	C12—C11—H11	123.4
C13—O2—C14	122.5 (3)	C11—C12—C8	103.4 (4)
C1—C2—C3	121.7 (4)	C11—C12—H12A	111.1
C1—C2—H2	119.2	C8—C12—H12A	111.1
C3—C2—H2	119.2	C11—C12—H12B	111.1
C4—C3—C2	119.4 (4)	C8—C12—H12B	111.1
C4—C3—H3	120.3	H12A—C12—H12B	109.1
C2—C3—H3	120.3	O3—C13—O2	125.3 (4)
C5—C4—C3	120.2 (4)	O3—C13—C8	124.9 (4)
C5—C4—H4	119.9	O2—C13—C8	109.7 (3)
C3—C4—H4	119.9	O2—C14—C16	102.5 (4)
O1—C7—C1	121.2 (4)	O2—C14—C15	109.0 (4)
O1—C7—C8	121.5 (4)	C16—C14—C15	110.4 (5)
C1—C7—C8	117.1 (3)	O2—C14—C17	109.1 (4)
C5—C6—C1	119.9 (4)	C16—C14—C17	111.1 (5)
C5—C6—I1	116.5 (3)	C15—C14—C17	114.1 (6)
C1—C6—I1	123.4 (3)	C14—C15—H15A	109.5
C4—C5—C6	120.5 (4)	C14—C15—H15B	109.5
C4—C5—H5	119.8	H15A—C15—H15B	109.5
C6—C5—H5	119.8	C14—C15—H15C	109.5
C13—C8—C7	111.9 (3)	H15A—C15—H15C	109.5
C13—C8—C12	111.1 (3)	H15B—C15—H15C	109.5
C7—C8—C12	110.5 (3)	C14—C16—H16A	109.5
C13—C8—C9	107.8 (3)	C14—C16—H16B	109.5
C7—C8—C9	110.7 (3)	H16A—C16—H16B	109.5
C12—C8—C9	104.7 (3)	C14—C16—H16C	109.5
C10—C9—C8	103.7 (4)	H16A—C16—H16C	109.5
C10—C9—H9A	111.0	H16B—C16—H16C	109.5
C8—C9—H9A	111.0	C14—C17—H17A	109.5
C10—C9—H9B	111.0	C14—C17—H17B	109.5
C8—C9—H9B	111.0	H17A—C17—H17B	109.5
H9A—C9—H9B	109.0	C14—C17—H17C	109.5
C11—C10—C9	112.8 (4)	H17A—C17—H17C	109.5
C11—C10—H10	123.6	H17B—C17—H17C	109.5
C9—C10—H10	123.6		

C6—C1—C2—C3	−1.1 (7)	C13—C8—C9—C10	104.1 (4)
C7—C1—C2—C3	−179.9 (4)	C7—C8—C9—C10	−133.3 (4)
C1—C2—C3—C4	−0.9 (7)	C12—C8—C9—C10	−14.3 (5)
C2—C3—C4—C5	0.6 (8)	C8—C9—C10—C11	9.5 (5)
C2—C1—C7—O1	130.7 (5)	C9—C10—C11—C12	−0.2 (6)
C6—C1—C7—O1	−48.0 (6)	C10—C11—C12—C8	−9.2 (5)
C2—C1—C7—C8	−45.7 (5)	C13—C8—C12—C11	−101.9 (4)

C6—C1—C7—C8	135.7 (4)	C7—C8—C12—C11	133.3 (4)
C2—C1—C6—C5	3.4 (6)	C9—C8—C12—C11	14.1 (4)
C7—C1—C6—C5	−177.9 (4)	C14—O2—C13—O3	−0.9 (6)
C2—C1—C6—I1	179.2 (3)	C14—O2—C13—C8	−178.2 (3)
C7—C1—C6—I1	−2.2 (6)	C7—C8—C13—O3	133.6 (4)
C3—C4—C5—C6	1.7 (8)	C12—C8—C13—O3	9.6 (5)
C1—C6—C5—C4	−3.7 (7)	C9—C8—C13—O3	−104.5 (5)
I1—C6—C5—C4	−179.8 (4)	C7—C8—C13—O2	−49.1 (4)
O1—C7—C8—C13	150.6 (4)	C12—C8—C13—O2	−173.1 (3)
C1—C7—C8—C13	−33.0 (5)	C9—C8—C13—O2	72.8 (4)
O1—C7—C8—C12	−85.0 (5)	C13—O2—C14—C16	−180.0 (4)
C1—C7—C8—C12	91.3 (4)	C13—O2—C14—C15	63.0 (6)
O1—C7—C8—C9	30.4 (6)	C13—O2—C14—C17	−62.2 (6)
C1—C7—C8—C9	−153.2 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O3^{i}	0.93	2.48	3.219 (5)	136

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.