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3-(4-Fluorophenylsulfinyl)-2-methyl-1-benzofuran

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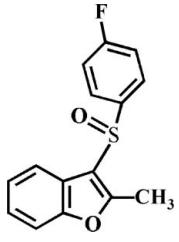
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.101; data-to-parameter ratio = 16.6.

In the title compound, $C_{15}H_{11}FO_2S$, the O atom and the 4-fluorophenyl group of the 4-fluorophenylsulfinyl substituent lie on opposite sides of the plane of the benzofuran fragment; the 4-fluorophenyl ring is almost perpendicular to this plane [dihedral angle = 89.59 (5)°]. Intermolecular C—H···F and C—H···O hydrogen bonds link the molecules together in the crystal structure.

Related literature

For the crystal structures of similar 2-methyl-3-phenylsulfinyl-1-benzofuran derivatives, see: Choi *et al.* (2008*a*,*b*,*c*). 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).



Experimental

Crystal data

$C_{15}H_{11}FO_2S$
M_r = 274.30
Orthorhombic, *Pbcn*
a = 14.992 (1) Å
b = 10.4661 (8) Å
c = 16.008 (1) Å
V = 2511.8 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 173 K
0.50 × 0.50 × 0.25 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.880, T_{max} = 0.937
14681 measured reflections
2878 independent reflections
2315 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.101
S = 1.10
2878 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···F^{i}	0.93	2.52	3.346 (2)	148
C9—H9B···O2^{ii}	0.96	2.41	3.189 (2)	138

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

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: BG2329).

References

Akgul, Y. Y. & Anil, H. (2003). *Phytochemistry*, **63**, 939–943.
Aslam, S. N., Stevenson, P. C., Phythian, S. J., Veitch, N. C. & Hall, D. R. (2006). *Tetrahedron*, **62**, 4214–4226.
Brandenburg, K. (1998). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2009). *SADABS*. *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2008*a*). *Acta Cryst.* E**64**, o1395.
Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2008*b*). *Acta Cryst.* E**64**, o1476.
Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2008*c*). *Acta Cryst.* E**64**, o1477.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Galal, S. A., Abd El-All, A. S., Abdallah, M. M. & El-Diwani, H. I. (2009). *Bioorg. Med. Chem. Lett.* **19**, 2420–2428.
Khan, M. W., Alam, M. J., Rashid, M. A. & Chowdhury, R. (2005). *Bioorg. Med. Chem.* **13**, 4796–4805.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Soekamto, N. H., Achmad, S. A., Ghisalberti, E. L., Hakim, E. H. & Syah, Y. M. (2003). *Phytochemistry*, **64**, 831–834.

supporting information

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3-(4-Fluorophenylsulfinyl)-2-methyl-1-benzofuran

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S1. Comment

Molecules containing benzofuran skeleton show significant pharmacological activities such as antifungal (Aslam *et al.*, 2006), antitumor and antiviral (Galal *et al.*, 2009), antimicrobial (Khan *et al.*, 2005) properties. These compounds are widely occurring in nature (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our ongoing studies of the effect of side chain substituents on the solid state structures of 2-methyl-3-phenylsulfinyl-1-benzofuran analogues (Choi *et al.*, 2008*a,b,c*), we report the crystal structure of the title compound (Fig. 1).

The benzofuran unit is essentially planar, with a mean deviation of 0.012 (1) Å from the least-squares plane defined by the nine constituent atoms. The 4-fluorophenyl ring is almost perpendicular to the plane of the benzofuran fragment [89.59 (5)°] and is tilted slightly towards it. The crystal packing (Fig. 2) is stabilized by two different intermolecular hydrogen bonds; the first one a C—H···F contact between the benzene H atom and the fluorine (Table 1, first entry), and the second, a C—H···O one between one methyl H atom and the oxygen of the S═O unit (Table 1, second entry).

S2. Experimental

77% 3-Chloroperoxybenzoic acid (359 mg, 1.6 mmol) was added in small portions to a stirred solution of 3-(4-fluorophenylsulfanyl)-2-methyl-1-benzofuran (387 mg, 1.5 mmol) in dichloromethane (40 mL) at 273 K. After being stirred at room temperature for 4h, the mixture was washed with saturated sodium bicarbonate solution and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated in vacuum. The residue was purified by column chromatography (hexane-ethyl acetate, 1:1 v/v) to afford the title compound as a colorless solid [yield 78%, m.p. 415–416 K; R_f = 0.63 (hexane-ethyl acetate, 1:1 v/v)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title compound in benzene at room temperature.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å for aryl and 0.96 Å for methyl H atoms. U_{iso}(H) = 1.2U_{eq}(C) for aryl and 1.5U_{eq}(C) for methyl H atoms.

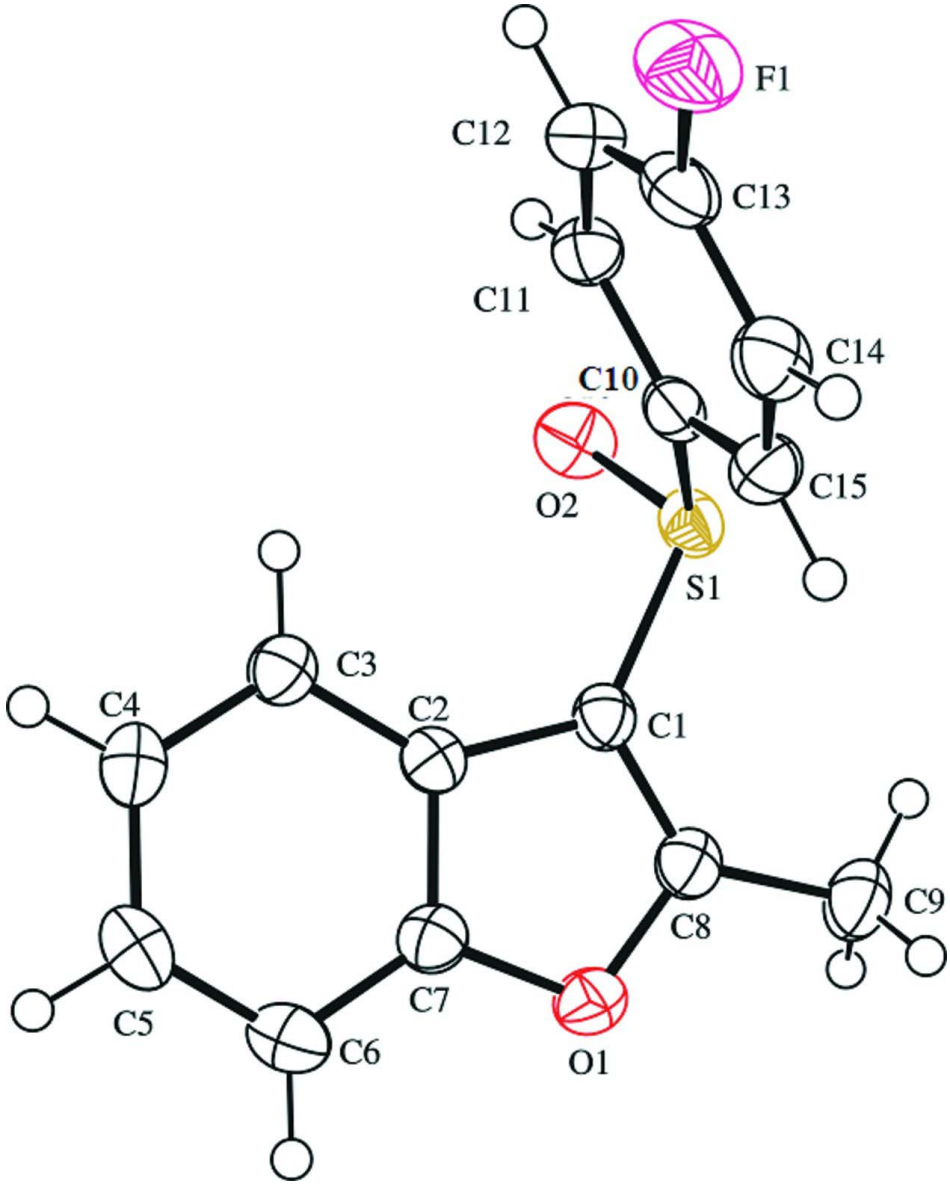

Figure 1

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 a small spheres of arbitrary radius.

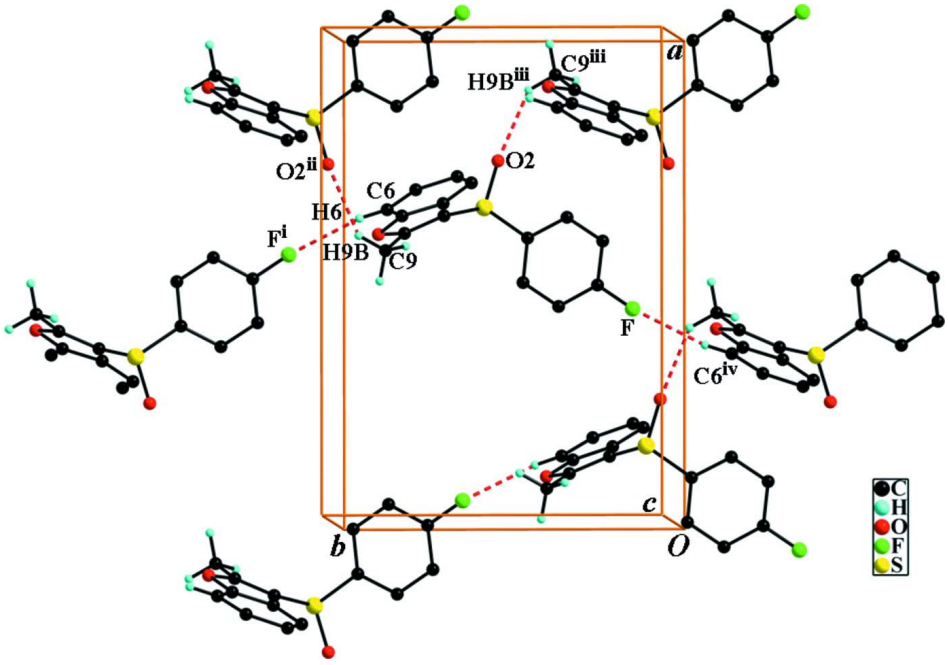

Figure 2

C—H···F and C—H···O interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: i) - *x* + 1, *y* + 1, - *z* + 1/2; ii) - *x* + 3/2, *y* + 1/2, *z*; iii) - *x* + 3/2, *y* - 1/2, *z*; iv) - *x* + 1, *y* - 1, - *z* + 1/2.]

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Crystal data

$C_{15}H_{11}FO_2S$
$M_r = 274.30$
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
$a = 14.992\ (1)$ Å
$b = 10.4661\ (8)$ Å
$c = 16.008\ (1)$ Å
$V = 2511.8\ (3)$ Å^3
$Z = 8$
$F(000) = 1136$
$D_x = 1.451$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6779 reflections
$\theta = 2.4$–$27.5°$
$\mu = 0.26$ mm^{-1}
$T = 173$ K
Block, colourless
0.50 × 0.50 × 0.25 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: Rotating Anode
Bruker HELIOS graded multilayer optics monochromator
Detector resolution: 10.0 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.880$, $T_{max} = 0.937$
14681 measured reflections
2878 independent reflections
2315 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.4°$
$h = -18 \rightarrow 19$
$k = -13 \rightarrow 13$
$l = -15 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.101$
$S = 1.10$
2878 reflections
173 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
$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 1.1695P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ 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}
S	0.65767 (3)	0.58401 (4)	0.06490 (3)	0.03017 (13)
F	0.44627 (8)	0.14149 (11)	0.17017 (8)	0.0492 (3)
O1	0.59892 (8)	0.88631 (11)	0.19868 (8)	0.0342 (3)
O2	0.75317 (9)	0.54319 (13)	0.06877 (8)	0.0394 (3)
C1	0.63870 (11)	0.69730 (16)	0.14353 (10)	0.0276 (3)
C2	0.66131 (10)	0.69382 (15)	0.23170 (10)	0.0265 (3)
C3	0.70180 (11)	0.60712 (17)	0.28570 (11)	0.0310 (4)
H3	0.7212	0.5278	0.2668	0.037*
C4	0.71236 (12)	0.64306 (18)	0.36876 (11)	0.0352 (4)
H4	0.7384	0.5862	0.4062	0.042*
C5	0.68456 (13)	0.76314 (19)	0.39714 (11)	0.0374 (4)
H5	0.6926	0.7844	0.4531	0.045*
C6	0.64547 (12)	0.85086 (18)	0.34404 (11)	0.0362 (4)
H6	0.6272	0.9310	0.3625	0.043*
C7	0.63504 (11)	0.81283 (16)	0.26195 (11)	0.0299 (4)
C8	0.60331 (11)	0.81418 (16)	0.12734 (11)	0.0306 (4)
C9	0.57041 (13)	0.87542 (19)	0.04971 (12)	0.0399 (4)
H9A	0.5808	0.8195	0.0032	0.060*
H9B	0.6015	0.9545	0.0410	0.060*
H9C	0.5076	0.8919	0.0547	0.060*
C10	0.59373 (11)	0.45389 (15)	0.10668 (10)	0.0274 (3)
C11	0.63578 (12)	0.33736 (17)	0.11793 (11)	0.0316 (4)
H11	0.6971	0.3304	0.1102	0.038*
C12	0.58623 (13)	0.23096 (17)	0.14081 (11)	0.0360 (4)
H12	0.6134	0.1521	0.1493	0.043*

C13	0.49582 (12)	0.24576 (16)	0.15059 (11)	0.0341 (4)
C14	0.45240 (12)	0.36075 (18)	0.14095 (11)	0.0359 (4)
H14	0.3912	0.3671	0.1494	0.043*
C15	0.50226 (12)	0.46665 (16)	0.11837 (11)	0.0329 (4)
H15	0.4748	0.5456	0.1111	0.040*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S	0.0341 (2)	0.0313 (2)	0.0251 (2)	−0.00272 (17)	−0.00071 (16)	−0.00052 (16)
F	0.0562 (7)	0.0355 (6)	0.0558 (7)	−0.0171 (5)	−0.0002 (6)	0.0001 (5)
O1	0.0408 (7)	0.0264 (6)	0.0354 (6)	0.0025 (5)	−0.0010 (5)	0.0017 (5)
O2	0.0311 (6)	0.0435 (7)	0.0437 (7)	−0.0024 (5)	0.0071 (6)	−0.0052 (6)
C1	0.0280 (8)	0.0273 (8)	0.0276 (8)	−0.0023 (6)	−0.0021 (6)	0.0010 (6)
C2	0.0253 (8)	0.0270 (8)	0.0273 (8)	−0.0037 (6)	0.0007 (6)	0.0000 (6)
C3	0.0317 (9)	0.0301 (8)	0.0311 (9)	0.0002 (7)	−0.0003 (7)	0.0017 (7)
C4	0.0347 (9)	0.0397 (10)	0.0312 (9)	−0.0023 (7)	−0.0049 (7)	0.0057 (7)
C5	0.0409 (10)	0.0442 (10)	0.0270 (9)	−0.0082 (8)	−0.0001 (8)	−0.0041 (8)
C6	0.0422 (10)	0.0307 (9)	0.0357 (9)	−0.0039 (7)	0.0052 (8)	−0.0053 (7)
C7	0.0310 (9)	0.0266 (8)	0.0320 (9)	−0.0026 (6)	0.0005 (7)	0.0024 (7)
C8	0.0287 (8)	0.0294 (8)	0.0337 (9)	−0.0033 (7)	−0.0028 (7)	0.0019 (7)
C9	0.0414 (10)	0.0371 (10)	0.0412 (10)	0.0005 (8)	−0.0091 (8)	0.0097 (8)
C10	0.0311 (8)	0.0274 (8)	0.0236 (8)	−0.0021 (6)	−0.0033 (6)	−0.0037 (6)
C11	0.0306 (9)	0.0320 (9)	0.0324 (9)	0.0038 (7)	−0.0009 (7)	−0.0045 (7)
C12	0.0453 (10)	0.0265 (8)	0.0364 (9)	0.0037 (7)	−0.0036 (8)	−0.0042 (7)
C13	0.0422 (10)	0.0287 (8)	0.0314 (9)	−0.0099 (7)	−0.0028 (7)	−0.0040 (7)
C14	0.0276 (8)	0.0398 (10)	0.0402 (10)	−0.0024 (7)	−0.0023 (7)	−0.0042 (8)
C15	0.0304 (8)	0.0291 (9)	0.0393 (9)	0.0028 (7)	−0.0049 (7)	−0.0010 (7)

Geometric parameters (Å, º)

S—O2	1.4953 (14)	C6—C7	1.382 (2)
S—C1	1.7525 (17)	C6—H6	0.9300
S—C10	1.7948 (17)	C8—C9	1.483 (2)
F—C13	1.357 (2)	C9—H9A	0.9600
O1—C8	1.371 (2)	C9—H9B	0.9600
O1—C7	1.382 (2)	C9—H9C	0.9600
C1—C8	1.358 (2)	C10—C11	1.385 (2)
C1—C2	1.452 (2)	C10—C15	1.390 (2)
C2—C3	1.393 (2)	C11—C12	1.388 (3)
C2—C7	1.393 (2)	C11—H11	0.9300
C3—C4	1.391 (2)	C12—C13	1.373 (3)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.400 (3)	C13—C14	1.377 (3)
C4—H4	0.9300	C14—C15	1.385 (3)
C5—C6	1.382 (3)	C14—H14	0.9300
C5—H5	0.9300	C15—H15	0.9300

O2—S—C1	108.60 (8)	C1—C8—C9	132.78 (17)
O2—S—C10	106.21 (8)	O1—C8—C9	116.38 (15)
C1—S—C10	99.15 (8)	C8—C9—H9A	109.5
C8—O1—C7	106.58 (13)	C8—C9—H9B	109.5
C8—C1—C2	107.42 (15)	H9A—C9—H9B	109.5
C8—C1—S	122.38 (13)	C8—C9—H9C	109.5
C2—C1—S	130.04 (13)	H9A—C9—H9C	109.5
C3—C2—C7	119.34 (15)	H9B—C9—H9C	109.5
C3—C2—C1	136.18 (16)	C11—C10—C15	121.07 (16)
C7—C2—C1	104.45 (14)	C11—C10—S	118.27 (13)
C4—C3—C2	117.83 (16)	C15—C10—S	120.27 (13)
C4—C3—H3	121.1	C10—C11—C12	119.83 (16)
C2—C3—H3	121.1	C10—C11—H11	120.1
C3—C4—C5	121.28 (17)	C12—C11—H11	120.1
C3—C4—H4	119.4	C13—C12—C11	117.90 (16)
C5—C4—H4	119.4	C13—C12—H12	121.1
C6—C5—C4	121.55 (17)	C11—C12—H12	121.1
C6—C5—H5	119.2	F—C13—C12	118.42 (16)
C4—C5—H5	119.2	F—C13—C14	118.04 (16)
C5—C6—C7	116.21 (17)	C12—C13—C14	123.54 (16)
C5—C6—H6	121.9	C13—C14—C15	118.26 (16)
C7—C6—H6	121.9	C13—C14—H14	120.9
C6—C7—O1	125.51 (16)	C15—C14—H14	120.9
C6—C7—C2	123.78 (16)	C14—C15—C10	119.38 (16)
O1—C7—C2	110.70 (14)	C14—C15—H15	120.3
C1—C8—O1	110.84 (15)	C10—C15—H15	120.3

O2—S—C1—C8	125.82 (15)	C2—C1—C8—O1	−1.56 (19)
C10—S—C1—C8	−123.54 (15)	S—C1—C8—O1	−177.39 (11)
O2—S—C1—C2	−48.99 (17)	C2—C1—C8—C9	178.10 (18)
C10—S—C1—C2	61.65 (16)	S—C1—C8—C9	2.3 (3)
C8—C1—C2—C3	−176.81 (19)	C7—O1—C8—C1	1.47 (18)
S—C1—C2—C3	−1.4 (3)	C7—O1—C8—C9	−178.25 (15)
C8—C1—C2—C7	1.00 (18)	O2—S—C10—C11	−12.66 (15)
S—C1—C2—C7	176.41 (13)	C1—S—C10—C11	−125.19 (13)
C7—C2—C3—C4	1.4 (2)	O2—S—C10—C15	174.41 (13)
C1—C2—C3—C4	178.99 (18)	C1—S—C10—C15	61.88 (15)
C2—C3—C4—C5	−1.0 (3)	C15—C10—C11—C12	0.3 (3)
C3—C4—C5—C6	0.1 (3)	S—C10—C11—C12	−172.52 (13)
C4—C5—C6—C7	0.4 (3)	C10—C11—C12—C13	0.7 (3)
C5—C6—C7—O1	−178.95 (16)	C11—C12—C13—F	177.80 (15)
C5—C6—C7—C2	0.1 (3)	C11—C12—C13—C14	−1.7 (3)
C8—O1—C7—C6	178.34 (17)	F—C13—C14—C15	−177.99 (15)
C8—O1—C7—C2	−0.79 (18)	C12—C13—C14—C15	1.5 (3)
C3—C2—C7—C6	−1.0 (3)	C13—C14—C15—C10	−0.3 (3)
C1—C2—C7—C6	−179.27 (16)	C11—C10—C15—C14	−0.6 (3)
C3—C2—C7—O1	178.14 (14)	S—C10—C15—C14	172.18 (13)
C1—C2—C7—O1	−0.12 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···F^{i}	0.93	2.52	3.346 (2)	148
C9—H9*B*···O2^{ii}	0.96	2.41	3.189 (2)	138

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