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3-(4-Bromophenylsulfinyl)-5-cyclohexyl-2-methyl-1-benzofuran

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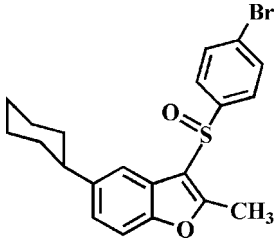
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.097; data-to-parameter ratio = 20.5.

In the title compound, $C_{21}H_{21}BrO_2S$, the cyclohexyl ring adopts a chair conformation. The 4-bromophenyl ring makes a dihedral angle of 81.62 (6)° with the mean plane of the benzofuran fragment. In the crystal, molecules are linked by weak C—H···O and C—H···π interactions. The crystal structure also exhibits a slipped π–π interaction between the furan rings of neighbouring molecules [centroid–centroid distances = 3.540 (3) Å, interplanar distance = 3.481 (3) Å and slippage = 0.644 (3) Å].

Related literature

For the biological 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 the crystal structures of related compounds, see: Choi *et al.* (2011*a*,*b*).



Experimental

Crystal data

$C_{21}H_{21}BrO_2S$
M_r = 417.35
Monoclinic, $P2_1/c$
a = 16.7340 (4) Å
b = 8.8290 (2) Å
c = 13.0178 (3) Å
β = 105.197 (1)°
V = 1856.05 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.34 mm^{-1}
T = 173 K
0.25 × 0.23 × 0.11 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.561, T_{max} = 0.746
17836 measured reflections
4653 independent reflections
3467 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.097
S = 1.04
4653 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

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

*Cg*2 is the centroid of the C2–C7 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17···O2^{i}	0.95	2.47	3.112 (3)	125
C15—H15B···*Cg*2^{ii}	0.98	3.06	3.532 (3)	111

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FF2048).

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supplementary materials

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3-(4-Bromophenylsulfinyl)-5-cyclohexyl-2-methyl-1-benzofuran

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Comment

Substituted benzofuran derivatives have drawn much interest due to their valuable biological 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 benzofuran derivatives occur in a wide range of natural products (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our ongoing study of 5-cyclohexyl-1-benzofuran derivatives containing either 3-(4-fluorophenylsulfinyl) (Choi *et al.*, 2011*a*) or 3-phenylsulfinyl (Choi *et al.*, 2011*b*) substituents, 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 (2) Å from the least-squares plane defined by the nine constituent atoms. The cyclohexyl ring has the chair form. The dihedral angle formed by the 4-bromophenyl ring and the mean plane of the benzofuran fragment is 81.62 (6)°. The crystal packing (Fig. 2) is stabilized by weak intermolecular C—H···O hydrogen bonds (Table 1; first entry) and intermolecular C—H···π interactions (Table 1; second entry, Cg2 is the centroid of the C2–C7 benzene ring). The crystal packing (Fig. 2) is further stabilized by a weak slipped π···π interaction between the furan rings of adjacent molecules, with a Cg1···Cg1^{ii} distance of 3.540 (3) Å and an interplanar distance of 3.481 (3) Å resulting in a slippage of 0.644 (3) Å (Cg1 is the centroid of the C1/C2/C7/O1/C8 furan ring).

Experimental

77% 3-chloroperoxybenzoic acid (202 mg, 0.9 mmol) was added in small portions to a stirred solution of 3-(4-bromophenylsulfanyl)-5-cyclohexyl-2-methyl-1-benzofuran (321 mg, 0.8 mmol) in dichloromethane (30 mL) at 273 K. After being stirred at room temperature for 6h, 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, 2:1 v/v) to afford the title compound as a colorless solid [yield 71%, m.p. 461–462 K; R_f = 0.47 (hexane–ethyl acetate, 2:1 v/v)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title compound in ethyl acetate at room temperature.

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_{iso}(H) =1.2U_{eq}(C) for aryl, methine and methylene, and 1.5U_{eq}(C) for methyl H atoms.

Figures

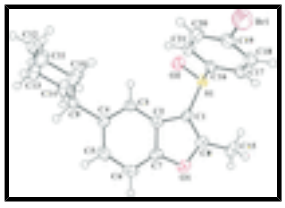


Fig. 1. The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

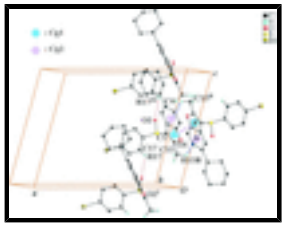


Fig. 2. A view of the C—H···O, C—H···π and π···π interactions (dotted lines). H atoms non-participating in hydrogen-bonding were omitted for clarity. [Symmetry codes: (i) *x*, - *y* + 3/2, *z* - 1/2; (ii) - *x*, - *y* + 1, - *z* + 1; (iii) *x*, - *y* + 3/2, *z* + 1/2 .]

3-(4-Bromophenylsulfinyl)-5-cyclohexyl-2-methyl-1-benzofuran

Crystal data

$C_{21}H_{21}BrO_2S$	$F(000) = 856$
$M_r = 417.35$	$D_x = 1.494$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 6823 reflections
$a = 16.7340$ (4) Å	$\theta = 2.5$–$25.9°$
$b = 8.8290$ (2) Å	$\mu = 2.34$ mm^{-1}
$c = 13.0178$ (3) Å	$T = 173$ K
$\beta = 105.197$ (1)°	Block, colourless
$V = 1856.05$ (7) Å^3	0.25 × 0.23 × 0.11 mm
$Z = 4$	

Data collection

Bruker SMART APEXII CCD diffractometer	4653 independent reflections
Radiation source: rotating anode	3467 reflections with $I > 2\sigma(I)$
graphite multilayer	$R_{int} = 0.039$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 28.4°$, $\theta_{min} = 1.3°$
φ and ω scans	$h = -21 \rightarrow 22$
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)	$k = -9 \rightarrow 11$
$T_{min} = 0.561$, $T_{max} = 0.746$	$l = -17 \rightarrow 15$
17836 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods

Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.037$	Hydrogen site location: difference Fourier map
$wR(F^2) = 0.097$	H-atom parameters constrained
$S = 1.04$	$w = 1/[\sigma^2(F_o^2) + (0.0422P)^2 + 0.7692P]$ where $P = (F_o^2 + 2F_c^2)/3$
4653 reflections	$(\Delta/\sigma)_{max} = 0.001$
227 parameters	$\Delta\rho_{max} = 0.52$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.61$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.468766 (17)	0.59993 (4)	0.30483 (2)	0.06137 (12)
S1	0.13569 (3)	0.72783 (5)	0.44840 (4)	0.03017 (13)
O1	0.03213 (8)	0.32472 (16)	0.40283 (11)	0.0312 (3)
O2	0.15901 (10)	0.78663 (16)	0.55882 (12)	0.0384 (4)
C1	0.10321 (12)	0.5392 (2)	0.45372 (15)	0.0259 (4)
C2	0.13294 (12)	0.4289 (2)	0.53755 (16)	0.0246 (4)
C3	0.19099 (12)	0.4260 (2)	0.63618 (16)	0.0253 (4)
H3	0.2228	0.5135	0.6625	0.030*
C4	0.20162 (12)	0.2931 (2)	0.69560 (16)	0.0267 (4)
C5	0.15359 (13)	0.1661 (2)	0.65496 (18)	0.0328 (5)
H5	0.1613	0.0759	0.6962	0.039*
C6	0.09542 (13)	0.1663 (2)	0.55754 (18)	0.0335 (5)
H6	0.0635	0.0790	0.5309	0.040*
C7	0.08631 (12)	0.2995 (2)	0.50145 (16)	0.0279 (4)
C8	0.04359 (12)	0.4725 (2)	0.37654 (16)	0.0285 (4)
C9	0.26423 (12)	0.2852 (2)	0.80359 (16)	0.0287 (4)
H9	0.2630	0.1795	0.8308	0.034*
C10	0.35211 (13)	0.3162 (3)	0.79681 (18)	0.0404 (5)
H10A	0.3547	0.4182	0.7663	0.048*
H10B	0.3675	0.2412	0.7487	0.048*
C11	0.41427 (14)	0.3071 (3)	0.90723 (19)	0.0435 (6)
H11A	0.4164	0.2018	0.9340	0.052*
H11B	0.4702	0.3341	0.9008	0.052*

C12	0.39071 (16)	0.4119 (3)	0.9856 (2)	0.0460 (6)
H12A	0.3950	0.5181	0.9633	0.055*
H12B	0.4298	0.3982	1.0566	0.055*
C13	0.30362 (16)	0.3820 (3)	0.99321 (19)	0.0480 (6)
H13A	0.2887	0.4573	1.0414	0.058*
H13B	0.3009	0.2801	1.0238	0.058*
C14	0.24169 (15)	0.3912 (3)	0.88407 (19)	0.0409 (5)
H14A	0.1859	0.3648	0.8911	0.049*
H14B	0.2397	0.4966	0.8575	0.049*
C15	−0.00823 (13)	0.5249 (3)	0.27284 (17)	0.0374 (5)
H15A	−0.0039	0.6352	0.2681	0.056*
H15B	−0.0660	0.4967	0.2660	0.056*
H15C	0.0108	0.4774	0.2154	0.056*
C16	0.22978 (13)	0.6877 (2)	0.41199 (15)	0.0275 (4)
C17	0.22676 (14)	0.6868 (2)	0.30470 (16)	0.0320 (5)
H17	0.1759	0.7059	0.2532	0.038*
C18	0.29773 (15)	0.6579 (2)	0.27262 (17)	0.0358 (5)
H18	0.2960	0.6548	0.1991	0.043*
C19	0.37075 (15)	0.6337 (3)	0.34865 (19)	0.0374 (5)
C20	0.37513 (14)	0.6356 (3)	0.45633 (19)	0.0388 (5)
H20	0.4263	0.6186	0.5076	0.047*
C21	0.30379 (13)	0.6628 (2)	0.48822 (17)	0.0337 (5)
H21	0.3055	0.6644	0.5617	0.040*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.04820 (18)	0.0874 (2)	0.0565 (2)	−0.00961 (14)	0.02786 (14)	−0.00300 (14)
S1	0.0388 (3)	0.0241 (2)	0.0259 (3)	0.0038 (2)	0.0053 (2)	0.0013 (2)
O1	0.0262 (7)	0.0341 (8)	0.0312 (8)	−0.0033 (6)	0.0036 (6)	−0.0058 (6)
O2	0.0513 (9)	0.0334 (8)	0.0294 (8)	−0.0014 (7)	0.0086 (7)	−0.0065 (6)
C1	0.0268 (10)	0.0256 (10)	0.0244 (10)	0.0022 (8)	0.0050 (8)	−0.0019 (8)
C2	0.0238 (9)	0.0232 (9)	0.0277 (10)	0.0023 (7)	0.0083 (8)	−0.0011 (8)
C3	0.0250 (10)	0.0229 (9)	0.0278 (10)	−0.0009 (7)	0.0068 (8)	−0.0013 (8)
C4	0.0245 (9)	0.0268 (10)	0.0295 (11)	0.0028 (8)	0.0079 (8)	0.0023 (8)
C5	0.0322 (11)	0.0257 (10)	0.0412 (13)	0.0000 (8)	0.0110 (9)	0.0056 (9)
C6	0.0292 (11)	0.0263 (10)	0.0445 (13)	−0.0068 (8)	0.0089 (9)	−0.0030 (9)
C7	0.0215 (9)	0.0319 (11)	0.0302 (11)	−0.0005 (8)	0.0065 (8)	−0.0048 (8)
C8	0.0260 (10)	0.0318 (10)	0.0286 (11)	0.0031 (8)	0.0085 (8)	−0.0037 (8)
C9	0.0278 (10)	0.0243 (10)	0.0323 (11)	0.0014 (8)	0.0051 (8)	0.0069 (8)
C10	0.0278 (11)	0.0626 (15)	0.0306 (12)	0.0051 (10)	0.0074 (9)	0.0004 (11)
C11	0.0280 (11)	0.0610 (16)	0.0385 (13)	0.0035 (11)	0.0034 (10)	0.0069 (11)
C12	0.0514 (15)	0.0446 (14)	0.0345 (13)	−0.0050 (11)	−0.0023 (11)	0.0016 (10)
C13	0.0556 (16)	0.0619 (16)	0.0264 (12)	0.0096 (12)	0.0105 (11)	0.0013 (11)
C14	0.0390 (13)	0.0524 (14)	0.0341 (13)	0.0105 (10)	0.0145 (10)	0.0074 (10)
C15	0.0310 (11)	0.0516 (14)	0.0268 (11)	0.0063 (10)	0.0022 (9)	−0.0037 (10)
C16	0.0378 (11)	0.0208 (9)	0.0232 (10)	−0.0040 (8)	0.0067 (9)	0.0006 (7)
C17	0.0428 (12)	0.0264 (10)	0.0238 (10)	−0.0037 (9)	0.0033 (9)	0.0026 (8)

C18	0.0509 (14)	0.0330 (11)	0.0247 (11)	−0.0086 (10)	0.0120 (10)	0.0007 (9)
C19	0.0391 (12)	0.0377 (12)	0.0382 (13)	−0.0088 (10)	0.0151 (10)	−0.0013 (10)
C20	0.0341 (12)	0.0480 (13)	0.0311 (12)	−0.0070 (10)	0.0026 (9)	−0.0006 (10)
C21	0.0403 (12)	0.0374 (11)	0.0212 (10)	−0.0064 (9)	0.0040 (9)	−0.0003 (9)

Geometric parameters (Å, °)

Br1—C19	1.896 (2)	C11—C12	1.505 (4)
S1—O2	1.4812 (15)	C11—H11A	0.9900
S1—C1	1.759 (2)	C11—H11B	0.9900
S1—C16	1.795 (2)	C12—C13	1.510 (4)
O1—C8	1.375 (3)	C12—H12A	0.9900
O1—C7	1.382 (2)	C12—H12B	0.9900
C1—C8	1.351 (3)	C13—C14	1.525 (3)
C1—C2	1.450 (3)	C13—H13A	0.9900
C2—C3	1.392 (3)	C13—H13B	0.9900
C2—C7	1.394 (3)	C14—H14A	0.9900
C3—C4	1.391 (3)	C14—H14B	0.9900
C3—H3	0.9500	C15—H15A	0.9800
C4—C5	1.400 (3)	C15—H15B	0.9800
C4—C9	1.519 (3)	C15—H15C	0.9800
C5—C6	1.382 (3)	C16—C17	1.384 (3)
C5—H5	0.9500	C16—C21	1.386 (3)
C6—C7	1.372 (3)	C17—C18	1.382 (3)
C6—H6	0.9500	C17—H17	0.9500
C8—C15	1.475 (3)	C18—C19	1.373 (3)
C9—C10	1.521 (3)	C18—H18	0.9500
C9—C14	1.524 (3)	C19—C20	1.384 (3)
C9—H9	1.0000	C20—C21	1.384 (3)
C10—C11	1.540 (3)	C20—H20	0.9500
C10—H10A	0.9900	C21—H21	0.9500
C10—H10B	0.9900		
O2—S1—C1	107.40 (9)	C10—C11—H11B	109.3
O2—S1—C16	107.42 (9)	H11A—C11—H11B	108.0
C1—S1—C16	97.18 (9)	C11—C12—C13	111.4 (2)
C8—O1—C7	106.49 (15)	C11—C12—H12A	109.3
C8—C1—C2	107.95 (17)	C13—C12—H12A	109.3
C8—C1—S1	123.96 (16)	C11—C12—H12B	109.3
C2—C1—S1	128.09 (15)	C13—C12—H12B	109.3
C3—C2—C7	119.31 (18)	H12A—C12—H12B	108.0
C3—C2—C1	136.49 (18)	C12—C13—C14	111.2 (2)
C7—C2—C1	104.20 (17)	C12—C13—H13A	109.4
C4—C3—C2	119.01 (18)	C14—C13—H13A	109.4
C4—C3—H3	120.5	C12—C13—H13B	109.4
C2—C3—H3	120.5	C14—C13—H13B	109.4
C3—C4—C5	119.23 (18)	H13A—C13—H13B	108.0
C3—C4—C9	120.69 (17)	C9—C14—C13	112.17 (19)
C5—C4—C9	120.08 (17)	C9—C14—H14A	109.2
C6—C5—C4	122.86 (19)	C13—C14—H14A	109.2

C6—C5—H5	118.6	C9—C14—H14B	109.2
C4—C5—H5	118.6	C13—C14—H14B	109.2
C7—C6—C5	116.29 (19)	H14A—C14—H14B	107.9
C7—C6—H6	121.9	C8—C15—H15A	109.5
C5—C6—H6	121.9	C8—C15—H15B	109.5
C6—C7—O1	125.95 (18)	H15A—C15—H15B	109.5
C6—C7—C2	123.30 (19)	C8—C15—H15C	109.5
O1—C7—C2	110.74 (17)	H15A—C15—H15C	109.5
C1—C8—O1	110.62 (17)	H15B—C15—H15C	109.5
C1—C8—C15	133.38 (19)	C17—C16—C21	120.7 (2)
O1—C8—C15	115.99 (17)	C17—C16—S1	117.72 (16)
C4—C9—C10	112.38 (17)	C21—C16—S1	121.55 (16)
C4—C9—C14	111.90 (17)	C18—C17—C16	119.9 (2)
C10—C9—C14	110.29 (18)	C18—C17—H17	120.0
C4—C9—H9	107.3	C16—C17—H17	120.0
C10—C9—H9	107.3	C19—C18—C17	118.9 (2)
C14—C9—H9	107.3	C19—C18—H18	120.5
C9—C10—C11	111.30 (18)	C17—C18—H18	120.5
C9—C10—H10A	109.4	C18—C19—C20	121.9 (2)
C11—C10—H10A	109.4	C18—C19—Br1	118.97 (18)
C9—C10—H10B	109.4	C20—C19—Br1	119.09 (18)
C11—C10—H10B	109.4	C21—C20—C19	119.0 (2)
H10A—C10—H10B	108.0	C21—C20—H20	120.5
C12—C11—C10	111.59 (19)	C19—C20—H20	120.5
C12—C11—H11A	109.3	C20—C21—C16	119.5 (2)
C10—C11—H11A	109.3	C20—C21—H21	120.3
C12—C11—H11B	109.3	C16—C21—H21	120.3
O2—S1—C1—C8	146.84 (17)	C7—O1—C8—C15	179.75 (17)
C16—S1—C1—C8	−102.33 (18)	C3—C4—C9—C10	−60.3 (2)
O2—S1—C1—C2	−32.9 (2)	C5—C4—C9—C10	119.9 (2)
C16—S1—C1—C2	77.98 (19)	C3—C4—C9—C14	64.4 (2)
C8—C1—C2—C3	−178.9 (2)	C5—C4—C9—C14	−115.3 (2)
S1—C1—C2—C3	0.8 (4)	C4—C9—C10—C11	−179.87 (18)
C8—C1—C2—C7	0.1 (2)	C14—C9—C10—C11	54.5 (3)
S1—C1—C2—C7	179.79 (15)	C9—C10—C11—C12	−55.4 (3)
C7—C2—C3—C4	0.8 (3)	C10—C11—C12—C13	55.4 (3)
C1—C2—C3—C4	179.7 (2)	C11—C12—C13—C14	−55.1 (3)
C2—C3—C4—C5	−0.2 (3)	C4—C9—C14—C13	179.11 (19)
C2—C3—C4—C9	−179.96 (17)	C10—C9—C14—C13	−55.0 (3)
C3—C4—C5—C6	0.0 (3)	C12—C13—C14—C9	55.4 (3)
C9—C4—C5—C6	179.74 (19)	O2—S1—C16—C17	−156.18 (15)
C4—C5—C6—C7	−0.3 (3)	C1—S1—C16—C17	92.99 (16)
C5—C6—C7—O1	179.92 (18)	O2—S1—C16—C21	21.95 (19)
C5—C6—C7—C2	0.9 (3)	C1—S1—C16—C21	−88.88 (18)
C8—O1—C7—C6	−179.9 (2)	C21—C16—C17—C18	1.2 (3)
C8—O1—C7—C2	−0.8 (2)	S1—C16—C17—C18	179.39 (15)
C3—C2—C7—C6	−1.2 (3)	C16—C17—C18—C19	−1.4 (3)
C1—C2—C7—C6	179.60 (19)	C17—C18—C19—C20	0.8 (3)
C3—C2—C7—O1	179.69 (17)	C17—C18—C19—Br1	−178.19 (15)

C1—C2—C7—O1	0.5 (2)	C18—C19—C20—C21	−0.1 (3)
C2—C1—C8—O1	−0.6 (2)	Br1—C19—C20—C21	178.94 (17)
S1—C1—C8—O1	179.68 (13)	C19—C20—C21—C16	−0.1 (3)
C2—C1—C8—C15	−179.2 (2)	C17—C16—C21—C20	−0.5 (3)
S1—C1—C8—C15	1.1 (3)	S1—C16—C21—C20	−178.55 (17)
C7—O1—C8—C1	0.9 (2)		

Hydrogen-bond geometry (Å, °)

Cg2 is the centroid of the C2–C7 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17···O2^{i}	0.95	2.47	3.112 (3)	125.
C15—H15B···Cg2^{ii}	0.98	3.06	3.532 (3)	111.

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

Fig. 1

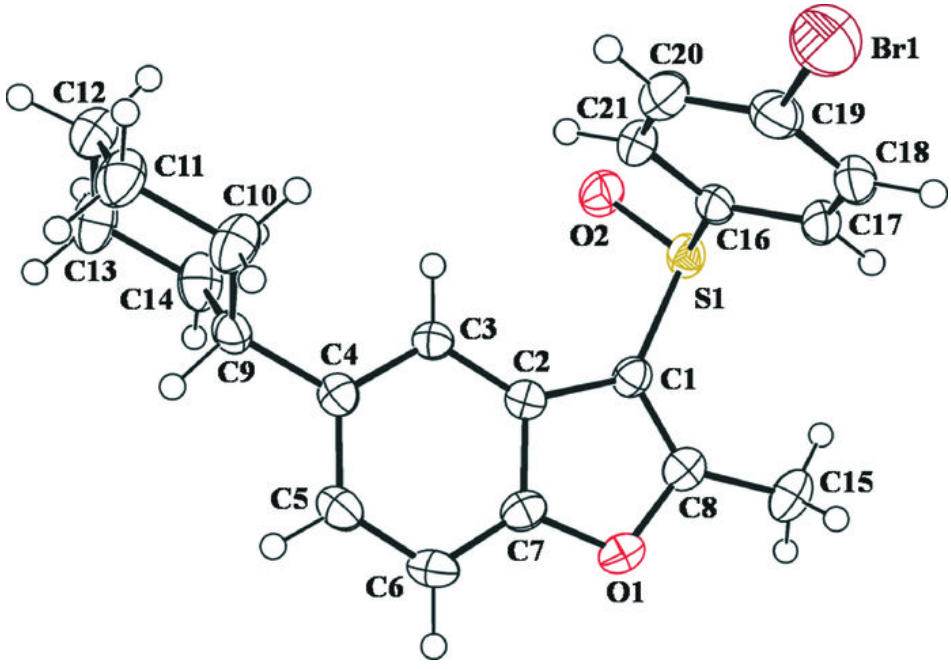
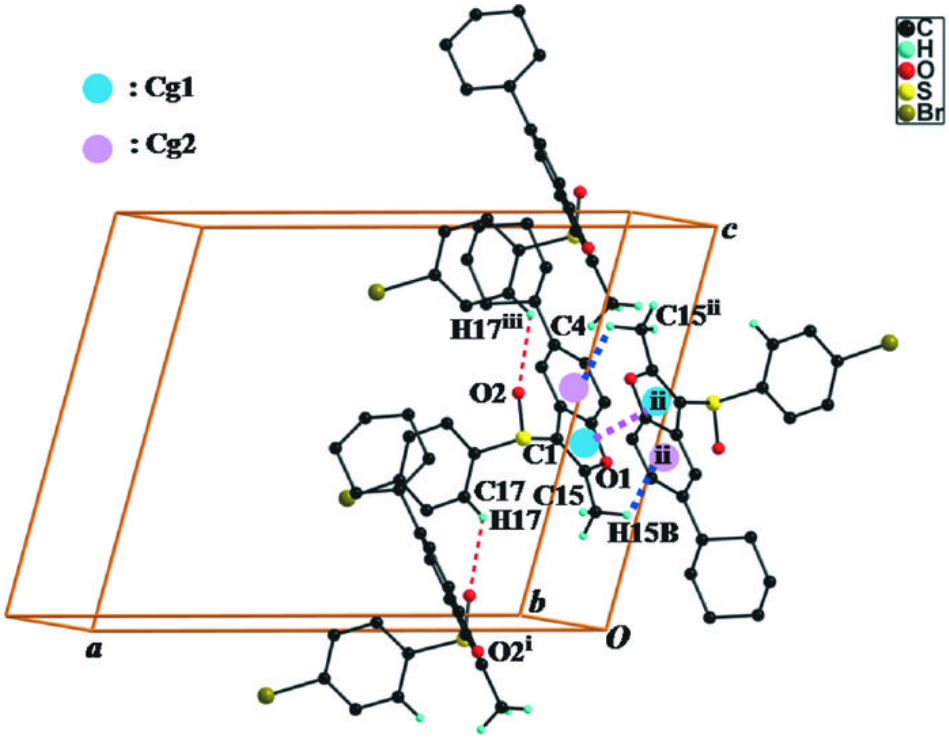

C12
C11
C10
C13
C14
C9
C4
C3
C2
C1
C5
C6
C7
C8
C15
O1
S1
O2
C16
C17
C18
C19
C20
C21
Br1

Fig. 2


: Cg1
: Cg2
C
H
O
S
Br
c
H17iii
C4
C15ii
O2
ii
C1
O1
C17
C15
H17
H15B
b
a
O
O2i