3-(3-Fluorophenylsulfonyl)-2,5,7-trimethyl-1-benzofuran

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In the title compound, $C_{17}H_{15}FO_3S$, the 3-fluorophenyl ring makes a dihedral angle of 73.39 (4)° with the mean plane of the benzofuran fragment. In the crystal, molecules are linked by weak intermolecular C—H···O hydrogen bonds. The crystal structure also exhibits a slipped π–π interaction between the furan and benzene rings of neighboring molecules [centroid–centroid distance = 3.743 (2) Å, interplanar distance = 3.543 (2) Å and slippage = 1.207 (2) 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, 2011).
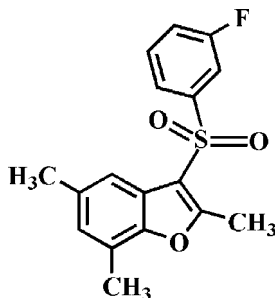
Experimental

Crystal data

C₁₇H₁₅FO₃S

M_r = 318.35

Triclinic, $P\overline{1}$

a = 7.3603 (1) Å

b = 10.3121 (2) Å

c = 11.0590 (2) Å

α = 111.753 (1)°

β = 92.864 (1)°

γ = 101.623 (1)°

V = 756.42 (2) Å³

Z = 2

Mo $K\alpha$ radiation

μ = 0.23 mm⁻¹

T = 173 K

0.21 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEXII CCD diffractometer

Absorption correction: multi-scan (*SADABS*; Bruker, 2009)

T_{min} = 0.953, T_{max} = 0.959

13459 measured reflections

3468 independent reflections

3111 reflections with $I > 2\sigma(I)$

R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036

$wR(F^2)$ = 0.096

S = 1.04

3468 reflections

202 parameters

H-atom parameters constrained

$\Delta\rho_{max}$ = 0.30 e Å⁻³

$\Delta\rho_{min}$ = −0.42 e Å⁻³

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2ⁱ	0.95	2.60	3.4890 (18)	156
C13—H13···O2ⁱ	0.95	2.51	3.4482 (18)	170
C17—H17···O3ⁱⁱ	0.95	2.41	3.3432 (18)	168

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

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: TK5019).

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supporting information

3-(3-Fluorophenylsulfonyl)-2,5,7-trimethyl-1-benzofuran

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S1. Comment

Recently, substituted benzofuran derivatives have drawn much attention due to their valuable 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 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 benzofuran derivatives containing either 3-(4-fluorophenyl-sulfonyl) (Choi *et al.*, 2010) or 3-(3-fluorophenylsulfinyl) (Choi *et al.*, 2011) 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 0.012 (1) Å from the least-squares plane defined by the nine constituent atoms. The dihedral angle formed by the 3-fluorobenzene ring and the mean plane of the benzofuran fragment is 73.39 (4)°. The crystal packing (Fig. 2) is stabilized by weak intermolecular C—H⋯O hydrogen bonds (Table 1) and further stabilized by a weak slipped π–π interaction between the furan and benzene rings of adjacent molecules, with a Cg1⋯Cg2^{iii} distance of 3.743 (2) Å and an interplanar distance of 3.543 (2) Å resulting in a slippage of 1.207 (2) Å (Cg1 and Cg2 are the centroids of the C1/C2/C7/O1/C8 furan ring and the C2-C7 benzene ring, respectively; *iii*: -*x*+1, -*y*+1, -*z*).

S2. Experimental

77% 3-Chloroperoxybenzoic acid (448 mg, 2.0 mmol) was added in small portions to a stirred solution of 3-(3-fluoro-phenylsulfanyl)-2,5,7-trimethyl-1-benzofuran (257 mg, 0.9 mmol) in dichloromethane (30 mL) at 273 K. After being stirred at room temperature for 6 h, 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 73%, *M*.pt. 403–404 K; R_f = 0.51 (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 diisopropyl ether 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) aryl and 1.5U_{eq}(C) for methyl H atoms.
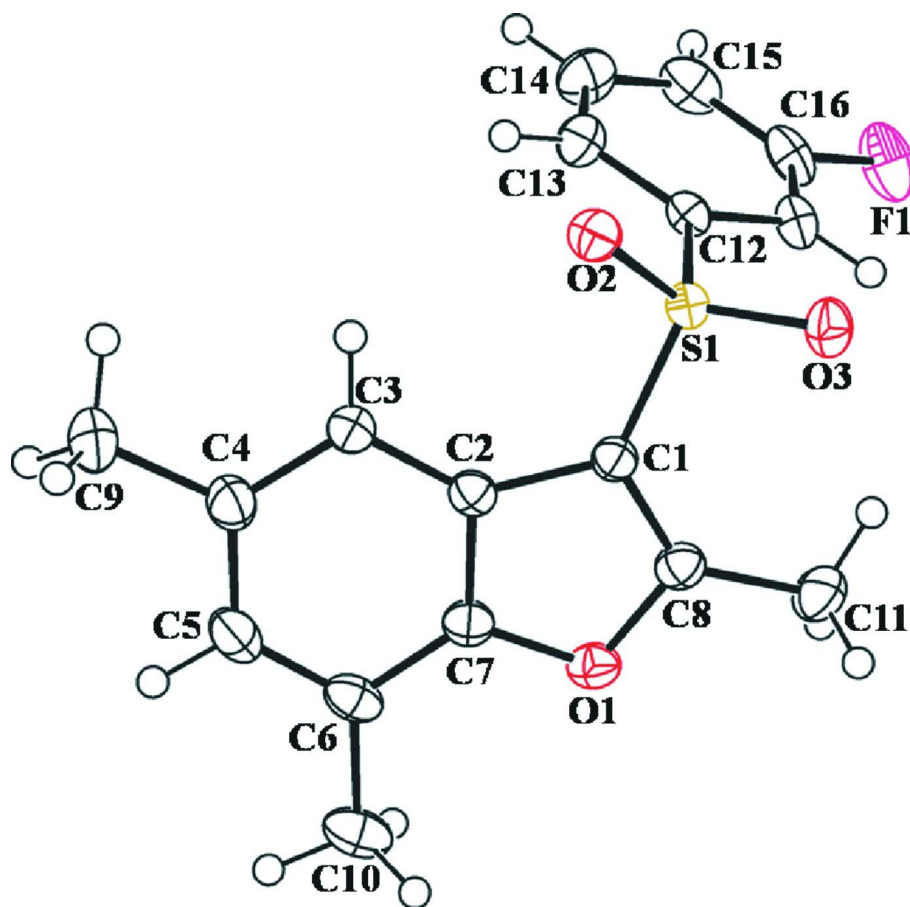
Figure 1

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.
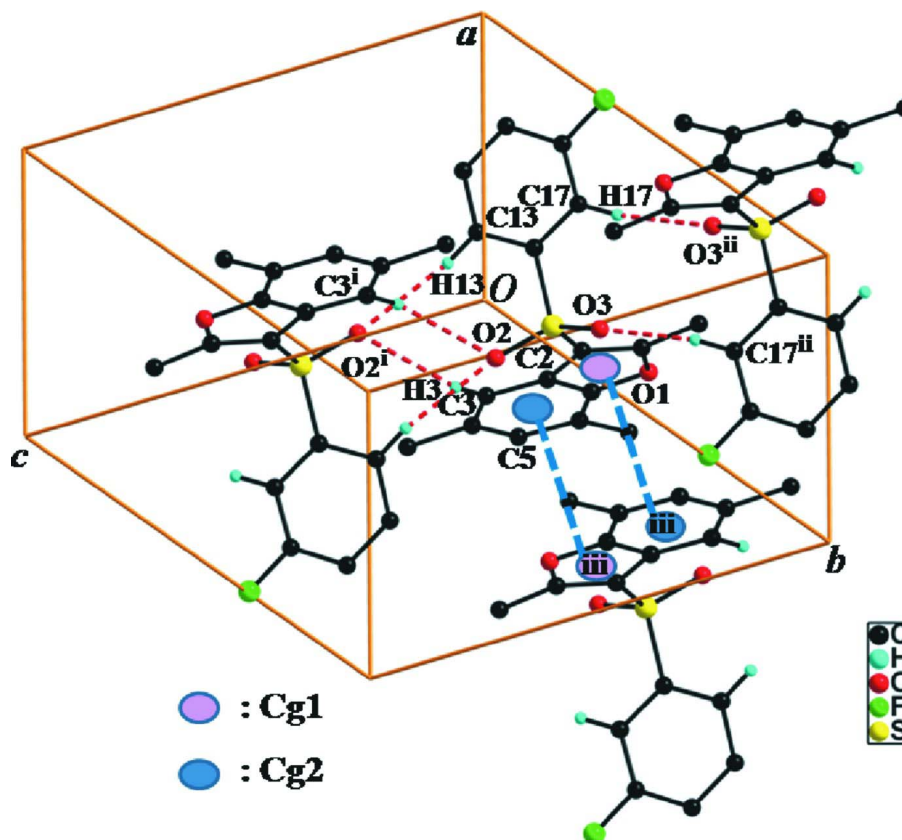
Figure 2

A view of the C—H⋯O and π–π interactions (dotted lines) in the crystal structure of the title compound. H atoms non-participating in hydrogen-bonding were omitted for clarity. [Symmetry codes: (i) - x + 1, - y + 1, - z + 1; (ii) - x + 1, - y + 1, - z; (iii) - x + 1, - y + 2, - z + 1]

3-(3-Fluorophenylsulfonyl)-2,5,7-trimethyl-1-benzofuran

Crystal data

$C_{17}H_{15}FO_3S$	$Z = 2$
$M_r = 318.35$	$F(000) = 332$
Triclinic, $P\overline{1}$	$D_x = 1.398$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.3603$ (1) Å	Cell parameters from 7569 reflections
$b = 10.3121$ (2) Å	$\theta = 2.9$–$27.5°$
$c = 11.0590$ (2) Å	$\mu = 0.23$ mm^{-1}
$\alpha = 111.753$ (1)°	$T = 173$ K
$\beta = 92.864$ (1)°	Block, colourless
$\gamma = 101.623$ (1)°	$0.21 \times 0.20 \times 0.18$ mm
$V = 756.42$ (2) Å^3	

Data collection

Bruker SMART APEXII CCD diffractometer	φ and ω scans
Radiation source: rotating anode	Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
Graphite multilayer monochromator	$T_{min} = 0.953$, $T_{max} = 0.959$
Detector resolution: 10.0 pixels mm^{-1}	13459 measured reflections

3468 independent reflections	$h = -9 \rightarrow 9$
3111 reflections with $I > 2\sigma(I)$	$k = -13 \rightarrow 13$
$R_{int} = 0.024$	$l = -14 \rightarrow 14$
$\theta_{max} = 27.6°$, $\theta_{min} = 2.0°$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.036$	Hydrogen site location: difference Fourier map
$wR(F^2) = 0.096$	H-atom parameters constrained
$S = 1.04$	$w = 1/[\sigma^2(F_o^2) + (0.0484P)^2 + 0.3468P]$
3468 reflections	where $P = (F_o^2 + 2F_c^2)/3$
202 parameters	$(\Delta/\sigma)_{max} < 0.001$
0 restraints	$\Delta\rho_{max} = 0.30$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{min} = -0.42$ 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 > 2sigma(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	$U_{iso}*/U_{eq}$
S1	0.51024 (4)	0.55990 (3)	0.27097 (3)	0.02048 (10)
F1	0.98547 (15)	0.34469 (13)	−0.00478 (10)	0.0483 (3)
O1	0.73981 (14)	0.96817 (11)	0.36726 (10)	0.0264 (2)
O2	0.41075 (14)	0.52113 (11)	0.36588 (10)	0.0255 (2)
O3	0.41181 (15)	0.52758 (12)	0.14377 (10)	0.0286 (2)
C1	0.61238 (19)	0.74265 (14)	0.34366 (13)	0.0212 (3)
C2	0.65279 (19)	0.82907 (14)	0.48360 (13)	0.0215 (3)
C3	0.6301 (2)	0.80574 (16)	0.59909 (14)	0.0256 (3)
H3	0.5802	0.7121	0.5963	0.031*
C4	0.6823 (2)	0.92315 (17)	0.71796 (15)	0.0307 (3)
C5	0.7596 (2)	1.06062 (17)	0.72026 (15)	0.0314 (3)
H5	0.7951	1.1389	0.8031	0.038*
C6	0.7865 (2)	1.08763 (15)	0.60761 (16)	0.0277 (3)
C7	0.72972 (19)	0.96719 (15)	0.49131 (14)	0.0237 (3)
C8	0.6676 (2)	0.83088 (15)	0.27950 (14)	0.0246 (3)
C9	0.6531 (3)	0.9053 (2)	0.84564 (17)	0.0472 (5)
H9A	0.5433	0.9401	0.8779	0.071*
H9B	0.7640	0.9607	0.9109	0.071*
H9C	0.6332	0.8034	0.8310	0.071*
C10	0.8689 (2)	1.23324 (16)	0.60873 (18)	0.0362 (4)
H10A	0.9853	1.2318	0.5695	0.054*

H10B	0.8955	1.3042	0.6995	0.054*
H10C	0.7798	1.2590	0.5579	0.054*
C11	0.6663 (3)	0.80980 (19)	0.13943 (16)	0.0353 (4)
H11A	0.6324	0.7067	0.0844	0.053*
H11B	0.7910	0.8525	0.1257	0.053*
H11C	0.5747	0.8562	0.1156	0.053*
C12	0.69861 (19)	0.47456 (14)	0.24581 (13)	0.0212 (3)
C13	0.7727 (2)	0.44175 (16)	0.34553 (15)	0.0279 (3)
H13	0.7234	0.4647	0.4267	0.033*
C14	0.9203 (2)	0.37478 (19)	0.32442 (18)	0.0364 (4)
H14	0.9728	0.3513	0.3916	0.044*
C15	0.9921 (2)	0.34180 (18)	0.20595 (18)	0.0371 (4)
H15	1.0931	0.2956	0.1912	0.045*
C16	0.9148 (2)	0.37706 (17)	0.11057 (15)	0.0323 (3)
C17	0.7679 (2)	0.44305 (16)	0.12597 (14)	0.0265 (3)
H17	0.7163	0.4660	0.0582	0.032*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02052 (17)	0.02127 (17)	0.01861 (17)	0.00476 (12)	0.00231 (12)	0.00675 (13)
F1	0.0390 (6)	0.0602 (7)	0.0312 (5)	0.0154 (5)	0.0133 (4)	−0.0012 (5)
O1	0.0280 (5)	0.0234 (5)	0.0305 (5)	0.0062 (4)	0.0071 (4)	0.0132 (4)
O2	0.0254 (5)	0.0253 (5)	0.0263 (5)	0.0054 (4)	0.0083 (4)	0.0105 (4)
O3	0.0276 (5)	0.0333 (6)	0.0225 (5)	0.0072 (4)	−0.0016 (4)	0.0088 (4)
C1	0.0224 (6)	0.0212 (6)	0.0211 (6)	0.0070 (5)	0.0040 (5)	0.0082 (5)
C2	0.0199 (6)	0.0214 (6)	0.0233 (7)	0.0074 (5)	0.0030 (5)	0.0075 (5)
C3	0.0311 (7)	0.0235 (7)	0.0232 (7)	0.0088 (6)	0.0043 (6)	0.0089 (6)
C4	0.0373 (8)	0.0306 (8)	0.0239 (7)	0.0141 (6)	0.0031 (6)	0.0072 (6)
C5	0.0328 (8)	0.0263 (7)	0.0276 (7)	0.0100 (6)	−0.0015 (6)	0.0011 (6)
C6	0.0216 (7)	0.0214 (7)	0.0355 (8)	0.0060 (5)	0.0012 (6)	0.0059 (6)
C7	0.0215 (7)	0.0234 (7)	0.0275 (7)	0.0074 (5)	0.0042 (5)	0.0101 (6)
C8	0.0249 (7)	0.0252 (7)	0.0265 (7)	0.0089 (6)	0.0054 (6)	0.0114 (6)
C9	0.0783 (14)	0.0416 (10)	0.0234 (8)	0.0234 (10)	0.0089 (8)	0.0094 (7)
C10	0.0287 (8)	0.0220 (7)	0.0509 (10)	0.0028 (6)	0.0031 (7)	0.0084 (7)
C11	0.0464 (10)	0.0374 (9)	0.0293 (8)	0.0127 (7)	0.0115 (7)	0.0190 (7)
C12	0.0200 (6)	0.0190 (6)	0.0210 (6)	0.0029 (5)	0.0022 (5)	0.0047 (5)
C13	0.0271 (7)	0.0314 (7)	0.0268 (7)	0.0066 (6)	0.0045 (6)	0.0133 (6)
C14	0.0308 (8)	0.0410 (9)	0.0430 (9)	0.0128 (7)	0.0014 (7)	0.0209 (8)
C15	0.0266 (8)	0.0329 (8)	0.0458 (10)	0.0119 (6)	0.0031 (7)	0.0061 (7)
C16	0.0261 (7)	0.0310 (8)	0.0265 (7)	0.0044 (6)	0.0055 (6)	−0.0027 (6)
C17	0.0260 (7)	0.0278 (7)	0.0194 (6)	0.0039 (6)	0.0019 (5)	0.0038 (6)

Geometric parameters (Å, º)

S1—O2	1.4380 (10)	C9—H9A	0.9800
S1—O3	1.4380 (10)	C9—H9B	0.9800
S1—C1	1.7345 (14)	C9—H9C	0.9800

S1—C12	1.7672 (14)	C10—H10A	0.9800
F1—C16	1.3526 (18)	C10—H10B	0.9800
O1—C8	1.3622 (18)	C10—H10C	0.9800
O1—C7	1.3813 (17)	C11—H11A	0.9800
C1—C8	1.3619 (19)	C11—H11B	0.9800
C1—C2	1.4500 (19)	C11—H11C	0.9800
C2—C7	1.3917 (19)	C12—C13	1.385 (2)
C2—C3	1.3965 (19)	C12—C17	1.3920 (19)
C3—C4	1.387 (2)	C13—C14	1.386 (2)
C3—H3	0.9500	C13—H13	0.9500
C4—C5	1.407 (2)	C14—C15	1.387 (2)
C4—C9	1.510 (2)	C14—H14	0.9500
C5—C6	1.389 (2)	C15—C16	1.370 (2)
C5—H5	0.9500	C15—H15	0.9500
C6—C7	1.387 (2)	C16—C17	1.375 (2)
C6—C10	1.497 (2)	C17—H17	0.9500
C8—C11	1.482 (2)		
O2—S1—O3	119.31 (6)	C4—C9—H9C	109.5
O2—S1—C1	107.39 (6)	H9A—C9—H9C	109.5
O3—S1—C1	109.06 (7)	H9B—C9—H9C	109.5
O2—S1—C12	107.29 (6)	C6—C10—H10A	109.5
O3—S1—C12	107.42 (6)	C6—C10—H10B	109.5
C1—S1—C12	105.55 (6)	H10A—C10—H10B	109.5
C8—O1—C7	107.03 (11)	C6—C10—H10C	109.5
C8—C1—C2	107.76 (12)	H10A—C10—H10C	109.5
C8—C1—S1	126.11 (11)	H10B—C10—H10C	109.5
C2—C1—S1	126.13 (10)	C8—C11—H11A	109.5
C7—C2—C3	119.43 (13)	C8—C11—H11B	109.5
C7—C2—C1	104.13 (12)	H11A—C11—H11B	109.5
C3—C2—C1	136.43 (13)	C8—C11—H11C	109.5
C4—C3—C2	118.13 (14)	H11A—C11—H11C	109.5
C4—C3—H3	120.9	H11B—C11—H11C	109.5
C2—C3—H3	120.9	C13—C12—C17	122.22 (13)
C3—C4—C5	120.14 (14)	C13—C12—S1	119.21 (11)
C3—C4—C9	120.40 (15)	C17—C12—S1	118.57 (11)
C5—C4—C9	119.45 (14)	C12—C13—C14	118.59 (14)
C6—C5—C4	123.35 (14)	C12—C13—H13	120.7
C6—C5—H5	118.3	C14—C13—H13	120.7
C4—C5—H5	118.3	C13—C14—C15	120.51 (15)
C7—C6—C5	114.29 (14)	C13—C14—H14	119.7
C7—C6—C10	121.84 (15)	C15—C14—H14	119.7
C5—C6—C10	123.87 (14)	C16—C15—C14	118.77 (15)
O1—C7—C6	124.66 (13)	C16—C15—H15	120.6
O1—C7—C2	110.69 (12)	C14—C15—H15	120.6
C6—C7—C2	124.65 (14)	F1—C16—C15	118.52 (14)
C1—C8—O1	110.39 (12)	F1—C16—C17	118.28 (15)
C1—C8—C11	134.46 (14)	C15—C16—C17	123.20 (15)

O1—C8—C11	115.15 (13)	C16—C17—C12	116.71 (14)
C4—C9—H9A	109.5	C16—C17—H17	121.6
C4—C9—H9B	109.5	C12—C17—H17	121.6
H9A—C9—H9B	109.5		
O2—S1—C1—C8	−158.08 (13)	C1—C2—C7—O1	−0.78 (15)
O3—S1—C1—C8	−27.46 (15)	C3—C2—C7—C6	−0.4 (2)
C12—S1—C1—C8	87.68 (14)	C1—C2—C7—C6	178.54 (14)
O2—S1—C1—C2	21.36 (14)	C2—C1—C8—O1	−0.35 (16)
O3—S1—C1—C2	151.98 (12)	S1—C1—C8—O1	179.17 (10)
C12—S1—C1—C2	−92.88 (13)	C2—C1—C8—C11	179.45 (16)
C8—C1—C2—C7	0.68 (15)	S1—C1—C8—C11	−1.0 (3)
S1—C1—C2—C7	−178.84 (10)	C7—O1—C8—C1	−0.13 (16)
C8—C1—C2—C3	179.38 (16)	C7—O1—C8—C11	−179.98 (12)
S1—C1—C2—C3	−0.1 (2)	O2—S1—C12—C13	−26.71 (13)
C7—C2—C3—C4	1.3 (2)	O3—S1—C12—C13	−156.14 (11)
C1—C2—C3—C4	−177.26 (15)	C1—S1—C12—C13	87.59 (12)
C2—C3—C4—C5	−1.3 (2)	O2—S1—C12—C17	153.52 (11)
C2—C3—C4—C9	177.35 (15)	O3—S1—C12—C17	24.09 (13)
C3—C4—C5—C6	0.5 (2)	C1—S1—C12—C17	−92.18 (12)
C9—C4—C5—C6	−178.17 (16)	C17—C12—C13—C14	−0.3 (2)
C4—C5—C6—C7	0.3 (2)	S1—C12—C13—C14	179.97 (12)
C4—C5—C6—C10	−179.86 (15)	C12—C13—C14—C15	0.1 (2)
C8—O1—C7—C6	−178.73 (14)	C13—C14—C15—C16	0.2 (3)
C8—O1—C7—C2	0.60 (15)	C14—C15—C16—F1	179.97 (15)
C5—C6—C7—O1	178.85 (13)	C14—C15—C16—C17	−0.4 (3)
C10—C6—C7—O1	−1.0 (2)	F1—C16—C17—C12	179.90 (13)
C5—C6—C7—C2	−0.4 (2)	C15—C16—C17—C12	0.3 (2)
C10—C6—C7—C2	179.80 (13)	C13—C12—C17—C16	0.0 (2)
C3—C2—C7—O1	−179.75 (12)	S1—C12—C17—C16	179.81 (11)

Hydrogen-bond geometry (Å, °)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C3—H3⋯O2[i]	0.95	2.60	3.4890 (18)	156
C13—H13⋯O2[i]	0.95	2.51	3.4482 (18)	170
C17—H17⋯O3[ii]	0.95	2.41	3.3432 (18)	168

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