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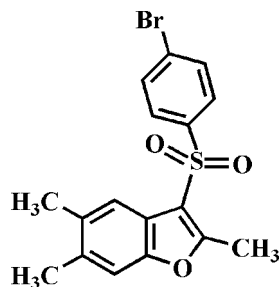
Crystal structure of 3-(4-bromophenylsulfonyl)-2,5,6-trimethyl-1-benzofuran

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In the title compound, C₁₇H₁₅BrO₃S, the dihedral angle between the planes of the benzofuran ring system [r.m.s. deviation = 0.015 (2) Å] and the 4-bromophenyl ring is 89.29 (6)°. In the crystal, molecules are linked into a chain along the *b*-axis direction by C—H... π hydrogen bonds and C—Br... π [3.626 (1) Å] interactions.

1. Chemical context

Molecules containing a benzofuran ring show significant biological properties, such as antibacterial and antifungal (Aslam *et al.*, 2009), antitumor and antiviral (Galal *et al.*, 2009) and antimicrobial activities (Wahab Khan *et al.*, 2005), and are potential inhibitors of β -amyloid aggregation (Ono *et al.*, 2002). Benzofuran compounds occur widely in nature (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our continuing project concerning 3-(arylsulfonyl)-2,5,7-trimethyl-1-benzofuran derivatives, we report herein on the synthesis and crystal structure of the title compound.

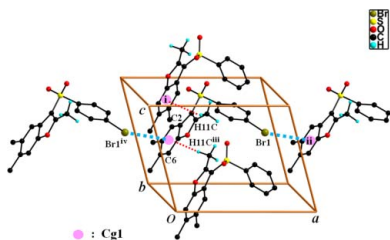


2. Structural commentary

In the title molecule (Fig. 1), the benzofuran unit (O1/C1–C8) is essentially planar, with a mean deviation of 0.015 (2) Å from the mean plane defined by the nine constituent atoms. The 4-bromophenyl ring (C12–C17) is inclined to the benzofuran ring by 89.29 (6)°. The title compound crystallized in the non-centrosymmetric space group *Pc* in spite of having no asymmetric C atoms.

3. Supramolecular features

In the crystal, molecules are linked into a chain along the *b*-axis direction by C—H... π hydrogen bonds (Fig. 2 and Table 1), and by C15—Br1... π interactions between the Br



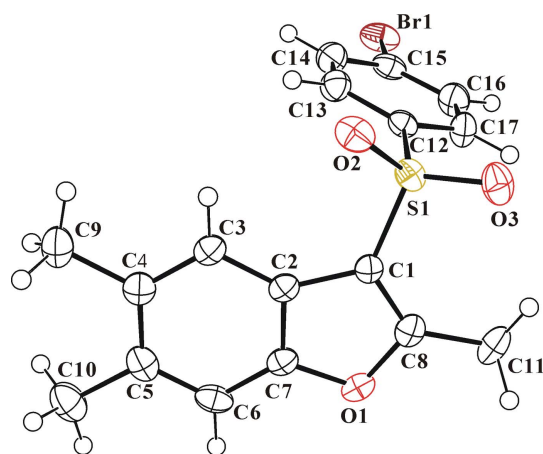


Figure 1
The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

atom and the benzene ring of a neighbouring molecule with a $\text{Br1} \cdots \text{Cg1}^{\text{ii}}$ separation of 3.626 (1) Å [illustrated in Fig. 2; Cg1 is the centroid of the C2–C7 benzene ring; symmetry code: (ii) $x + 1, y, z$].

4. Database survey

A search of the Cambridge Structural Database (Version 5.35, last update May 2014; Groom & Allen, 2014) for 3-(aryl-sulfonyl)benzofuran gave 66 hits. Six of these are 3-aryl-sulfonyl-2,5,7-trimethyl-1-benzofuran derivatives whose structures are closely related to that of the title compound. In these six compounds, the dihedral angle between the aryl-sulfonyl ring and the benzofuran ring varies from *ca* 72.67° in 3-(4-fluorophenylsulfonyl)-2,5,7-trimethyl-1-benzofuran (Choi *et al.*, 2010) to 87.61° in 3-(2-fluorophenylsulfonyl)-2,5,7-trimethyl-1-benzofuran (Choi *et al.*, 2014). These dihedral angles are slightly smaller than the same angle of the title compound [89.29 (6)°].

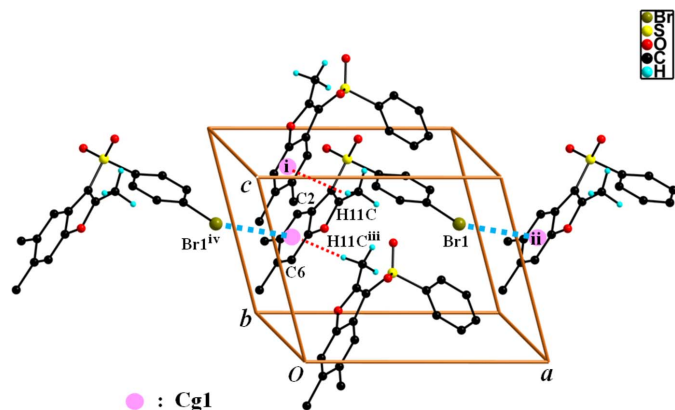


Figure 2
A view of the C–H... π and C–Br... π interactions (dotted lines) in the crystal structure of the title compound. H atoms not participating in hydrogen bonding have been omitted for clarity. [Symmetry codes: (i) $x, -y + 1, z + \frac{1}{2}$; (ii) $x + 1, y, z$; (iii) $x, -y + 1, z - \frac{1}{2}$; (iv) $x - 1, y, z$.]

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

Cg1 is the centroid of the C2–C7 benzene ring.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{C11}-\text{H11B} \cdots \text{Cg1}^{\text{i}}$	0.98	2.89	3.504 (3)	122

Symmetry code: (i) $x, -y + 1, z + \frac{1}{2}$.

5. Synthesis and crystallization

The starting material 3-(4-bromophenylsulfanyl)-2,5,6-trimethyl-1-benzofuran was prepared by a literature method (Choi *et al.*, 1999). 3-Chloroperoxybenzoic acid (77%, 448 mg, 2.0 mmol) was added in small portions to a stirred solution of 3-(4-bromophenylsulfanyl)-2,5,6-trimethyl-1-benzofuran (312 mg, 0.9 mmol) in dichloromethane (30 ml) at 273 K. After being stirred at room temperature for 10 h, the mixture was washed with saturated sodium bicarbonate solution (2×10 ml) 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, 2:1 *v/v*) to afford the title compound as a colorless solid [yield 77%, 263 mg; m.p. 452–453 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 a solution of the title compound (24 mg) in ethyl acetate (20 ml) at room temperature.

Table 2
Experimental details.

Crystal data	
Chemical formula	$\text{C}_{17}\text{H}_{15}\text{BrO}_3\text{S}$
M_r	379.26
Crystal system, space group	Monoclinic, Pc
Temperature (K)	173
a, b, c (Å)	11.3395 (3), 8.0093 (2), 9.0439 (2)
β (°)	108.800 (1)
V (Å ³)	777.56 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	2.79
Crystal size (mm)	0.21 \times 0.17 \times 0.15
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (SADABS; Bruker, 2009)
$T_{\text{min}}, T_{\text{max}}$	0.643, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12777, 3392, 3136
R_{int}	0.030
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.639
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.024, 0.056, 1.00
No. of reflections	3392
No. of parameters	202
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.32, -0.37
Absolute structure	Flack (1983), 1710 Friedel pairs
Absolute structure parameter	-0.001 (6)

Computer programs: APEX2 and SAINT (Bruker, 2009), SHELXS97 and SHELXL97 (Sheldrick, 2008), ORTEP-3 for Windows (Farrugia, 2012) and DIAMOND (Brandenburg, 1998).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were positioned geometrically and refined using a riding model, with C–H = 0.95 for aryl and 0.98 Å for methyl H atoms, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aryl and $1.5U_{\text{eq}}(\text{C})$ for methyl H atoms.

Acknowledgements

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supporting information

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Crystal structure of 3-(4-bromophenylsulfonyl)-2,5,6-trimethyl-1-benzofuran

Hong Dae Choi and Uk Lee

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); 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, 2012) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

3-(4-Bromophenylsulfonyl)-2,5,6-trimethyl-1-benzofuran

Crystal data

$C_{17}H_{15}BrO_3S$

$M_r = 379.26$

Monoclinic, *Pc*

Hall symbol: P -2yc

$a = 11.3395$ (3) Å

$b = 8.0093$ (2) Å

$c = 9.0439$ (2) Å

$\beta = 108.800$ (1)°

$V = 777.56$ (3) Å³

$Z = 2$

$F(000) = 384$

$D_x = 1.620$ Mg m⁻³

Melting point = 453–452 K

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

Cell parameters from 6185 reflections

$\theta = 2.5$ – 27.5 °

$\mu = 2.79$ mm⁻¹

$T = 173$ K

Block, colourless

$0.21 \times 0.17 \times 0.15$ 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)

$T_{\min} = 0.643$, $T_{\max} = 0.746$

12777 measured reflections

3392 independent reflections

3136 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\max} = 27.0$ °, $\theta_{\min} = 1.9$ °

$h = -14 \rightarrow 14$

$k = -10 \rightarrow 10$

$l = -11 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.056$

$S = 1.00$

3392 reflections

202 parameters

2 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

$w = 1/[\sigma^2(F_o^2) + (0.0201P)^2]$

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

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

$\Delta\rho_{\max} = 0.32$ e Å⁻³

$\Delta\rho_{\min} = -0.37$ e Å⁻³

Absolute structure: Flack (1983), 1710 Friedel pairs

Absolute structure parameter: $-0.001(6)$

Special details

Experimental. ^1H NMR (δ p.p.m., CDCl_3 , 400 Hz): 7.85 (d, $J = 8.56$ Hz, 2H), 7.63 (d, $J = 8.21$ Hz, 2H), 7.58 (s, 1H), 7.20(s, 1H), 2.76 (s, 3H), 2.34 (s, 3H), 2.32 (s, 3H).

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	0.89314 (3)	0.76274 (4)	0.54426 (3)	0.04023 (8)
S1	0.49513 (5)	0.71962 (7)	0.90695 (6)	0.02534 (13)
O1	0.27996 (15)	0.39863 (18)	0.61667 (18)	0.0275 (4)
O2	0.44621 (15)	0.8818 (2)	0.92194 (19)	0.0325 (4)
O3	0.54542 (16)	0.6177 (2)	1.04338 (19)	0.0357 (4)
C1	0.3808 (2)	0.6097 (2)	0.7663 (2)	0.0212 (4)
C2	0.2883 (2)	0.6820 (3)	0.6333 (2)	0.0229 (4)
C3	0.2506 (2)	0.8416 (3)	0.5766 (3)	0.0256 (5)
H3	0.2894	0.9370	0.6343	0.031*
C4	0.1567 (2)	0.8602 (3)	0.4364 (3)	0.0278 (5)
C5	0.0994 (2)	0.7185 (3)	0.3471 (3)	0.0301 (6)
C6	0.1362 (2)	0.5613 (3)	0.4028 (3)	0.0305 (5)
H6	0.0986	0.4653	0.3451	0.037*
C7	0.22934 (19)	0.5462 (3)	0.5449 (3)	0.0239 (5)
C8	0.3733 (2)	0.4408 (3)	0.7508 (3)	0.0258 (5)
C9	0.1161 (3)	1.0346 (3)	0.3779 (3)	0.0373 (6)
H9A	0.1698	1.1164	0.4489	0.056*
H9B	0.0295	1.0520	0.3740	0.056*
H9C	0.1224	1.0485	0.2731	0.056*
C10	$-0.0008(3)$	0.7398 (3)	0.1912 (3)	0.0429 (7)
H10A	-0.0211	0.6310	0.1397	0.064*
H10B	0.0289	0.8152	0.1255	0.064*
H10C	-0.0755	0.7872	0.2071	0.064*
C11	0.4438 (3)	0.3001 (3)	0.8427 (3)	0.0360 (6)
H11A	0.4959	0.3405	0.9453	0.054*
H11B	0.4968	0.2505	0.7876	0.054*
H11C	0.3856	0.2157	0.8564	0.054*
C12	0.6123 (2)	0.7434 (3)	0.8190 (3)	0.0238 (5)
C13	0.6082 (2)	0.8757 (3)	0.7190 (3)	0.0303 (5)
H12	0.5469	0.9605	0.7046	0.036*
C14	0.6935 (2)	0.8833 (3)	0.6407 (3)	0.0334 (6)

H13	0.6915	0.9737	0.5719	0.040*
C15	0.7818 (3)	0.7605 (3)	0.6615 (3)	0.0293 (5)
C16	0.7893 (2)	0.6306 (3)	0.7645 (3)	0.0349 (6)
H15	0.8527	0.5485	0.7810	0.042*
C17	0.7032 (2)	0.6216 (3)	0.8436 (3)	0.0303 (5)
H16	0.7065	0.5325	0.9141	0.036*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03614 (13)	0.05357 (16)	0.03812 (15)	−0.01553 (15)	0.02190 (11)	−0.01138 (13)
S1	0.0241 (3)	0.0324 (3)	0.0203 (3)	0.0013 (3)	0.0082 (2)	−0.0013 (2)
O1	0.0323 (9)	0.0210 (8)	0.0336 (9)	−0.0030 (7)	0.0169 (8)	−0.0009 (6)
O2	0.0313 (9)	0.0347 (9)	0.0323 (9)	0.0021 (7)	0.0112 (7)	−0.0124 (7)
O3	0.0357 (9)	0.0502 (11)	0.0226 (8)	0.0051 (8)	0.0114 (7)	0.0069 (7)
C1	0.0213 (11)	0.0242 (10)	0.0208 (10)	0.0003 (9)	0.0103 (9)	0.0011 (8)
C2	0.0228 (11)	0.0243 (11)	0.0255 (12)	−0.0008 (9)	0.0133 (9)	0.0007 (8)
C3	0.0251 (11)	0.0244 (11)	0.0317 (12)	0.0005 (9)	0.0153 (9)	0.0010 (9)
C4	0.0250 (12)	0.0338 (13)	0.0299 (13)	0.0008 (9)	0.0161 (10)	0.0038 (9)
C5	0.0234 (13)	0.0464 (14)	0.0242 (13)	0.0020 (10)	0.0129 (11)	0.0049 (10)
C6	0.0252 (12)	0.0384 (13)	0.0309 (14)	−0.0081 (10)	0.0134 (11)	−0.0089 (10)
C7	0.0238 (11)	0.0229 (11)	0.0296 (13)	−0.0006 (9)	0.0148 (10)	−0.0005 (9)
C8	0.0270 (12)	0.0294 (11)	0.0273 (12)	0.0029 (9)	0.0174 (10)	0.0043 (9)
C9	0.0347 (13)	0.0419 (16)	0.0367 (13)	0.0083 (12)	0.0133 (11)	0.0108 (11)
C10	0.0337 (15)	0.0618 (19)	0.0312 (16)	0.0002 (12)	0.0075 (13)	0.0040 (12)
C11	0.0455 (15)	0.0251 (12)	0.0447 (16)	0.0075 (11)	0.0245 (13)	0.0107 (10)
C12	0.0223 (11)	0.0286 (11)	0.0198 (12)	−0.0025 (9)	0.0058 (10)	−0.0033 (8)
C13	0.0296 (12)	0.0283 (12)	0.0331 (13)	0.0018 (10)	0.0105 (10)	0.0006 (10)
C14	0.0346 (14)	0.0358 (14)	0.0305 (13)	−0.0040 (11)	0.0117 (11)	0.0044 (10)
C15	0.0241 (12)	0.0400 (13)	0.0256 (13)	−0.0092 (10)	0.0107 (10)	−0.0073 (9)
C16	0.0268 (12)	0.0400 (14)	0.0399 (14)	0.0035 (11)	0.0135 (11)	0.0043 (11)
C17	0.0280 (12)	0.0338 (13)	0.0308 (13)	0.0070 (10)	0.0115 (10)	0.0095 (10)

Geometric parameters (Å, °)

Br1—C15	1.892 (3)	C9—H9A	0.9800
S1—O3	1.4354 (17)	C9—H9B	0.9800
S1—O2	1.4360 (17)	C9—H9C	0.9800
S1—C1	1.735 (2)	C10—H10A	0.9800
S1—C12	1.765 (3)	C10—H10B	0.9800
O1—C8	1.371 (3)	C10—H10C	0.9800
O1—C7	1.381 (2)	C11—H11A	0.9800
C1—C8	1.360 (3)	C11—H11B	0.9800
C1—C2	1.439 (3)	C11—H11C	0.9800
C2—C7	1.388 (3)	C12—C17	1.384 (3)
C2—C3	1.392 (3)	C12—C13	1.384 (3)
C3—C4	1.376 (3)	C13—C14	1.372 (3)
C3—H3	0.9500	C13—H12	0.9500

C4—C5	1.423 (3)	C14—C15	1.372 (4)
C4—C9	1.512 (3)	C14—H13	0.9500
C5—C6	1.370 (3)	C15—C16	1.381 (4)
C5—C10	1.508 (4)	C16—C17	1.386 (3)
C6—C7	1.381 (3)	C16—H15	0.9500
C6—H6	0.9500	C17—H16	0.9500
C8—C11	1.473 (3)		
O3—S1—O2	119.46 (10)	C4—C9—H9C	109.5
O3—S1—C1	109.74 (10)	H9A—C9—H9C	109.5
O2—S1—C1	107.95 (10)	H9B—C9—H9C	109.5
O3—S1—C12	107.50 (11)	C5—C10—H10A	109.5
O2—S1—C12	108.34 (11)	C5—C10—H10B	109.5
C1—S1—C12	102.55 (11)	H10A—C10—H10B	109.5
C8—O1—C7	106.92 (16)	C5—C10—H10C	109.5
C8—C1—C2	108.04 (19)	H10A—C10—H10C	109.5
C8—C1—S1	125.97 (18)	H10B—C10—H10C	109.5
C2—C1—S1	125.47 (16)	C8—C11—H11A	109.5
C7—C2—C3	118.3 (2)	C8—C11—H11B	109.5
C7—C2—C1	104.63 (19)	H11A—C11—H11B	109.5
C3—C2—C1	137.1 (2)	C8—C11—H11C	109.5
C4—C3—C2	119.6 (2)	H11A—C11—H11C	109.5
C4—C3—H3	120.2	H11B—C11—H11C	109.5
C2—C3—H3	120.2	C17—C12—C13	120.7 (2)
C3—C4—C5	120.8 (2)	C17—C12—S1	118.77 (18)
C3—C4—C9	118.7 (2)	C13—C12—S1	120.39 (19)
C5—C4—C9	120.4 (2)	C14—C13—C12	119.4 (2)
C6—C5—C4	119.7 (2)	C14—C13—H12	120.3
C6—C5—C10	119.8 (2)	C12—C13—H12	120.3
C4—C5—C10	120.6 (2)	C15—C14—C13	120.1 (2)
C5—C6—C7	118.3 (2)	C15—C14—H13	119.9
C5—C6—H6	120.8	C13—C14—H13	119.9
C7—C6—H6	120.8	C14—C15—C16	121.1 (3)
O1—C7—C6	126.2 (2)	C14—C15—Br1	120.3 (2)
O1—C7—C2	110.48 (19)	C16—C15—Br1	118.5 (2)
C6—C7—C2	123.3 (2)	C15—C16—C17	119.1 (2)
C1—C8—O1	109.9 (2)	C15—C16—H15	120.4
C1—C8—C11	134.3 (2)	C17—C16—H15	120.4
O1—C8—C11	115.8 (2)	C12—C17—C16	119.5 (2)
C4—C9—H9A	109.5	C12—C17—H16	120.2
C4—C9—H9B	109.5	C16—C17—H16	120.2
H9A—C9—H9B	109.5		
O3—S1—C1—C8	-26.6 (2)	C1—C2—C7—O1	0.4 (2)
O2—S1—C1—C8	-158.29 (18)	C3—C2—C7—C6	0.7 (3)
C12—S1—C1—C8	87.4 (2)	C1—C2—C7—C6	-177.6 (2)
O3—S1—C1—C2	162.75 (18)	C2—C1—C8—O1	-0.9 (2)
O2—S1—C1—C2	31.0 (2)	S1—C1—C8—O1	-172.93 (15)

C12—S1—C1—C2	-83.2 (2)	C2—C1—C8—C11	177.4 (3)
C8—C1—C2—C7	0.3 (2)	S1—C1—C8—C11	5.4 (4)
S1—C1—C2—C7	172.36 (16)	C7—O1—C8—C1	1.2 (2)
C8—C1—C2—C3	-177.5 (2)	C7—O1—C8—C11	-177.5 (2)
S1—C1—C2—C3	-5.4 (4)	O3—S1—C12—C17	25.8 (2)
C7—C2—C3—C4	0.3 (3)	O2—S1—C12—C17	156.21 (19)
C1—C2—C3—C4	177.8 (2)	C1—S1—C12—C17	-89.8 (2)
C2—C3—C4—C5	-1.3 (3)	O3—S1—C12—C13	-158.47 (19)
C2—C3—C4—C9	179.2 (2)	O2—S1—C12—C13	-28.1 (2)
C3—C4—C5—C6	1.4 (4)	C1—S1—C12—C13	85.9 (2)
C9—C4—C5—C6	-179.1 (2)	C17—C12—C13—C14	1.6 (4)
C3—C4—C5—C10	-178.2 (2)	S1—C12—C13—C14	-173.97 (18)
C9—C4—C5—C10	1.3 (4)	C12—C13—C14—C15	0.1 (4)
C4—C5—C6—C7	-0.4 (4)	C13—C14—C15—C16	-2.1 (4)
C10—C5—C6—C7	179.2 (2)	C13—C14—C15—Br1	176.07 (19)
C8—O1—C7—C6	177.0 (2)	C14—C15—C16—C17	2.3 (4)
C8—O1—C7—C2	-1.0 (2)	Br1—C15—C16—C17	-175.84 (18)
C5—C6—C7—O1	-178.3 (2)	C13—C12—C17—C16	-1.4 (4)
C5—C6—C7—C2	-0.6 (3)	S1—C12—C17—C16	174.32 (19)
C3—C2—C7—O1	178.70 (17)	C15—C16—C17—C12	-0.6 (4)

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the C2—C7 benzene ring.

<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>
C11—H11B \cdots Cg1 ⁱ	0.98	2.89	3.504 (3)	122

Symmetry code: (i) *x*, -*y*+1, *z*+1/2.