Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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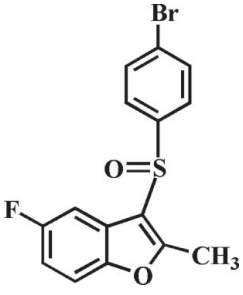
Received 24 January 2012; accepted 9 February 2012

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.035; wR factor = 0.087; data-to-parameter ratio = 17.8.

There are two symmetry-independent molecules, *A* and *B*, in the asymmetric unit of the title compound, $C_{15}H_{10}BrFO_2S$. The dihedral angle formed by the 4-bromophenyl ring and the mean plane of the benzofuran fragment is 88.26 (6)° in molecule *A* and 88.25 (6)° in molecule *B*. In the crystal, molecules are linked by weak intermolecular C—H···F, C—H···O and C—H···π interactions. The crystal structure also exhibits intermolecular C—Br···π [3.737 (3) Å] interactions, and weak π–π interactions between the benzene and furan rings of neighbouring molecules [centroid–centroid distance = 3.557 (3) Å, interplanar distance = 3.421 (3) Å and slippage = 0.974 (3) 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 the crystal structures of related compounds, see: Choi *et al.* (2010*a*,*b*,*c*).



Experimental

Crystal data

$C_{15}H_{10}BrFO_2S$
M_r = 353.20
Triclinic, $P\overline{1}$
a = 9.6576 (1) Å
b = 11.9134 (2) Å
c = 13.5395 (2) Å
α = 94.038 (1)°
β = 101.096 (1)°
γ = 112.610 (1)°
V = 1393.13 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.11 mm^{-1}
T = 173 K
0.34 × 0.27 × 0.17 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.554, T_{max} = 0.746
24788 measured reflections
6444 independent reflections
4958 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.087
S = 1.02
6444 reflections
363 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}

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

*Cg*1 is the centroid of the C17–C22 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···F1^{i}	0.95	2.44	3.316 (3)	154
C15—H15···O4^{ii}	0.95	2.42	3.323 (3)	158
C24—H24*C*···O2^{iii}	0.98	2.59	3.502 (3)	154
C5—H5···*Cg*1^{iv}	0.95	2.74	3.612 (3)	154

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

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*.

This work was supported by Blue-Bio Industry Regional Innovation Center (grant No. RIC08-06-07) at Dongeui University as an RIC program under the Ministry of Knowledge Economy and Busan city.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2180).

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supporting information

Acta Cryst. (2012). E**68**, o750–o751 [doi:10.1107/S1600536812005715]

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

Hong Dae Choi, Pil Ja Seo and Uk Lee

S1. Comment

Benzofuran derivatives have drawn considerable attention owing 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 continuing study of 5-fluoro-2-methyl-1-benzofuran analoques containing 3-phenylsulfonyl (Choi *et al.*, 2010*a*), 3-(4-fluorophenylsulfinyl) (Choi *et al.*, 2010*b*) and 3-(4-fluorophenylsufonyl) (Choi *et al.*, 2010*c*) substituents, we report herein the crystal structure of the title compound which crystallizes with two unique molecule, A & B, in the asymmetric unit.

In the title molecule (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.002 (2) Å, for A, and 0.009 (2) Å, for B, respectively, from the least-squares plane defined by the nine constituent atoms. The dihedral angles between the 4-bromophenyl ring and the mean plane of the benzofurn fragment are 88.26 (6)° in molecule A and 88.25 (6)° in molecule B, respectively. The crystal packing (Fig. 2) is stabilized by weak intermolecular C–H···F (Table 1; first entry) and C–H···O (Table 1; second and third entry) hydrogen bonds. The crystal packing (Fig. 3) is further stabilized by intermolecular C–H···π interactions (Table 1; fourth entry, Cg1 is the centroid of the C17-C22 benzene ring), and by intermolecular C28–Br2···π interactions between the bromine atom and the 4-bromophenyl ring of a neighbouring molecule with Br2···Cg3^{iv} being 3.737 (3) Å (Cg3 is the centroid of the C9–C14 4-bromophenyl ring). Additionally, the crystal packing (Fig. 3) exhibits weak slipped π–π interactions between the benzene and furan rings of neighbouring molecules, with a Cg1···Cg2^{ii} distance of 3.557 (3) Å and an interplanar distance of 3.421 (3) Å resulting in a slippage of 0.974 (3) Å (Cg2 is the centroid of the C1/C2/C7/O1/C8 furan ring).

S2. Experimental

3-Chloroperoxybenzoic acid (77%) (224 mg, 1.0 mmol) was added in small portions to a stirred solution of 3-(4-bromophenylsulfanyl)-5-fluoro-2-methyl-1-benzofuran (303 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, 2:1 v/v) to afford the title compound as a colorless solid [yield 71%, m.p. 382-383 K; R_f = 0.45 (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 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 and 0.98 Å for methyl H atoms. U_{iso}(H) = 1.2U_{eq}(C) for aryl and 1.5U_{eq}(C) for methyl H atoms.

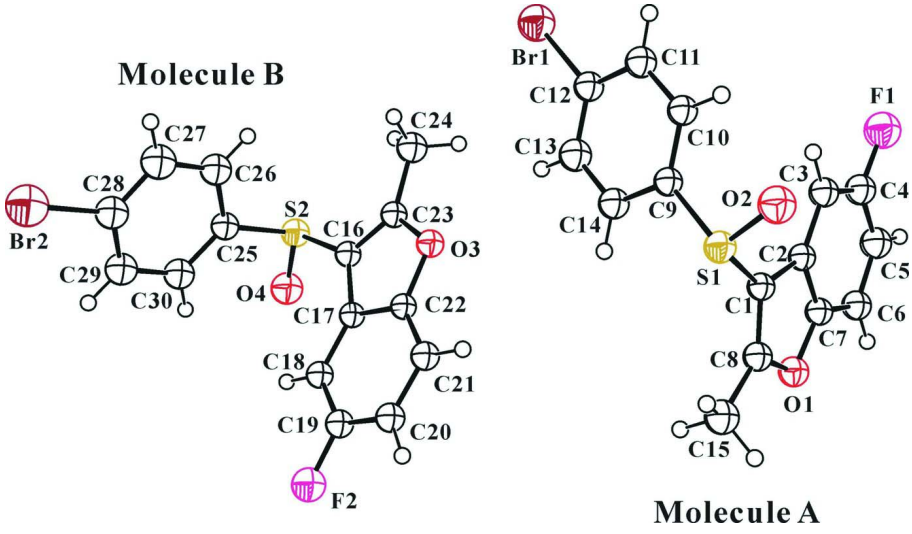

Figure 1

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

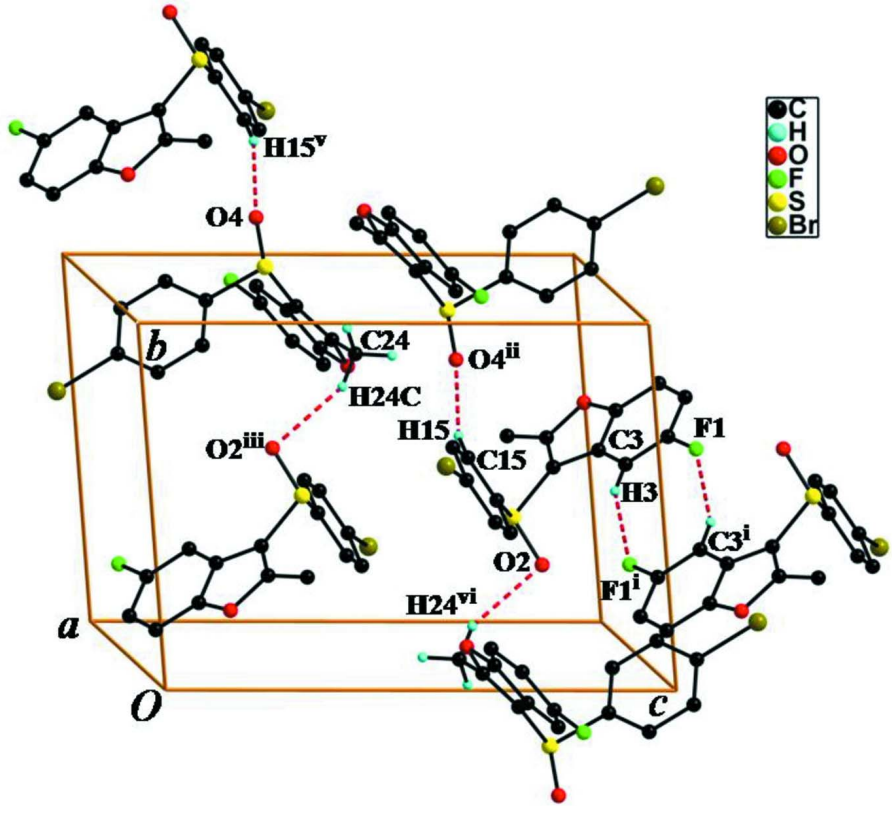

Figure 2

A view of the C–H···O and C–H···F interactions (dotted lines) in the crystal structure of the title compound. H atoms non-participating in hydrogen-bonding were omitted for clarity. For symmetry codes: (v) - *x* + 1, - *y* + 2, - *z* + 1; (vi) - *x*, - *y* + 1, - *z* + 1]. For other codes, see Table 1.

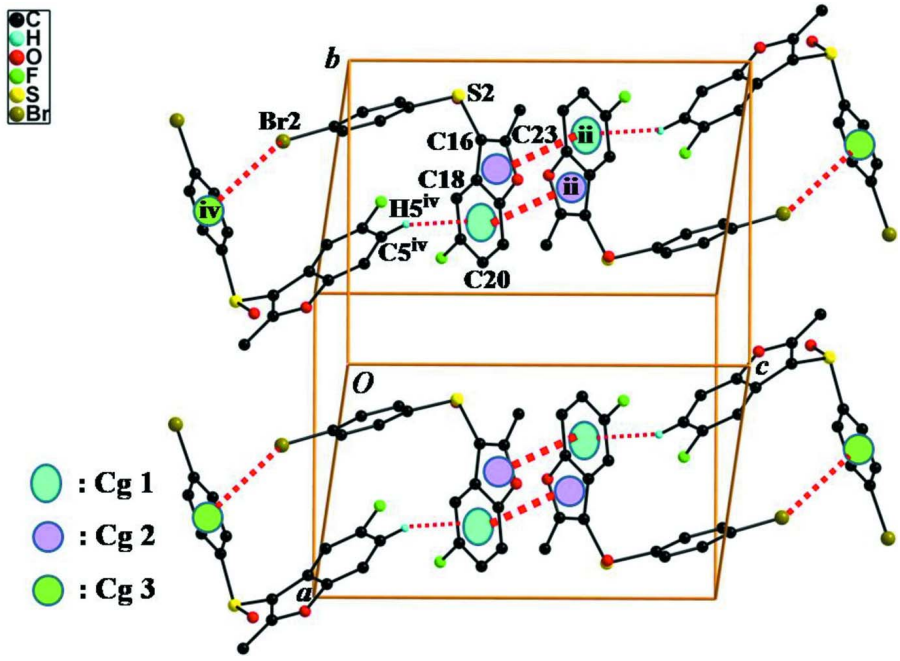

Figure 3

A view of the C–H···π, C–Br···π and π–π interactions (dotted lines) in the crystal structure of the title compound. H atoms non-participating in hydrogen-bonding were omitted for clarity. For symmetry codes, see Table 1.

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

Crystal data

$C_{15}H_{10}BrFO_2S$
$M_r = 353.20$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.6576$ (1) Å
$b = 11.9134$ (2) Å
$c = 13.5395$ (2) Å
$\alpha = 94.038$ (1)°
$\beta = 101.096$ (1)°
$\gamma = 112.610$ (1)°
$V = 1393.13$ (3) Å^3
$Z = 4$
$F(000) = 704$
$D_x = 1.684$ Mg m^{-3}
Melting point = 382–383 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8290 reflections
$\theta = 2.2$–27.2°
$\mu = 3.11$ mm^{-1}
$T = 173$ K
Block, colourless
0.34 × 0.27 × 0.17 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)
$T_{min} = 0.554$, $T_{max} = 0.746$
24788 measured reflections
6444 independent reflections
4958 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 27.6°$, $\theta_{min} = 1.6°$
$h = -12 \rightarrow 12$
$k = -15 \rightarrow 15$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.087$
$S = 1.02$
6444 reflections
363 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
$w = 1/[\sigma^2(F_o^2) + (0.0348P)^2 + 0.8229P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.73$ 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	−0.19888 (4)	0.64684 (3)	0.55467 (2)	0.05801 (11)
S1	0.27869 (7)	0.41871 (5)	0.74250 (5)	0.03725 (14)
O1	0.62608 (18)	0.66639 (14)	0.94699 (13)	0.0358 (4)
O2	0.1845 (2)	0.30693 (15)	0.78067 (15)	0.0497 (5)
F1	0.12944 (19)	0.63331 (15)	1.09105 (13)	0.0607 (5)
C1	0.4009 (3)	0.5329 (2)	0.84628 (17)	0.0305 (5)
C2	0.3666 (3)	0.58567 (19)	0.93269 (16)	0.0282 (4)
C3	0.2340 (3)	0.5723 (2)	0.96518 (18)	0.0359 (5)
H3	0.1341	0.5171	0.9271	0.043*
C4	0.2560 (3)	0.6437 (2)	1.05536 (19)	0.0392 (5)
C5	0.3978 (3)	0.7245 (2)	1.11426 (18)	0.0406 (6)
H5	0.4044	0.7711	1.1762	0.049*
C6	0.5302 (3)	0.7375 (2)	1.08299 (18)	0.0376 (5)
H6	0.6297	0.7920	1.1222	0.045*
C7	0.5101 (3)	0.66719 (19)	0.99181 (17)	0.0309 (5)
C8	0.5566 (3)	0.5840 (2)	0.85873 (18)	0.0335 (5)
C9	0.6600 (3)	0.5691 (3)	0.7962 (2)	0.0472 (6)
H15A	0.7009	0.6429	0.7647	0.071*
H15B	0.6019	0.4970	0.7428	0.071*
H15C	0.7457	0.5577	0.8396	0.071*
C10	0.1497 (3)	0.4894 (2)	0.69659 (16)	0.0312 (5)
C11	−0.0031 (3)	0.4298 (2)	0.69762 (18)	0.0351 (5)
H11	−0.0371	0.3567	0.7269	0.042*
C12	−0.1076 (3)	0.4776 (2)	0.65540 (18)	0.0372 (5)
H12	−0.2135	0.4382	0.6562	0.045*

C13	−0.0552 (3)	0.5827 (2)	0.61246 (17)	0.0366 (5)
C14	0.0986 (3)	0.6429 (2)	0.61141 (18)	0.0417 (6)
H14	0.1325	0.7160	0.5821	0.050*
C15	0.2025 (3)	0.5955 (2)	0.65345 (18)	0.0389 (5)
H15	0.3084	0.6350	0.6528	0.047*
Br2	0.08498 (5)	0.79746 (3)	−0.15733 (2)	0.07262 (12)
S2	0.28070 (7)	1.09998 (5)	0.29462 (5)	0.03822 (15)
O3	0.28658 (18)	0.82877 (14)	0.44327 (12)	0.0327 (3)
O4	0.4310 (2)	1.20632 (15)	0.30530 (15)	0.0517 (5)
F2	0.80169 (17)	0.96487 (15)	0.29759 (12)	0.0505 (4)
C16	0.3202 (3)	0.98537 (19)	0.35506 (17)	0.0297 (5)
C17	0.4479 (2)	0.95086 (18)	0.35492 (16)	0.0275 (4)
C18	0.5797 (3)	0.9915 (2)	0.31620 (17)	0.0316 (5)
H18	0.6039	1.0589	0.2796	0.038*
C19	0.6722 (3)	0.9282 (2)	0.33421 (18)	0.0342 (5)
C20	0.6434 (3)	0.8299 (2)	0.38744 (18)	0.0357 (5)
H20	0.7118	0.7896	0.3965	0.043*
C21	0.5147 (3)	0.7908 (2)	0.42724 (17)	0.0345 (5)
H21	0.4921	0.7240	0.4647	0.041*
C22	0.4202 (2)	0.85308 (19)	0.41017 (16)	0.0287 (5)
C23	0.2295 (2)	0.91161 (19)	0.40823 (17)	0.0307 (5)
C24	0.0814 (3)	0.9007 (2)	0.4318 (2)	0.0407 (6)
H24A	0.0626	0.9736	0.4169	0.061*
H24B	0.0869	0.8945	0.5041	0.061*
H24C	−0.0031	0.8269	0.3900	0.061*
C25	0.2258 (3)	1.0190 (2)	0.16674 (19)	0.0357 (5)
C26	0.0802 (3)	0.9237 (2)	0.1333 (2)	0.0427 (6)
H26	0.0107	0.9038	0.1767	0.051*
C27	0.0376 (3)	0.8582 (2)	0.0363 (2)	0.0495 (7)
H27	−0.0615	0.7925	0.0122	0.059*
C28	0.1403 (3)	0.8894 (2)	−0.0250 (2)	0.0459 (6)
C29	0.2847 (3)	0.9855 (2)	0.0071 (2)	0.0462 (6)
H29	0.3537	1.0057	−0.0367	0.055*
C30	0.3269 (3)	1.0515 (2)	0.1042 (2)	0.0414 (6)
H30	0.4248	1.1188	0.1274	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0696 (2)	0.0880 (2)	0.04255 (16)	0.05785 (19)	0.01397 (14)	0.01981 (14)
S1	0.0372 (3)	0.0393 (3)	0.0347 (3)	0.0205 (3)	0.0007 (3)	−0.0048 (2)
O1	0.0243 (8)	0.0350 (8)	0.0434 (9)	0.0086 (7)	0.0046 (7)	0.0069 (7)
O2	0.0450 (11)	0.0296 (8)	0.0623 (12)	0.0122 (8)	−0.0068 (9)	0.0031 (8)
F1	0.0488 (10)	0.0662 (10)	0.0585 (10)	0.0102 (8)	0.0284 (8)	−0.0102 (8)
C1	0.0279 (11)	0.0346 (11)	0.0290 (11)	0.0135 (9)	0.0048 (9)	0.0058 (9)
C2	0.0289 (11)	0.0261 (10)	0.0261 (10)	0.0089 (9)	0.0032 (9)	0.0052 (8)
C3	0.0259 (12)	0.0381 (12)	0.0338 (12)	0.0045 (10)	0.0050 (10)	0.0000 (10)
C4	0.0362 (13)	0.0401 (13)	0.0379 (13)	0.0092 (11)	0.0154 (11)	0.0035 (10)

C5	0.0509 (16)	0.0361 (12)	0.0276 (12)	0.0124 (12)	0.0065 (11)	−0.0001 (10)
C6	0.0374 (13)	0.0305 (11)	0.0336 (12)	0.0075 (10)	−0.0022 (10)	0.0020 (9)
C7	0.0272 (11)	0.0284 (10)	0.0342 (12)	0.0100 (9)	0.0025 (9)	0.0089 (9)
C8	0.0331 (12)	0.0332 (11)	0.0389 (12)	0.0171 (10)	0.0088 (10)	0.0131 (10)
C9	0.0398 (15)	0.0505 (15)	0.0619 (18)	0.0232 (13)	0.0228 (13)	0.0177 (13)
C10	0.0335 (12)	0.0347 (11)	0.0228 (10)	0.0147 (10)	0.0013 (9)	−0.0024 (9)
C11	0.0367 (13)	0.0334 (11)	0.0342 (12)	0.0146 (10)	0.0072 (10)	0.0012 (9)
C12	0.0296 (12)	0.0421 (13)	0.0375 (13)	0.0143 (11)	0.0060 (10)	−0.0016 (10)
C13	0.0452 (14)	0.0496 (14)	0.0235 (11)	0.0304 (12)	0.0043 (10)	0.0036 (10)
C14	0.0516 (16)	0.0463 (14)	0.0338 (13)	0.0231 (13)	0.0155 (12)	0.0137 (11)
C15	0.0362 (13)	0.0467 (14)	0.0347 (12)	0.0167 (11)	0.0105 (10)	0.0073 (11)
Br2	0.0903 (3)	0.0663 (2)	0.03856 (16)	0.01303 (19)	0.00546 (16)	0.00434 (14)
S2	0.0365 (3)	0.0280 (3)	0.0498 (4)	0.0175 (2)	0.0019 (3)	0.0015 (2)
O3	0.0291 (8)	0.0357 (8)	0.0324 (8)	0.0132 (7)	0.0063 (7)	0.0034 (6)
O4	0.0482 (11)	0.0252 (8)	0.0664 (12)	0.0073 (8)	−0.0022 (9)	0.0010 (8)
F2	0.0352 (8)	0.0640 (10)	0.0606 (10)	0.0256 (7)	0.0184 (7)	0.0110 (8)
C16	0.0281 (11)	0.0249 (10)	0.0314 (11)	0.0116 (9)	−0.0018 (9)	−0.0043 (8)
C17	0.0261 (11)	0.0257 (10)	0.0255 (10)	0.0100 (9)	−0.0010 (8)	−0.0054 (8)
C18	0.0276 (12)	0.0311 (11)	0.0331 (12)	0.0113 (9)	0.0034 (9)	0.0008 (9)
C19	0.0246 (11)	0.0410 (12)	0.0340 (12)	0.0131 (10)	0.0039 (9)	−0.0033 (10)
C20	0.0329 (13)	0.0405 (12)	0.0356 (12)	0.0237 (11)	−0.0022 (10)	−0.0045 (10)
C21	0.0370 (13)	0.0344 (11)	0.0316 (12)	0.0179 (10)	0.0004 (10)	0.0030 (9)
C22	0.0265 (11)	0.0301 (10)	0.0255 (10)	0.0109 (9)	0.0009 (9)	−0.0030 (8)
C23	0.0260 (11)	0.0301 (10)	0.0299 (11)	0.0103 (9)	−0.0010 (9)	−0.0066 (9)
C24	0.0279 (12)	0.0470 (14)	0.0439 (14)	0.0140 (11)	0.0078 (11)	−0.0040 (11)
C25	0.0324 (12)	0.0298 (11)	0.0430 (13)	0.0142 (10)	−0.0002 (10)	0.0101 (10)
C26	0.0319 (13)	0.0458 (14)	0.0424 (14)	0.0091 (11)	0.0044 (11)	0.0097 (11)
C27	0.0375 (15)	0.0456 (14)	0.0453 (15)	0.0013 (12)	−0.0023 (12)	0.0077 (12)
C28	0.0537 (17)	0.0392 (13)	0.0371 (13)	0.0148 (12)	0.0006 (12)	0.0097 (11)
C29	0.0460 (16)	0.0464 (14)	0.0451 (15)	0.0154 (13)	0.0120 (12)	0.0181 (12)
C30	0.0328 (13)	0.0327 (12)	0.0518 (15)	0.0073 (10)	0.0052 (12)	0.0129 (11)

Geometric parameters (Å, º)

Br1—C13	1.898 (2)	Br2—C28	1.897 (3)
S1—O2	1.4881 (19)	S2—O4	1.4876 (19)
S1—C1	1.754 (2)	S2—C16	1.766 (2)
S1—C10	1.797 (2)	S2—C25	1.797 (3)
O1—C8	1.364 (3)	O3—C23	1.374 (3)
O1—C7	1.375 (3)	O3—C22	1.380 (3)
F1—C4	1.365 (3)	F2—C19	1.360 (3)
C1—C8	1.358 (3)	C16—C23	1.341 (3)
C1—C2	1.442 (3)	C16—C17	1.442 (3)
C2—C3	1.388 (3)	C17—C18	1.395 (3)
C2—C7	1.391 (3)	C17—C22	1.396 (3)
C3—C4	1.369 (3)	C18—C19	1.373 (3)
C3—H3	0.9500	C18—H18	0.9500
C4—C5	1.377 (4)	C19—C20	1.383 (3)

C5—C6	1.379 (4)	C20—C21	1.379 (3)
C5—H5	0.9500	C20—H20	0.9500
C6—C7	1.379 (3)	C21—C22	1.379 (3)
C6—H6	0.9500	C21—H21	0.9500
C8—C9	1.479 (3)	C23—C24	1.484 (3)
C9—H15A	0.9800	C24—H24A	0.9800
C9—H15B	0.9800	C24—H24B	0.9800
C9—H15C	0.9800	C24—H24C	0.9800
C10—C11	1.373 (3)	C25—C30	1.377 (4)
C10—C15	1.386 (3)	C25—C26	1.388 (3)
C11—C12	1.391 (3)	C26—C27	1.380 (4)
C11—H11	0.9500	C26—H26	0.9500
C12—C13	1.375 (3)	C27—C28	1.374 (4)
C12—H12	0.9500	C27—H27	0.9500
C13—C14	1.382 (4)	C28—C29	1.384 (4)
C14—C15	1.382 (4)	C29—C30	1.383 (4)
C14—H14	0.9500	C29—H29	0.9500
C15—H15	0.9500	C30—H30	0.9500

O2—S1—C1	109.43 (11)	O4—S2—C16	107.26 (11)
O2—S1—C10	105.77 (11)	O4—S2—C25	107.02 (12)
C1—S1—C10	98.65 (10)	C16—S2—C25	96.12 (10)
C8—O1—C7	106.70 (17)	C23—O3—C22	106.26 (17)
C8—C1—C2	107.5 (2)	C23—C16—C17	107.87 (19)
C8—C1—S1	121.82 (18)	C23—C16—S2	124.12 (17)
C2—C1—S1	130.60 (17)	C17—C16—S2	127.99 (18)
C3—C2—C7	119.7 (2)	C18—C17—C22	119.4 (2)
C3—C2—C1	135.9 (2)	C18—C17—C16	136.2 (2)
C7—C2—C1	104.4 (2)	C22—C17—C16	104.42 (19)
C4—C3—C2	115.9 (2)	C19—C18—C17	116.0 (2)
C4—C3—H3	122.0	C19—C18—H18	122.0
C2—C3—H3	122.0	C17—C18—H18	122.0
C3—C4—F1	118.2 (2)	F2—C19—C18	117.8 (2)
C3—C4—C5	124.7 (2)	F2—C19—C20	117.6 (2)
F1—C4—C5	117.1 (2)	C18—C19—C20	124.6 (2)
C4—C5—C6	119.8 (2)	C21—C20—C19	119.5 (2)
C4—C5—H5	120.1	C21—C20—H20	120.2
C6—C5—H5	120.1	C19—C20—H20	120.2
C5—C6—C7	116.4 (2)	C20—C21—C22	116.9 (2)
C5—C6—H6	121.8	C20—C21—H21	121.6
C7—C6—H6	121.8	C22—C21—H21	121.6
O1—C7—C6	125.7 (2)	C21—C22—O3	126.0 (2)
O1—C7—C2	110.70 (19)	C21—C22—C17	123.6 (2)
C6—C7—C2	123.6 (2)	O3—C22—C17	110.39 (18)
C1—C8—O1	110.7 (2)	C16—C23—O3	111.06 (19)
C1—C8—C9	133.1 (2)	C16—C23—C24	132.7 (2)
O1—C8—C9	116.3 (2)	O3—C23—C24	116.2 (2)
C8—C9—H15A	109.5	C23—C24—H24A	109.5

C8—C9—H15B	109.5	C23—C24—H24B	109.5
H15A—C9—H15B	109.5	H24A—C24—H24B	109.5
C8—C9—H15C	109.5	C23—C24—H24C	109.5
H15A—C9—H15C	109.5	H24A—C24—H24C	109.5
H15B—C9—H15C	109.5	H24B—C24—H24C	109.5
C11—C10—C15	121.6 (2)	C30—C25—C26	121.3 (2)
C11—C10—S1	118.17 (18)	C30—C25—S2	120.24 (18)
C15—C10—S1	119.95 (18)	C26—C25—S2	118.5 (2)
C10—C11—C12	119.4 (2)	C27—C26—C25	119.3 (3)
C10—C11—H11	120.3	C27—C26—H26	120.3
C12—C11—H11	120.3	C25—C26—H26	120.3
C13—C12—C11	118.9 (2)	C28—C27—C26	119.1 (2)
C13—C12—H12	120.5	C28—C27—H27	120.5
C11—C12—H12	120.5	C26—C27—H27	120.5
C14—C13—C12	121.8 (2)	C27—C28—C29	122.0 (3)
C14—C13—Br1	119.60 (18)	C27—C28—Br2	119.5 (2)
C12—C13—Br1	118.60 (19)	C29—C28—Br2	118.5 (2)
C13—C14—C15	119.3 (2)	C30—C29—C28	118.8 (3)
C13—C14—H14	120.4	C30—C29—H29	120.6
C15—C14—H14	120.4	C28—C29—H29	120.6
C14—C15—C10	119.0 (2)	C25—C30—C29	119.4 (2)
C14—C15—H15	120.5	C25—C30—H30	120.3
C10—C15—H15	120.5	C29—C30—H30	120.3

O2—S1—C1—C8	122.96 (19)	O4—S2—C16—C23	143.29 (19)
C10—S1—C1—C8	−126.85 (19)	C25—S2—C16—C23	−106.7 (2)
O2—S1—C1—C2	−53.8 (2)	O4—S2—C16—C17	−38.7 (2)
C10—S1—C1—C2	56.4 (2)	C25—S2—C16—C17	71.3 (2)
C8—C1—C2—C3	−179.5 (3)	C23—C16—C17—C18	−178.5 (2)
S1—C1—C2—C3	−2.5 (4)	S2—C16—C17—C18	3.2 (4)
C8—C1—C2—C7	0.1 (2)	C23—C16—C17—C22	0.7 (2)
S1—C1—C2—C7	177.15 (17)	S2—C16—C17—C22	−177.64 (16)
C7—C2—C3—C4	0.5 (3)	C22—C17—C18—C19	1.5 (3)
C1—C2—C3—C4	−179.9 (2)	C16—C17—C18—C19	−179.4 (2)
C2—C3—C4—F1	−179.5 (2)	C17—C18—C19—F2	179.93 (19)
C2—C3—C4—C5	−0.6 (4)	C17—C18—C19—C20	−0.4 (3)
C3—C4—C5—C6	0.1 (4)	F2—C19—C20—C21	179.0 (2)
F1—C4—C5—C6	179.0 (2)	C18—C19—C20—C21	−0.7 (4)
C4—C5—C6—C7	0.5 (3)	C19—C20—C21—C22	0.6 (3)
C8—O1—C7—C6	179.6 (2)	C20—C21—C22—O3	−179.97 (19)
C8—O1—C7—C2	0.0 (2)	C20—C21—C22—C17	0.6 (3)
C5—C6—C7—O1	179.9 (2)	C23—O3—C22—C21	−179.3 (2)
C5—C6—C7—C2	−0.6 (3)	C23—O3—C22—C17	0.2 (2)
C3—C2—C7—O1	179.63 (19)	C18—C17—C22—C21	−1.6 (3)
C1—C2—C7—O1	−0.1 (2)	C16—C17—C22—C21	179.0 (2)
C3—C2—C7—C6	0.0 (3)	C18—C17—C22—O3	178.83 (18)
C1—C2—C7—C6	−179.7 (2)	C16—C17—C22—O3	−0.5 (2)
C2—C1—C8—O1	−0.1 (2)	C17—C16—C23—O3	−0.6 (2)

S1—C1—C8—O1	−177.45 (15)	S2—C16—C23—O3	177.83 (14)
C2—C1—C8—C9	−178.9 (2)	C17—C16—C23—C24	−178.0 (2)
S1—C1—C8—C9	3.7 (4)	S2—C16—C23—C24	0.4 (4)
C7—O1—C8—C1	0.0 (2)	C22—O3—C23—C16	0.2 (2)
C7—O1—C8—C9	179.08 (19)	C22—O3—C23—C24	178.11 (18)
O2—S1—C10—C11	−4.0 (2)	O4—S2—C25—C30	7.5 (2)
C1—S1—C10—C11	−117.14 (19)	C16—S2—C25—C30	−102.7 (2)
O2—S1—C10—C15	−178.55 (18)	O4—S2—C25—C26	−172.55 (18)
C1—S1—C10—C15	68.3 (2)	C16—S2—C25—C26	77.3 (2)
C15—C10—C11—C12	−0.7 (3)	C30—C25—C26—C27	1.7 (4)
S1—C10—C11—C12	−175.12 (17)	S2—C25—C26—C27	−178.2 (2)
C10—C11—C12—C13	0.8 (3)	C25—C26—C27—C28	−0.3 (4)
C11—C12—C13—C14	−0.9 (4)	C26—C27—C28—C29	−0.8 (4)
C11—C12—C13—Br1	179.82 (17)	C26—C27—C28—Br2	178.5 (2)
C12—C13—C14—C15	0.8 (4)	C27—C28—C29—C30	0.3 (4)
Br1—C13—C14—C15	−179.88 (18)	Br2—C28—C29—C30	−178.88 (19)
C13—C14—C15—C10	−0.7 (4)	C26—C25—C30—C29	−2.1 (4)
C11—C10—C15—C14	0.6 (3)	S2—C25—C30—C29	177.82 (19)
S1—C10—C15—C14	174.96 (18)	C28—C29—C30—C25	1.1 (4)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C17–C22 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···F1^{i}	0.95	2.44	3.316 (3)	154
C15—H15···O4^{ii}	0.95	2.42	3.323 (3)	158
C24—H24*C*···O2^{iii}	0.98	2.59	3.502 (3)	154
C5—H5···*Cg*1^{iv}	0.95	2.74	3.612 (3)	154

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