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5-Bromo-3-cyclohexylsulfonyl-2-methyl-1-benzofuran

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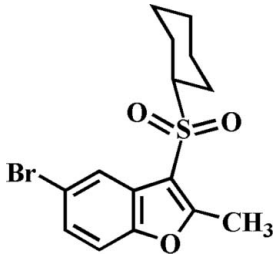
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.073; data-to-parameter ratio = 18.6.

In the title compound, $C_{15}H_{17}BrO_3S$, the cyclohexyl ring adopts a practically undistorted chair conformation [endocyclic torsion angles are within a 54.5–56.4 (3)° range] and the arylsulfonyl unit is positioned equatorial relative to the cyclohexyl group. In the crystal, molecules are linked through C—H···O hydrogen bonds and donor–acceptor Br···O contacts [3.250 (2) Å]. The crystal structure also exhibits aromatic π–π overlap between the benzene and furan rings of neighbouring molecules [centroid–centroid distance = 3.635 (2) Å].

Related literature

For the pharmacological activity of benzofuran compounds, see: Aslam *et al.* (2006); Galal *et al.* (2009); Khan *et al.* (2005). For natural products with benzofuran rings, see: Akgul & Anil (2003); Soekamto *et al.* (2003). For structural studies of related 3-arylsulfonyl-5-bromo-2-methyl-1-benzofuran derivatives, see: Choi *et al.* (2008, 2010). For a review of halogen bonding, see: Politzer *et al.* (2007).



Experimental

Crystal data

$C_{15}H_{17}BrO_3S$
M_r = 357.26
Triclinic, $P\overline{1}$
a = 6.3452 (1) Å
b = 8.2065 (1) Å
c = 14.4866 (2) Å
α = 98.842 (1)°
β = 97.693 (1)°
γ = 96.385 (1)°
V = 731.95 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.95 mm^{-1}
T = 173 K
0.33 × 0.26 × 0.23 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.585, T_{max} = 0.746
13107 measured reflections
3377 independent reflections
3109 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.073
S = 1.07
3377 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O1^{i}	0.95	2.57	3.518 (2)	174
C9—H9B···O3^{ii}	0.98	2.55	3.303 (2)	134

Symmetry codes: (i) $-x+2, -y+2, -z+1$; (ii) $x+1, y, z$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LD2001).

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supporting information

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5-Bromo-3-cyclohexylsulfonyl-2-methyl-1-benzofuran

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S1. Comment

Many compounds containing a benzofuran ring show diverse pharmacological properties such as antifungal, antitumor and antiviral, and antimicrobial activities (Aslam *et al.*, 2006, Galal *et al.*, 2009, Khan *et al.*, 2005). These compounds occur in a wide range of natural products (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our ongoing study of the substituent effect on the solid state structures of 3-arylsulfonyl-5-bromo-2-methyl-1-benzofuran analogues (Choi *et al.*, 2008, 2010), we report herein the crystal structure of the title compound.

In the title molecule (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.006 (2) Å from the least-squares plane defined by the nine constituent atoms. The cyclohexyl ring is in the chair form and arylsulfonyl moiety is positioned equatorial relative to the cyclohexyl group. The molecular packing (Fig. 2) is stabilized by intermolecular C—H···O hydrogen bonds - between an arene H atom and the furan O atom (Table 1; C6—H6···O1^{i}), and between a methyl H atom and a sulfonyl oxygen (Table 1; C9—H9B···O3^{ii}). The crystal structure is further stabilized by Br···O halogen bonding between the bromine and an oxygen of the sulfonyl group [Br1···O3^{iii} = 3.250 (2) Å, C4—Br1···O3^{iii} = 165.29 (6)°] (Politzer *et al.*, 2007). The crystal packing (Fig. 2) also exhibits π–π overlap between the benzene and furan rings of neighbouring molecules, with a Cg1···Cg2^{iv} distance of 3.633 (2) Å (Cg1 and Cg2 are the centroids of the C2-C7 benzene ring and the C1/C2/C7/O1/C8 furan ring, respectively), wherein the inter-planar distance between the benzene and furan rings is 3.391 (2) Å.

S2. Experimental

77% 3-chloroperoxybenzoic acid (381 mg, 1.7 mmol) was added in small portions to a stirred solution of 5-bromo-3-cyclohexylsulfanyl-2-methyl-1-benzofuran (260 mg, 0.8 mmol) in dichloromethane (40 mL) at 273 K. After being stirred at room temperature for 5h, the mixture was washed with saturated sodium bicarbonate solution and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated at reduced pressure. The residue was purified by column chromatography (hexane–ethyl acetate, 4:1 v/v) to afford the title compound as a colorless solid [yield 76%, m.p. 446–447 K; R_f = 0.58 (hexane–ethyl acetate, 4:1 v/v)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of acetone solution of the title compound at room temperature.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding and rotating model, with C—H = 0.95 Å for aryl, 1.00 Å for methine, 0.99 Å for methylene and 0.98 Å for methyl H atoms, respectively. U_{iso}(H) = 1.2U_{eq}(C) for aryl, methine, methylene and 1.5U_{eq}(C) for methyl H atoms.

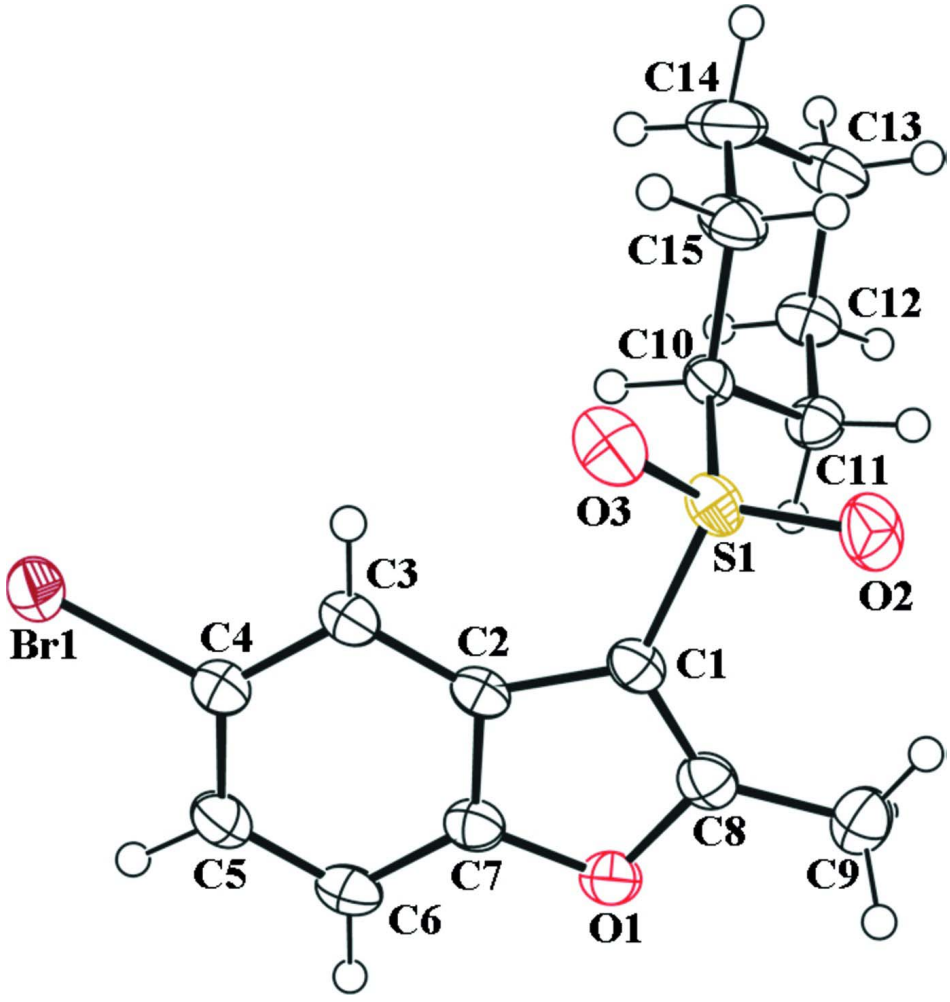

Figure 1

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radius.

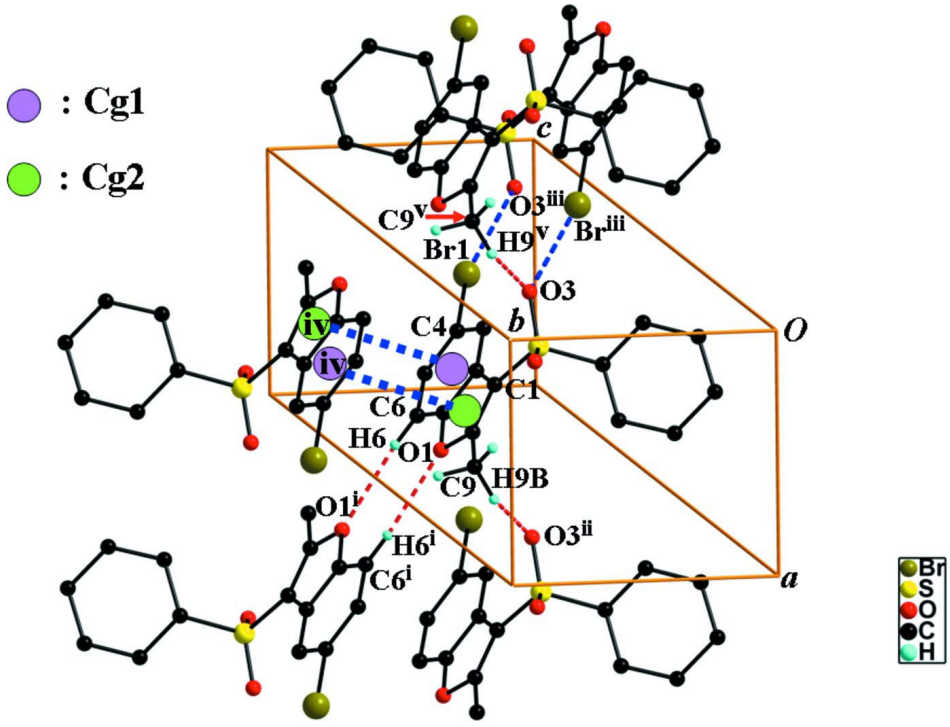

Figure 2

A view of the C—H···O, Br···O and π–π interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (i) - x + 2, - *y* + 2, - *z* + 1; (ii) x + 1, *y*, *z*; (iii) - x, - *y* + 1, - *z* + 1 ; (iv) - *x* + 1, - *y* + 2, - *z* + 1; (v) x - 1, *y*, *z* .]

5-Bromo-3-cyclohexylsulfonyl-2-methyl-1-benzofuran

Crystal data

$C_{15}H_{17}BrO_3S$
M_r = 357.26
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 6.3452 (1) Å
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c = 14.4866 (2) Å
α = 98.842 (1)°
β = 97.693 (1)°
γ = 96.385 (1)°
V = 731.95 (2) Å^3

Z = 2
F(000) = 364
D_x = 1.621 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 8112 reflections
θ = 2.7–27.5°
μ = 2.95 mm^{-1}
T = 173 K
Block, colourless
0.33 × 0.26 × 0.23 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: rotating anode
Graphite multilayer monochromator
Detector resolution: 10.0 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.585, T_{max} = 0.746

13107 measured reflections
3377 independent reflections
3109 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 27.6°, θ_{min} = 1.4°
h = −8→8
k = −10→10
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.073$
$S = 1.07$
3377 reflections
182 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 0.2624P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.70$ 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.

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 $F^2 > 2$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}
Br1	0.24178 (3)	0.58796 (3)	0.634104 (12)	0.03547 (8)
S1	0.21139 (7)	0.69361 (6)	0.22168 (3)	0.02801 (11)
O1	0.7467 (2)	0.92120 (16)	0.38017 (9)	0.0310 (3)
O2	0.2068 (3)	0.78049 (19)	0.14233 (10)	0.0400 (3)
O3	0.0254 (2)	0.6830 (2)	0.26875 (10)	0.0396 (3)
C1	0.4294 (3)	0.7824 (2)	0.30762 (12)	0.0267 (4)
C2	0.4500 (3)	0.7619 (2)	0.40566 (12)	0.0261 (3)
C3	0.3234 (3)	0.6829 (2)	0.46111 (12)	0.0284 (4)
H3	0.1862	0.6225	0.4355	0.034*
C4	0.4078 (3)	0.6967 (2)	0.55581 (13)	0.0286 (4)
C5	0.6076 (3)	0.7838 (3)	0.59542 (13)	0.0324 (4)
H5	0.6582	0.7887	0.6607	0.039*
C6	0.7337 (3)	0.8635 (3)	0.54056 (14)	0.0330 (4)
H6	0.8706	0.9243	0.5663	0.040*
C7	0.6495 (3)	0.8496 (2)	0.44644 (13)	0.0284 (4)
C8	0.6100 (3)	0.8776 (2)	0.29616 (13)	0.0290 (4)
C9	0.6862 (4)	0.9444 (3)	0.21558 (15)	0.0365 (4)
H9A	0.5693	0.9244	0.1619	0.055*
H9B	0.8070	0.8887	0.1974	0.055*
H9C	0.7330	1.0643	0.2340	0.055*
C10	0.2636 (3)	0.4859 (2)	0.18543 (12)	0.0244 (3)
H10	0.3071	0.4386	0.2436	0.029*
C11	0.4467 (3)	0.4811 (2)	0.12705 (13)	0.0288 (4)
H11A	0.5802	0.5433	0.1657	0.035*
H11B	0.4124	0.5353	0.0714	0.035*

C12	0.4807 (3)	0.3011 (3)	0.09420 (14)	0.0328 (4)
H12A	0.5919	0.2997	0.0523	0.039*
H12B	0.5334	0.2522	0.1498	0.039*
C13	0.2750 (3)	0.1955 (3)	0.04136 (16)	0.0419 (5)
H13A	0.2310	0.2363	−0.0182	0.050*
H13B	0.3015	0.0787	0.0249	0.050*
C14	0.0960 (4)	0.2023 (3)	0.10074 (18)	0.0474 (6)
H14A	0.1341	0.1512	0.1573	0.057*
H14B	−0.0373	0.1371	0.0636	0.057*
C15	0.0563 (3)	0.3812 (3)	0.13187 (14)	0.0358 (4)
H15A	−0.0560	0.3825	0.1732	0.043*
H15B	0.0050	0.4294	0.0757	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03585 (12)	0.04254 (13)	0.02647 (11)	0.00000 (9)	0.00393 (8)	0.00562 (8)
S1	0.0262 (2)	0.0334 (2)	0.0240 (2)	0.00874 (18)	0.00065 (16)	0.00314 (18)
O1	0.0298 (7)	0.0289 (7)	0.0321 (7)	0.0000 (6)	0.0053 (5)	0.0004 (5)
O2	0.0471 (8)	0.0414 (8)	0.0332 (7)	0.0134 (7)	−0.0016 (6)	0.0129 (6)
O3	0.0277 (7)	0.0553 (10)	0.0352 (7)	0.0134 (7)	0.0045 (6)	0.0009 (7)
C1	0.0294 (9)	0.0247 (9)	0.0243 (8)	0.0049 (7)	0.0024 (7)	−0.0003 (7)
C2	0.0272 (8)	0.0236 (8)	0.0248 (8)	0.0043 (7)	0.0017 (6)	−0.0026 (7)
C3	0.0280 (9)	0.0290 (9)	0.0251 (8)	0.0023 (7)	0.0012 (7)	−0.0013 (7)
C4	0.0308 (9)	0.0270 (9)	0.0266 (8)	0.0035 (7)	0.0038 (7)	0.0007 (7)
C5	0.0348 (10)	0.0330 (10)	0.0255 (8)	0.0026 (8)	−0.0020 (7)	−0.0002 (7)
C6	0.0278 (9)	0.0323 (10)	0.0327 (10)	−0.0025 (8)	−0.0031 (7)	−0.0025 (8)
C7	0.0282 (9)	0.0256 (9)	0.0296 (9)	0.0029 (7)	0.0045 (7)	−0.0009 (7)
C8	0.0337 (9)	0.0242 (9)	0.0287 (9)	0.0076 (7)	0.0051 (7)	0.0000 (7)
C9	0.0413 (11)	0.0336 (10)	0.0379 (10)	0.0078 (9)	0.0114 (9)	0.0098 (8)
C10	0.0228 (8)	0.0285 (9)	0.0197 (7)	0.0003 (7)	0.0004 (6)	0.0023 (6)
C11	0.0243 (8)	0.0303 (9)	0.0312 (9)	0.0018 (7)	0.0057 (7)	0.0032 (7)
C12	0.0284 (9)	0.0316 (10)	0.0353 (10)	0.0052 (8)	0.0019 (7)	−0.0018 (8)
C13	0.0363 (11)	0.0423 (12)	0.0377 (11)	0.0002 (9)	−0.0012 (9)	−0.0124 (9)
C14	0.0374 (11)	0.0441 (13)	0.0496 (13)	−0.0147 (10)	0.0052 (10)	−0.0107 (10)
C15	0.0213 (8)	0.0485 (12)	0.0313 (9)	−0.0042 (8)	0.0018 (7)	−0.0047 (9)

Geometric parameters (Å, º)

Br1—O3^{i}	3.250 (2)	C9—H9A	0.9800
Br1—C4	1.901 (2)	C9—H9B	0.9800
S1—O3	1.4409 (15)	C9—H9C	0.9800
S1—O2	1.4416 (15)	C10—C11	1.526 (2)
S1—C1	1.7408 (18)	C10—C15	1.530 (2)
S1—C10	1.7852 (18)	C10—H10	1.0000
O1—C8	1.370 (2)	C11—C12	1.529 (3)
O1—C7	1.378 (2)	C11—H11A	0.9900
C1—C8	1.357 (3)	C11—H11B	0.9900

C1—C2	1.446 (2)	C12—C13	1.523 (3)
C2—C3	1.388 (3)	C12—H12A	0.9900
C2—C7	1.392 (3)	C12—H12B	0.9900
C3—C4	1.387 (2)	C13—C14	1.515 (3)
C3—H3	0.9500	C13—H13A	0.9900
C4—C5	1.387 (3)	C13—H13B	0.9900
C5—C6	1.383 (3)	C14—C15	1.527 (3)
C5—H5	0.9500	C14—H14A	0.9900
C6—C7	1.379 (3)	C14—H14B	0.9900
C6—H6	0.9500	C15—H15A	0.9900
C8—C9	1.479 (3)	C15—H15B	0.9900

C4—Br1—O3^{i}	165.29 (6)	H9B—C9—H9C	109.5
O3—S1—O2	118.38 (9)	C11—C10—C15	112.06 (14)
O3—S1—C1	106.84 (9)	C11—C10—S1	111.82 (13)
O2—S1—C1	109.77 (9)	C15—C10—S1	108.98 (13)
O3—S1—C10	107.26 (9)	C11—C10—H10	107.9
O2—S1—C10	109.22 (9)	C15—C10—H10	107.9
C1—S1—C10	104.45 (8)	S1—C10—H10	107.9
C8—O1—C7	106.96 (14)	C10—C11—C12	110.24 (15)
C8—C1—C2	107.72 (16)	C10—C11—H11A	109.6
C8—C1—S1	127.65 (14)	C12—C11—H11A	109.6
C2—C1—S1	124.60 (14)	C10—C11—H11B	109.6
C3—C2—C7	119.65 (16)	C12—C11—H11B	109.6
C3—C2—C1	135.86 (17)	H11A—C11—H11B	108.1
C7—C2—C1	104.48 (16)	C13—C12—C11	111.97 (16)
C4—C3—C2	116.54 (17)	C13—C12—H12A	109.2
C4—C3—H3	121.7	C11—C12—H12A	109.2
C2—C3—H3	121.7	C13—C12—H12B	109.2
C3—C4—C5	123.20 (18)	C11—C12—H12B	109.2
C3—C4—Br1	118.01 (14)	H12A—C12—H12B	107.9
C5—C4—Br1	118.78 (14)	C14—C13—C12	111.09 (17)
C6—C5—C4	120.46 (17)	C14—C13—H13A	109.4
C6—C5—H5	119.8	C12—C13—H13A	109.4
C4—C5—H5	119.8	C14—C13—H13B	109.4
C7—C6—C5	116.23 (17)	C12—C13—H13B	109.4
C7—C6—H6	121.9	H13A—C13—H13B	108.0
C5—C6—H6	121.9	C13—C14—C15	111.34 (19)
O1—C7—C6	125.59 (17)	C13—C14—H14A	109.4
O1—C7—C2	110.49 (16)	C15—C14—H14A	109.4
C6—C7—C2	123.91 (18)	C13—C14—H14B	109.4
C1—C8—O1	110.33 (16)	C15—C14—H14B	109.4
C1—C8—C9	134.57 (18)	H14A—C14—H14B	108.0
O1—C8—C9	115.09 (17)	C14—C15—C10	110.09 (16)
C8—C9—H9A	109.5	C14—C15—H15A	109.6
C8—C9—H9B	109.5	C10—C15—H15A	109.6
H9A—C9—H9B	109.5	C14—C15—H15B	109.6
C8—C9—H9C	109.5	C10—C15—H15B	109.6

H9A—C9—H9C	109.5	H15A—C15—H15B	108.2
O3—S1—C1—C8	−150.39 (17)	C3—C2—C7—C6	0.4 (3)
O2—S1—C1—C8	−20.86 (19)	C1—C2—C7—C6	179.62 (18)
C10—S1—C1—C8	96.14 (18)	C2—C1—C8—O1	−0.3 (2)
O3—S1—C1—C2	31.47 (18)	S1—C1—C8—O1	−178.67 (13)
O2—S1—C1—C2	161.01 (15)	C2—C1—C8—C9	−179.0 (2)
C10—S1—C1—C2	−81.99 (16)	S1—C1—C8—C9	2.6 (3)
C8—C1—C2—C3	178.9 (2)	C7—O1—C8—C1	0.59 (19)
S1—C1—C2—C3	−2.7 (3)	C7—O1—C8—C9	179.58 (15)
C8—C1—C2—C7	−0.1 (2)	O3—S1—C10—C11	175.09 (12)
S1—C1—C2—C7	178.32 (13)	O2—S1—C10—C11	45.64 (14)
C7—C2—C3—C4	−0.3 (3)	C1—S1—C10—C11	−71.74 (14)
C1—C2—C3—C4	−179.25 (19)	O3—S1—C10—C15	50.66 (14)
C2—C3—C4—C5	−0.1 (3)	O2—S1—C10—C15	−78.79 (14)
C2—C3—C4—Br1	−179.16 (13)	C1—S1—C10—C15	163.83 (13)
C3—C4—C5—C6	0.4 (3)	C15—C10—C11—C12	−55.1 (2)
Br1—C4—C5—C6	179.53 (15)	S1—C10—C11—C12	−177.82 (12)
C4—C5—C6—C7	−0.4 (3)	C10—C11—C12—C13	54.5 (2)
C8—O1—C7—C6	−179.79 (18)	C11—C12—C13—C14	−55.5 (3)
C8—O1—C7—C2	−0.68 (19)	C12—C13—C14—C15	56.4 (3)
C5—C6—C7—O1	178.95 (17)	C13—C14—C15—C10	−56.4 (2)
C5—C6—C7—C2	0.0 (3)	C11—C10—C15—C14	56.2 (2)
C3—C2—C7—O1	−178.72 (15)	S1—C10—C15—C14	−179.50 (15)
C1—C2—C7—O1	0.5 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O1^{ii}	0.95	2.57	3.518 (2)	174
C9—H9*B*···O3^{iii}	0.98	2.55	3.303 (2)	134

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