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5-Bromo-3-cyclohexylsulfonyl-2,7-dimethyl-1-benzofuran

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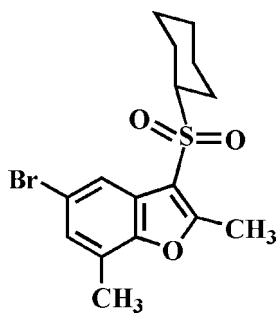
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 Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.025; wR factor = 0.066; data-to-parameter ratio = 18.4.

In the title compound, $\text{C}_{16}\text{H}_{19}\text{BrO}_3\text{S}$, the cyclohexyl ring adopts a chair conformation. In the crystal, molecules are linked through weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and $\text{Br}\cdots\text{O}$ contacts [3.211 (1) Å].

Related literature

For the pharmacological activity of benzofuran compounds, see: Aslam *et al.* (2009); 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-cyclohexylsulfonyl-5-halo-2-methyl-1-benzofuran derivatives, see: Choi *et al.* (2011a,b). For a review of halogen bonding, see: Politzer *et al.* (2007).



Experimental

Crystal data

 $\text{C}_{16}\text{H}_{19}\text{BrO}_3\text{S}$
 $M_r = 371.28$

 Triclinic, $P\bar{1}$
 $a = 6.6992$ (2) Å
 $b = 8.4654$ (2) Å
 $c = 14.1065$ (3) Å
 $\alpha = 101.773$ (1)°
 $\beta = 99.283$ (1)°
 $\gamma = 92.067$ (1)°

 $V = 770.94$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 2.81$ mm⁻¹
 $T = 173$ K
 $0.26 \times 0.25 \times 0.21$ mm

Data collection

 Bruker SMART APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2009)
 $T_{\min} = 0.525$, $T_{\max} = 0.591$

 13840 measured reflections
 3542 independent reflections
 3247 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.066$
 $S = 1.10$
 3542 reflections

 192 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.27$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.59$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}10-\text{H}10\text{B}\cdots\text{O}2^i$	0.98	2.55	3.384 (2)	143

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

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: LR2008).

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supporting information

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5-Bromo-3-cyclohexylsulfonyl-2,7-dimethyl-1-benzofuran

Hong Dae Choi, Pil Ja Seo, Byeng Wha Son and Uk Lee

S1. Comment

Many compounds containing a benzofuran skeleton have drawn much attention owing to diverse pharmacological properties such as antibacterial and antifungal, antitumor and antiviral, and antimicrobial activities (Aslam *et al.*, 2009, 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-cyclohexylsulfonyl-5-halo-2-methyl-1-benzofuran analogues (Choi *et al.*, 2011*a,b*), 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 0.004 (1) Å from the least-squares plane defined by the nine constituent atoms. The cyclohexyl ring is in the chair form. The molecular packing (Fig. 2) is stabilized by weak intermolecular C—H \cdots O hydrogen bonds between a methyl H atom and the O atom of the sulfonyl group (Table 1; C10—H10B \cdots O2ⁱⁱ). The crystal packing (Fig. 2) is further stabilized by a Br \cdots O halogen-bonding between the bromine and the O atom of the sulfonyl group [Br1 \cdots O2ⁱ = 3.211 (1) Å, C4—Br1 \cdots O2ⁱ = 168.13 (6)°] (Politzer *et al.*, 2007).

S2. Experimental

77% 3-chloroperoxybenzoic acid (448 mg, 2.0 mmol) was added in small portions to a stirred solution of 5-bromo-3-cyclohexylsulfonyl-2,7-dimethyl-1-benzofuran (305 mg, 0.9 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 72%, m.p. 440–441 K; R_f = 0.55 (hexane-ethyl acetate, 4:1 v/v)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title compound in acetone at room temperature.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding 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. $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aryl, methine and methylene, and $1.5U_{\text{eq}}(\text{C})$ for methyl H atoms.

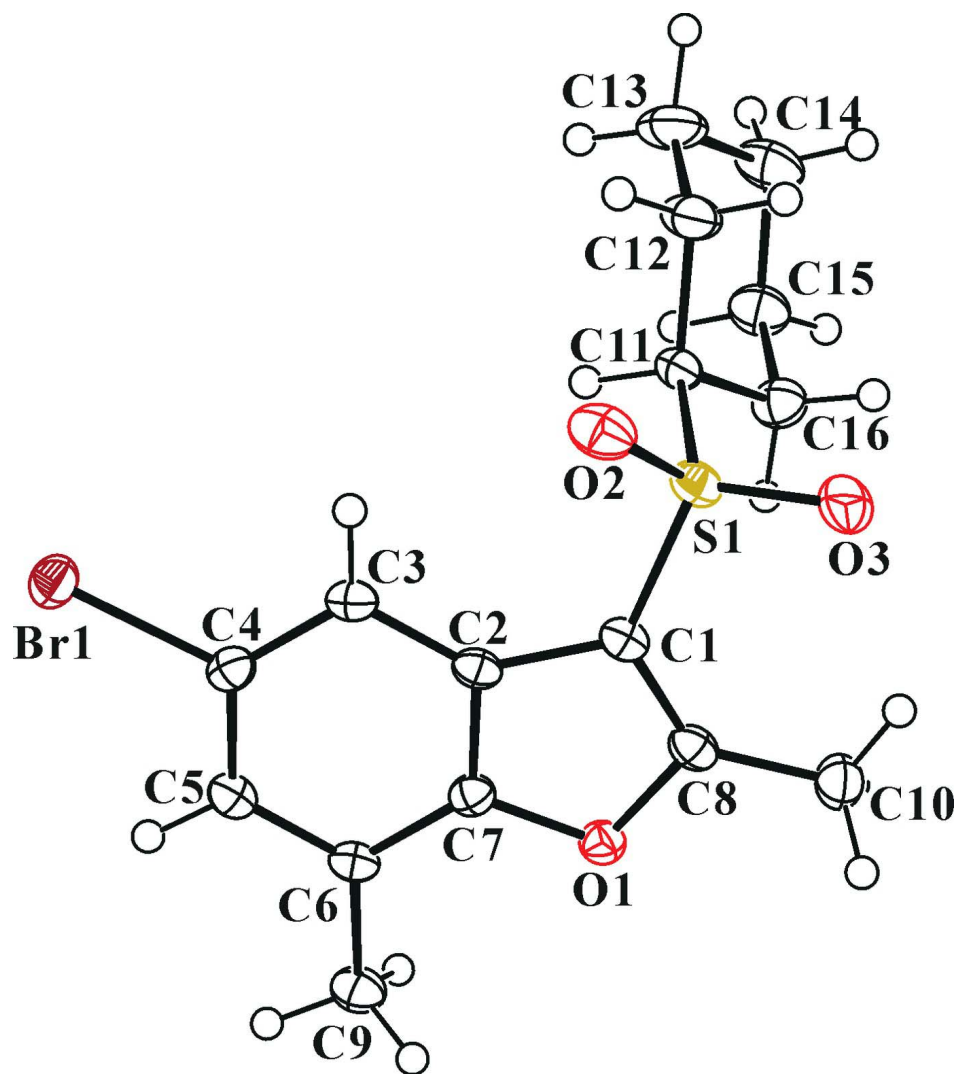


Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

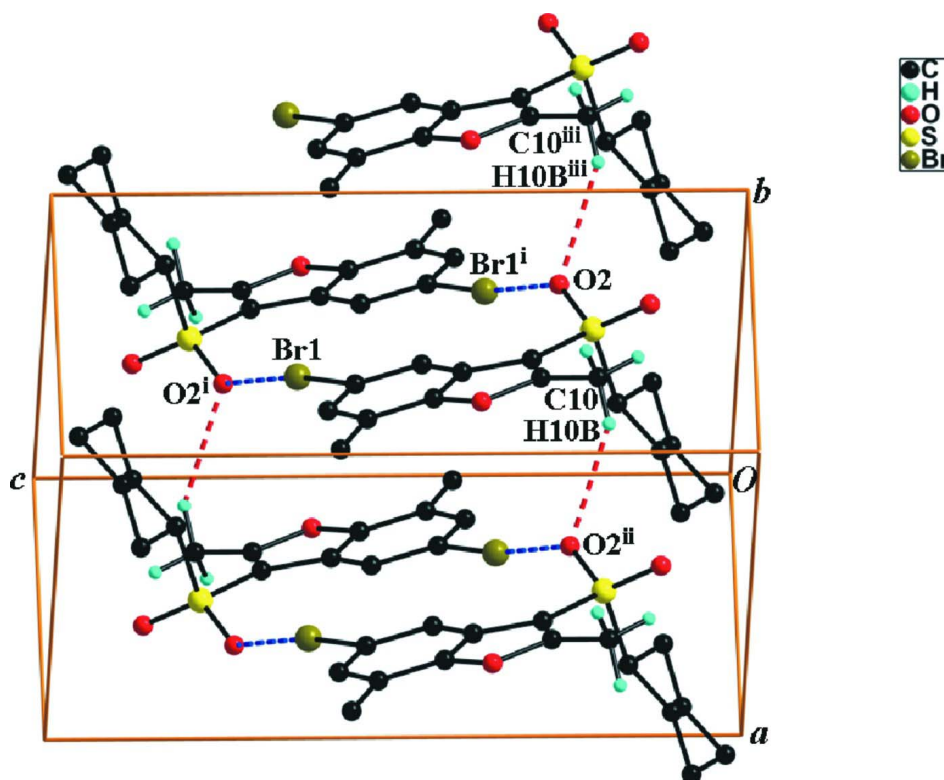


Figure 2

A view of the Br \cdots O and C—H \cdots O interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (i) $-x, -y + 1, -z + 1$; (ii) $x + 1, y, z$; (iii) $x - 1, y, z$.]

5-Bromo-3-cyclohexylsulfonyl-2,7-dimethyl-1-benzofuran

Crystal data

$C_{16}H_{19}BrO_3S$

$M_r = 371.28$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 6.6992$ (2) Å

$b = 8.4654$ (2) Å

$c = 14.1065$ (3) Å

$\alpha = 101.773$ (1) $^\circ$

$\beta = 99.283$ (1) $^\circ$

$\gamma = 92.067$ (1) $^\circ$

$V = 770.94$ (3) Å 3

$Z = 2$

$F(000) = 380$

$D_x = 1.599$ Mg m $^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 7893 reflections

$\theta = 2.5$ – 27.5°

$\mu = 2.81$ mm $^{-1}$

$T = 173$ K

Block, colourless

$0.26 \times 0.25 \times 0.21$ 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)

$T_{\min} = 0.525$, $T_{\max} = 0.591$

13840 measured reflections

3542 independent reflections

3247 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.032$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 1.5^\circ$

$h = -8 \rightarrow 8$

$k = -10 \rightarrow 11$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.066$

$S = 1.10$

3542 reflections

192 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

$w = 1/[\sigma^2(F_o^2) + (0.0331P)^2 + 0.2732P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.27 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.59 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.23387 (3)	0.56750 (2)	0.639762 (13)	0.02642 (7)
S1	0.18306 (6)	0.68046 (5)	0.21799 (3)	0.02179 (10)
O1	0.68271 (17)	0.88970 (14)	0.39103 (9)	0.0209 (2)
O2	0.00575 (19)	0.67623 (17)	0.26350 (10)	0.0308 (3)
O3	0.1772 (2)	0.76300 (17)	0.13792 (10)	0.0319 (3)
C1	0.3856 (3)	0.7638 (2)	0.31083 (12)	0.0199 (3)
C2	0.4083 (2)	0.7416 (2)	0.41070 (12)	0.0186 (3)
C3	0.2943 (2)	0.6642 (2)	0.46471 (12)	0.0205 (3)
H3	0.1661	0.6086	0.4362	0.025*
C4	0.3779 (3)	0.6731 (2)	0.56194 (13)	0.0205 (3)
C5	0.5655 (3)	0.7538 (2)	0.60597 (12)	0.0207 (3)
H5	0.6147	0.7562	0.6733	0.025*
C6	0.6817 (2)	0.8306 (2)	0.55345 (12)	0.0193 (3)
C7	0.5946 (2)	0.8214 (2)	0.45637 (12)	0.0187 (3)
C8	0.5527 (3)	0.8528 (2)	0.30300 (12)	0.0210 (3)
C9	0.8873 (3)	0.9137 (2)	0.59697 (14)	0.0259 (4)
H9A	0.9904	0.8546	0.5652	0.039*
H9B	0.9150	0.9161	0.6676	0.039*
H9C	0.8910	1.0246	0.5865	0.039*
C10	0.6222 (3)	0.9166 (2)	0.22308 (13)	0.0278 (4)
H10A	0.5172	0.8903	0.1641	0.042*
H10B	0.7471	0.8677	0.2085	0.042*
H10C	0.6483	1.0343	0.2435	0.042*
C11	0.2440 (3)	0.4760 (2)	0.17876 (12)	0.0212 (3)
H11	0.2926	0.4334	0.2389	0.025*

C12	0.0529 (3)	0.3725 (2)	0.12283 (14)	0.0305 (4)
H12A	-0.0521	0.3788	0.1652	0.037*
H12B	-0.0016	0.4137	0.0637	0.037*
C13	0.1038 (3)	0.1970 (3)	0.09238 (17)	0.0399 (5)
H13A	0.1455	0.1532	0.1519	0.048*
H13B	-0.0187	0.1316	0.0534	0.048*
C14	0.2727 (3)	0.1828 (3)	0.03208 (16)	0.0386 (5)
H14A	0.2253	0.2152	-0.0309	0.046*
H14B	0.3069	0.0686	0.0169	0.046*
C15	0.4616 (3)	0.2888 (2)	0.08642 (15)	0.0321 (4)
H15A	0.5648	0.2825	0.0431	0.039*
H15B	0.5189	0.2477	0.1452	0.039*
C16	0.4139 (3)	0.4651 (2)	0.11810 (14)	0.0277 (4)
H16A	0.5368	0.5293	0.1576	0.033*
H16B	0.3723	0.5107	0.0592	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02483 (10)	0.02977 (12)	0.02630 (10)	-0.00189 (7)	0.00582 (7)	0.00932 (8)
S1	0.0202 (2)	0.0225 (2)	0.0199 (2)	0.00190 (16)	-0.00183 (15)	0.00234 (17)
O1	0.0188 (6)	0.0227 (6)	0.0203 (6)	-0.0014 (5)	0.0035 (5)	0.0031 (5)
O2	0.0196 (6)	0.0361 (8)	0.0324 (7)	0.0021 (5)	0.0016 (5)	-0.0002 (6)
O3	0.0372 (8)	0.0301 (7)	0.0265 (7)	0.0024 (6)	-0.0058 (6)	0.0103 (6)
C1	0.0199 (8)	0.0190 (8)	0.0187 (8)	0.0020 (6)	0.0012 (6)	0.0007 (6)
C2	0.0190 (8)	0.0149 (8)	0.0196 (8)	0.0025 (6)	0.0017 (6)	-0.0005 (6)
C3	0.0177 (8)	0.0186 (8)	0.0228 (8)	-0.0010 (6)	0.0024 (6)	0.0004 (7)
C4	0.0205 (8)	0.0177 (8)	0.0235 (8)	0.0008 (6)	0.0056 (6)	0.0038 (7)
C5	0.0216 (8)	0.0196 (8)	0.0193 (8)	0.0035 (6)	0.0008 (6)	0.0019 (7)
C6	0.0169 (7)	0.0169 (8)	0.0216 (8)	0.0016 (6)	0.0012 (6)	-0.0003 (6)
C7	0.0187 (8)	0.0164 (8)	0.0209 (8)	0.0016 (6)	0.0051 (6)	0.0024 (6)
C8	0.0231 (8)	0.0189 (8)	0.0191 (8)	0.0044 (6)	0.0020 (6)	0.0003 (7)
C9	0.0190 (8)	0.0286 (10)	0.0270 (9)	-0.0014 (7)	-0.0007 (7)	0.0027 (8)
C10	0.0284 (9)	0.0320 (10)	0.0245 (9)	0.0009 (8)	0.0060 (7)	0.0085 (8)
C11	0.0235 (8)	0.0198 (8)	0.0176 (8)	-0.0012 (7)	0.0003 (6)	0.0010 (7)
C12	0.0256 (9)	0.0335 (11)	0.0267 (9)	-0.0072 (8)	0.0036 (7)	-0.0043 (8)
C13	0.0410 (12)	0.0302 (11)	0.0400 (12)	-0.0125 (9)	0.0069 (9)	-0.0095 (9)
C14	0.0407 (12)	0.0329 (11)	0.0334 (11)	0.0007 (9)	0.0038 (9)	-0.0107 (9)
C15	0.0304 (10)	0.0286 (10)	0.0339 (10)	0.0035 (8)	0.0047 (8)	-0.0008 (8)
C16	0.0258 (9)	0.0266 (10)	0.0300 (9)	0.0005 (7)	0.0068 (7)	0.0032 (8)

Geometric parameters (Å, °)

Br1—C4	1.9011 (17)	C9—H9C	0.9800
Br1—O2 ⁱ	3.2114 (14)	C10—H10A	0.9800
S1—O3	1.4406 (13)	C10—H10B	0.9800
S1—O2	1.4410 (14)	C10—H10C	0.9800
S1—C1	1.7420 (17)	C11—C16	1.525 (3)

S1—C11	1.7891 (18)	C11—C12	1.530 (2)
O1—C8	1.368 (2)	C11—H11	1.0000
O1—C7	1.379 (2)	C12—C13	1.526 (3)
C1—C8	1.359 (2)	C12—H12A	0.9900
C1—C2	1.444 (2)	C12—H12B	0.9900
C2—C7	1.390 (2)	C13—C14	1.515 (3)
C2—C3	1.396 (2)	C13—H13A	0.9900
C3—C4	1.381 (2)	C13—H13B	0.9900
C3—H3	0.9500	C14—C15	1.523 (3)
C4—C5	1.395 (2)	C14—H14A	0.9900
C5—C6	1.387 (2)	C14—H14B	0.9900
C5—H5	0.9500	C15—C16	1.529 (3)
C6—C7	1.385 (2)	C15—H15A	0.9900
C6—C9	1.500 (2)	C15—H15B	0.9900
C8—C10	1.476 (2)	C16—H16A	0.9900
C9—H9A	0.9800	C16—H16B	0.9900
C9—H9B	0.9800		
C4—Br1—O2 ⁱ	168.13 (6)	H10A—C10—H10B	109.5
O3—S1—O2	118.36 (9)	C8—C10—H10C	109.5
O3—S1—C1	109.59 (8)	H10A—C10—H10C	109.5
O2—S1—C1	107.06 (8)	H10B—C10—H10C	109.5
O3—S1—C11	109.54 (8)	C16—C11—C12	111.87 (15)
O2—S1—C11	107.55 (8)	C16—C11—S1	111.84 (12)
C1—S1—C11	103.73 (8)	C12—C11—S1	109.74 (13)
C8—O1—C7	107.00 (13)	C16—C11—H11	107.7
C8—C1—C2	107.69 (15)	C12—C11—H11	107.7
C8—C1—S1	127.55 (14)	S1—C11—H11	107.7
C2—C1—S1	124.69 (13)	C13—C12—C11	109.64 (16)
C7—C2—C3	119.34 (15)	C13—C12—H12A	109.7
C7—C2—C1	104.60 (15)	C11—C12—H12A	109.7
C3—C2—C1	136.06 (15)	C13—C12—H12B	109.7
C4—C3—C2	116.33 (15)	C11—C12—H12B	109.7
C4—C3—H3	121.8	H12A—C12—H12B	108.2
C2—C3—H3	121.8	C14—C13—C12	111.54 (18)
C3—C4—C5	123.20 (16)	C14—C13—H13A	109.3
C3—C4—Br1	118.84 (12)	C12—C13—H13A	109.3
C5—C4—Br1	117.95 (13)	C14—C13—H13B	109.3
C6—C5—C4	121.37 (15)	C12—C13—H13B	109.3
C6—C5—H5	119.3	H13A—C13—H13B	108.0
C4—C5—H5	119.3	C13—C14—C15	111.59 (17)
C7—C6—C5	114.55 (15)	C13—C14—H14A	109.3
C7—C6—C9	122.37 (16)	C15—C14—H14A	109.3
C5—C6—C9	123.07 (16)	C13—C14—H14B	109.3
O1—C7—C6	124.35 (15)	C15—C14—H14B	109.3
O1—C7—C2	110.43 (14)	H14A—C14—H14B	108.0
C6—C7—C2	125.21 (15)	C14—C15—C16	111.47 (17)
C1—C8—O1	110.27 (15)	C14—C15—H15A	109.3

C1—C8—C10	134.88 (16)	C16—C15—H15A	109.3
O1—C8—C10	114.85 (15)	C14—C15—H15B	109.3
C6—C9—H9A	109.5	C16—C15—H15B	109.3
C6—C9—H9B	109.5	H15A—C15—H15B	108.0
H9A—C9—H9B	109.5	C11—C16—C15	110.14 (16)
C6—C9—H9C	109.5	C11—C16—H16A	109.6
H9A—C9—H9C	109.5	C15—C16—H16A	109.6
H9B—C9—H9C	109.5	C11—C16—H16B	109.6
C8—C10—H10A	109.5	C15—C16—H16B	109.6
C8—C10—H10B	109.5	H16A—C16—H16B	108.1
O3—S1—C1—C8	-20.06 (19)	C9—C6—C7—C2	177.58 (17)
O2—S1—C1—C8	-149.60 (16)	C3—C2—C7—O1	-179.90 (14)
C11—S1—C1—C8	96.84 (17)	C1—C2—C7—O1	0.31 (18)
O3—S1—C1—C2	163.32 (14)	C3—C2—C7—C6	0.7 (3)
O2—S1—C1—C2	33.78 (17)	C1—C2—C7—C6	-179.11 (16)
C11—S1—C1—C2	-79.78 (16)	C2—C1—C8—O1	0.13 (19)
C8—C1—C2—C7	-0.26 (19)	S1—C1—C8—O1	-176.95 (12)
S1—C1—C2—C7	176.92 (13)	C2—C1—C8—C10	-179.71 (19)
C8—C1—C2—C3	179.99 (19)	S1—C1—C8—C10	3.2 (3)
S1—C1—C2—C3	-2.8 (3)	C7—O1—C8—C1	0.06 (18)
C7—C2—C3—C4	-0.2 (2)	C7—O1—C8—C10	179.94 (15)
C1—C2—C3—C4	179.56 (18)	O3—S1—C11—C16	43.02 (15)
C2—C3—C4—C5	0.0 (3)	O2—S1—C11—C16	172.87 (12)
C2—C3—C4—Br1	-178.90 (12)	C1—S1—C11—C16	-73.92 (14)
O2 ⁱ —Br1—C4—C3	56.5 (3)	O3—S1—C11—C12	-81.75 (14)
O2 ⁱ —Br1—C4—C5	-122.5 (3)	O2—S1—C11—C12	48.11 (14)
C3—C4—C5—C6	-0.4 (3)	C1—S1—C11—C12	161.32 (13)
Br1—C4—C5—C6	178.57 (13)	C16—C11—C12—C13	57.1 (2)
C4—C5—C6—C7	0.8 (2)	S1—C11—C12—C13	-178.14 (14)
C4—C5—C6—C9	-177.76 (17)	C11—C12—C13—C14	-56.2 (2)
C8—O1—C7—C6	179.18 (16)	C12—C13—C14—C15	55.8 (2)
C8—O1—C7—C2	-0.24 (18)	C13—C14—C15—C16	-55.0 (3)
C5—C6—C7—O1	179.69 (15)	C12—C11—C16—C15	-56.6 (2)
C9—C6—C7—O1	-1.8 (3)	S1—C11—C16—C15	179.81 (12)
C5—C6—C7—C2	-1.0 (3)	C14—C15—C16—C11	54.9 (2)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C10—H10B \cdots O2 ⁱⁱ	0.98	2.55	3.384 (2)	143

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