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

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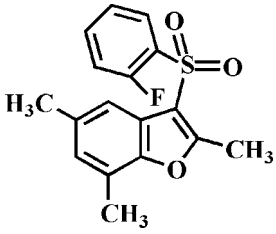
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.104; data-to-parameter ratio = 17.3.

In the title compound, $C_{17}H_{15}FO_3S$, the dihedral angle between the mean planes of the benzofuran and 2-fluorophenyl rings is 87.61 (4) Å. In the crystal, molecules are linked *via* pairs of C—H$\cdots\pi$ interactions into inversion-related dimers. These dimers are linked by C—H$\cdots$O hydrogen bonds into supramolecular chains running along the *a*-axis direction.

Related literature

For background information and the crystal structures of related compounds, see: Choi *et al.* (2010, 2012); Seo *et al.* (2011).



Experimental

Crystal data

$C_{17}H_{15}FO_3S$
M_r = 318.35
Triclinic, $P\overline{1}$
a = 7.7658 (2) Å
b = 8.3529 (3) Å
c = 12.9732 (4) Å
α = 74.253 (2)°
β = 75.048 (2)°
γ = 66.046 (1)°
V = 729.66 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 173 K
0.34 × 0.26 × 0.23 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.700, T_{max} = 0.746
13247 measured reflections
3498 independent reflections
3057 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.104
S = 1.04
3498 reflections
202 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

*Cg*1 is the centroid of the C2–C7 benzene ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C16—H16$\cdots$O2^{i}	0.95	2.58	3.462 (2)	155
C9—H9*C*$\cdots$*Cg*1^{ii}	0.98	2.79	3.612 (2)	142

Symmetry codes: (i) $x-1, y, z$; (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 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

Supporting information for this paper is available from the IUCr electronic archives (Reference: ZQ2222).

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supporting information

Acta Cryst. (2014). E**70**, o566 [doi:10.1107/S1600536814007909]

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

Hong Dae Choi, Pil Ja Seo and Uk Lee

S1. Comment

As a part of our ongoing study of 2,5,7-trimethyl-1-benzofuran derivatives containing 4-fluorophenylsulfonyl (Choi *et al.*, 2010), 3-fluorophenylsulfonyl (Seo *et al.*, 2011) and 4-methylphenylsulfonyl (Choi *et al.*, 2012) substituents in the 3-position, we report here on the crystal structure of the title compound.

In the title molecule (Fig. 1), the benzofuran ring system is essentially planar, with a mean deviation of 0.013 (1) Å from the least-squares plane defined by the nine constituent atoms. The 2-fluorophenyl ring is essentially planar, with a mean deviation of 0.004 (1) Å from the least-squares plane defined by the six constituent atoms. The dihedral angle formed by the benzofuran ring system and the 2-fluorophenyl ring is 87.61 (4)°. In the crystal structure (Fig. 2), molecules are linked via pairs of C—H···π interactions (Table 1, Cg1 is the centroid of the C2–C7 benzene ring) into inversion-related dimers. These dimers are further linked by C—H···O hydrogen bonds (Table 1), forming supramolecular chains running along the *a*-axis direction.

S2. Experimental

3-Chloroperoxybenzoic acid (77%, 448 mg, 2.0 mmol) was added in small portions to a stirred solution of 3-(2-fluorophenylsulfanyl)-2,5,7-trimethyl-1-benzofuran (257 mg, 0.9 mmol) in dichloromethane (35 mL) at 273 K. After being stirred at room temperature for 10h, 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 (benzene) to afford the title compound as a colorless solid [yield 71%, m.p. 409–410 K; R_f = 0.52 (benzene)]. Single crystals suitable for X-ray diffraction were prepared by slow vaporation 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, respectively. U_{iso} (H) = 1.2U_{eq} (C) for aryl and 1.5U_{eq} (C) for methyl H atoms. The positions of methyl hydrogens were optimized using the SHELXL-97's command AFIX 137 (Sheldrick, 2008).

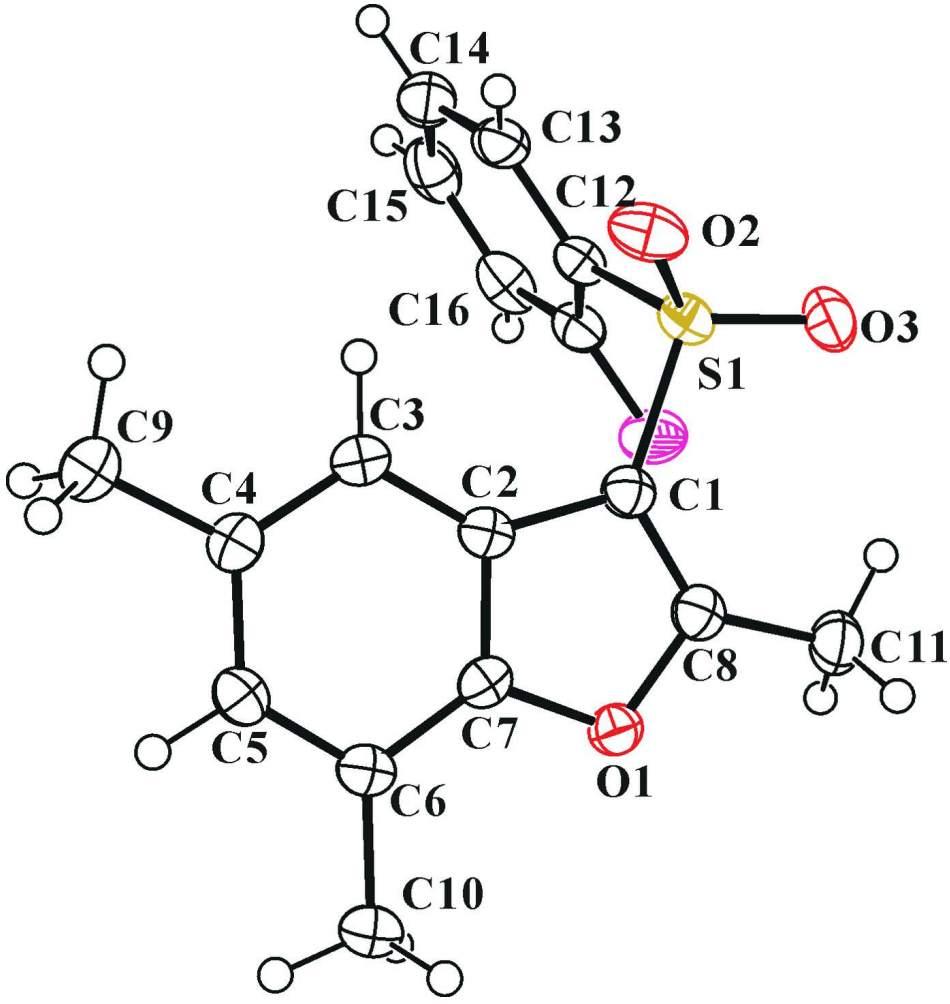

Figure 1

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

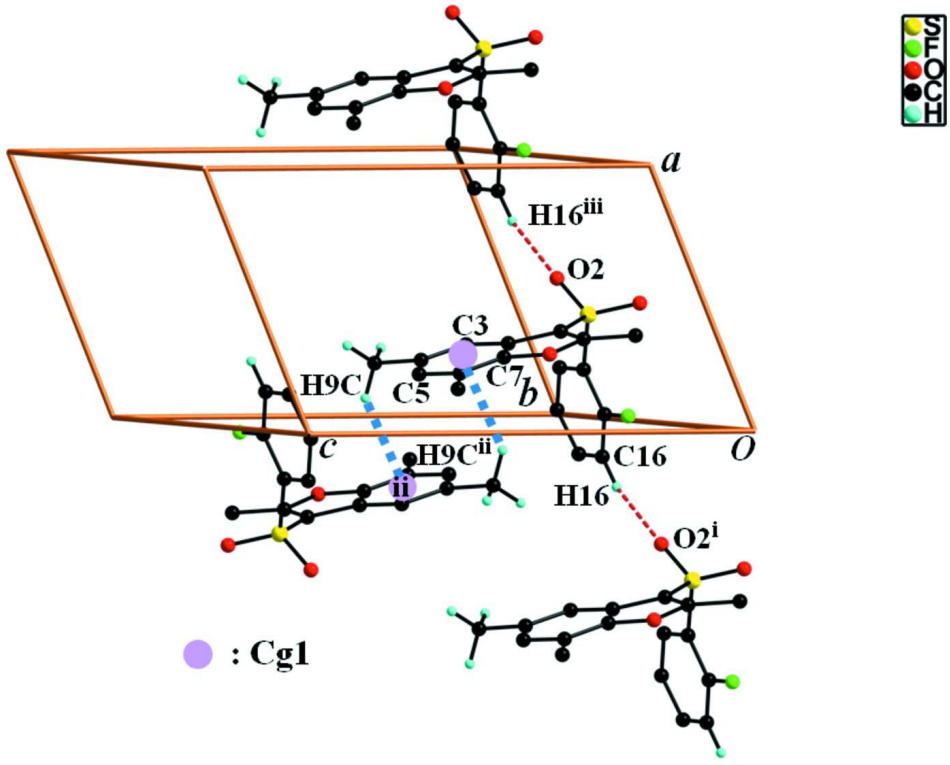

Figure 2

A view of the C—H···O and C—H···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, z; (ii) - x, - y + 1, - z + 1; (iii) x + 1, y, z.]

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Crystal data

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Triclinic, $P\overline{1}$
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α = 74.253 (2)°
β = 75.048 (2)°
γ = 66.046 (1)°
V = 729.66 (4) Å^3
Z = 2
$F(000)$ = 332
D_x = 1.449 Mg m^{-3}
Melting point = 410–409 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6186 reflections
θ = 2.7–28.2°
μ = 0.24 mm^{-1}
T = 173 K
Block, colourless
0.34 × 0.26 × 0.23 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} = 0.700, T_{max} = 0.746
13247 measured reflections
3498 independent reflections
3057 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

θ_{max} = 28.0°, θ_{min} = 1.7°
h = −10→10
k = −11→10
l = −16→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.104
S = 1.04
3498 reflections
202 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
$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.2699P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 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 $F^2 > 2\text{sigma}(F^2)$ 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}
S1	0.42141 (5)	0.28123 (5)	0.15133 (3)	0.02646 (12)
F1	0.04064 (14)	0.26625 (13)	0.15747 (8)	0.0372 (2)
O1	0.29698 (15)	−0.04837 (13)	0.41192 (8)	0.0261 (2)
O2	0.55334 (16)	0.35762 (16)	0.15685 (9)	0.0370 (3)
O3	0.47053 (17)	0.17497 (16)	0.07064 (9)	0.0368 (3)
C12	0.2034 (2)	0.4608 (2)	0.13354 (11)	0.0248 (3)
C17	0.0368 (2)	0.4340 (2)	0.13746 (12)	0.0281 (3)
C1	0.3680 (2)	0.16080 (19)	0.27862 (12)	0.0248 (3)
C2	0.3203 (2)	0.22449 (19)	0.37943 (11)	0.0236 (3)
C3	0.3066 (2)	0.37738 (19)	0.40990 (12)	0.0261 (3)
H3	0.3364	0.4706	0.3573	0.031*
C4	0.2485 (2)	0.3905 (2)	0.51883 (12)	0.0273 (3)
C5	0.2053 (2)	0.2505 (2)	0.59508 (12)	0.0274 (3)
H5	0.1650	0.2625	0.6691	0.033*
C6	0.2185 (2)	0.09579 (19)	0.56803 (12)	0.0249 (3)
C7	0.2774 (2)	0.08988 (18)	0.45848 (12)	0.0232 (3)
C8	0.3499 (2)	−0.0012 (2)	0.30262 (12)	0.0264 (3)
C9	0.2271 (3)	0.5540 (2)	0.55619 (14)	0.0358 (4)
H9A	0.2797	0.6306	0.4961	0.054*
H9B	0.2964	0.5184	0.6169	0.054*
H9C	0.0914	0.6196	0.5799	0.054*
C10	0.1698 (2)	−0.0525 (2)	0.64939 (12)	0.0301 (3)
H10A	0.0649	−0.0689	0.6300	0.045*

H10B	0.1306	−0.0223	0.7219	0.045*
H10C	0.2821	−0.1632	0.6493	0.045*
C11	0.3704 (2)	−0.1314 (2)	0.23854 (14)	0.0351 (4)
H11A	0.3914	−0.0806	0.1609	0.053*
H11B	0.2538	−0.1592	0.2568	0.053*
H11C	0.4796	−0.2408	0.2554	0.053*
C13	0.1995 (2)	0.6340 (2)	0.11204 (12)	0.0310 (3)
H13	0.3121	0.6552	0.1092	0.037*
C14	0.0312 (3)	0.7759 (2)	0.09474 (13)	0.0387 (4)
H14	0.0282	0.8946	0.0806	0.046*
C15	−0.1330 (3)	0.7457 (2)	0.09789 (13)	0.0403 (4)
H15	−0.2473	0.8439	0.0845	0.048*
C16	−0.1318 (2)	0.5737 (2)	0.12045 (13)	0.0359 (4)
H16	−0.2447	0.5525	0.1241	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0237 (2)	0.0311 (2)	0.02292 (18)	−0.01123 (15)	−0.00111 (13)	−0.00301 (14)
F1	0.0387 (5)	0.0397 (5)	0.0406 (5)	−0.0238 (4)	−0.0086 (4)	−0.0022 (4)
O1	0.0260 (5)	0.0235 (5)	0.0277 (5)	−0.0094 (4)	−0.0034 (4)	−0.0036 (4)
O2	0.0288 (6)	0.0478 (7)	0.0361 (6)	−0.0216 (5)	−0.0062 (5)	0.0025 (5)
O3	0.0379 (7)	0.0392 (6)	0.0272 (6)	−0.0096 (5)	0.0022 (5)	−0.0111 (5)
C12	0.0262 (7)	0.0287 (7)	0.0183 (6)	−0.0106 (6)	−0.0031 (5)	−0.0023 (5)
C17	0.0305 (8)	0.0335 (8)	0.0214 (6)	−0.0147 (6)	−0.0026 (6)	−0.0037 (6)
C1	0.0227 (7)	0.0255 (7)	0.0249 (7)	−0.0085 (6)	−0.0036 (5)	−0.0035 (5)
C2	0.0198 (7)	0.0255 (7)	0.0242 (7)	−0.0079 (5)	−0.0045 (5)	−0.0021 (5)
C3	0.0267 (7)	0.0238 (7)	0.0277 (7)	−0.0107 (6)	−0.0059 (6)	−0.0010 (6)
C4	0.0257 (7)	0.0267 (7)	0.0304 (7)	−0.0090 (6)	−0.0059 (6)	−0.0066 (6)
C5	0.0257 (7)	0.0320 (8)	0.0242 (7)	−0.0099 (6)	−0.0043 (6)	−0.0055 (6)
C6	0.0198 (7)	0.0267 (7)	0.0257 (7)	−0.0079 (6)	−0.0045 (5)	−0.0010 (6)
C7	0.0205 (7)	0.0211 (6)	0.0281 (7)	−0.0070 (5)	−0.0060 (5)	−0.0035 (5)
C8	0.0218 (7)	0.0273 (7)	0.0281 (7)	−0.0070 (6)	−0.0039 (6)	−0.0053 (6)
C9	0.0420 (10)	0.0316 (8)	0.0375 (9)	−0.0158 (7)	−0.0056 (7)	−0.0095 (7)
C10	0.0307 (8)	0.0308 (8)	0.0276 (7)	−0.0141 (6)	−0.0041 (6)	0.0003 (6)
C11	0.0369 (9)	0.0337 (8)	0.0369 (9)	−0.0136 (7)	−0.0005 (7)	−0.0141 (7)
C13	0.0393 (9)	0.0323 (8)	0.0228 (7)	−0.0171 (7)	−0.0049 (6)	−0.0015 (6)
C14	0.0528 (11)	0.0294 (8)	0.0276 (8)	−0.0112 (8)	−0.0075 (7)	−0.0007 (6)
C15	0.0381 (9)	0.0427 (10)	0.0255 (8)	−0.0001 (8)	−0.0070 (7)	−0.0046 (7)
C16	0.0266 (8)	0.0508 (10)	0.0261 (7)	−0.0107 (7)	−0.0037 (6)	−0.0064 (7)

Geometric parameters (Å, º)

S1—O3	1.4327 (12)	C6—C7	1.384 (2)
S1—O2	1.4336 (11)	C6—C10	1.5023 (19)
S1—C1	1.7305 (15)	C8—C11	1.477 (2)
S1—C12	1.7664 (15)	C9—H9A	0.9800
F1—C17	1.3430 (18)	C9—H9B	0.9800

O1—C8	1.3646 (18)	C9—H9C	0.9800
O1—C7	1.3820 (17)	C10—H10A	0.9800
C12—C13	1.386 (2)	C10—H10B	0.9800
C12—C17	1.387 (2)	C10—H10C	0.9800
C17—C16	1.376 (2)	C11—H11A	0.9800
C1—C8	1.361 (2)	C11—H11B	0.9800
C1—C2	1.449 (2)	C11—H11C	0.9800
C2—C7	1.3887 (19)	C13—C14	1.383 (2)
C2—C3	1.393 (2)	C13—H13	0.9500
C3—C4	1.388 (2)	C14—C15	1.386 (3)
C3—H3	0.9500	C14—H14	0.9500
C4—C5	1.406 (2)	C15—C16	1.383 (3)
C4—C9	1.504 (2)	C15—H15	0.9500
C5—C6	1.387 (2)	C16—H16	0.9500
C5—H5	0.9500		

O3—S1—O2	118.79 (7)	C1—C8—O1	110.21 (13)
O3—S1—C1	109.75 (7)	C1—C8—C11	135.02 (14)
O2—S1—C1	108.30 (7)	O1—C8—C11	114.75 (13)
O3—S1—C12	109.12 (7)	C4—C9—H9A	109.5
O2—S1—C12	106.32 (7)	C4—C9—H9B	109.5
C1—S1—C12	103.44 (7)	H9A—C9—H9B	109.5
C8—O1—C7	107.16 (11)	C4—C9—H9C	109.5
C13—C12—C17	118.81 (14)	H9A—C9—H9C	109.5
C13—C12—S1	119.15 (12)	H9B—C9—H9C	109.5
C17—C12—S1	122.02 (12)	C6—C10—H10A	109.5
F1—C17—C16	119.00 (14)	C6—C10—H10B	109.5
F1—C17—C12	118.90 (14)	H10A—C10—H10B	109.5
C16—C17—C12	122.09 (15)	C6—C10—H10C	109.5
C8—C1—C2	107.72 (13)	H10A—C10—H10C	109.5
C8—C1—S1	127.53 (12)	H10B—C10—H10C	109.5
C2—C1—S1	124.61 (11)	C8—C11—H11A	109.5
C7—C2—C3	119.30 (13)	C8—C11—H11B	109.5
C7—C2—C1	104.47 (12)	H11A—C11—H11B	109.5
C3—C2—C1	136.22 (13)	C8—C11—H11C	109.5
C4—C3—C2	118.53 (13)	H11A—C11—H11C	109.5
C4—C3—H3	120.7	H11B—C11—H11C	109.5
C2—C3—H3	120.7	C14—C13—C12	119.81 (15)
C3—C4—C5	119.61 (14)	C14—C13—H13	120.1
C3—C4—C9	120.90 (14)	C12—C13—H13	120.1
C5—C4—C9	119.47 (14)	C13—C14—C15	120.32 (16)
C6—C5—C4	123.54 (14)	C13—C14—H14	119.8
C6—C5—H5	118.2	C15—C14—H14	119.8
C4—C5—H5	118.2	C16—C15—C14	120.53 (16)
C7—C6—C5	114.35 (13)	C16—C15—H15	119.7
C7—C6—C10	122.18 (14)	C14—C15—H15	119.7
C5—C6—C10	123.46 (14)	C17—C16—C15	118.42 (16)
O1—C7—C6	124.88 (13)	C17—C16—H16	120.8

O1—C7—C2	110.44 (12)	C15—C16—H16	120.8
C6—C7—C2	124.67 (13)		
O3—S1—C12—C13	−119.82 (12)	C4—C5—C6—C7	−0.3 (2)
O2—S1—C12—C13	9.42 (14)	C4—C5—C6—C10	−179.14 (14)
C1—S1—C12—C13	123.39 (12)	C8—O1—C7—C6	177.56 (13)
O3—S1—C12—C17	58.37 (14)	C8—O1—C7—C2	−0.85 (15)
O2—S1—C12—C17	−172.39 (12)	C5—C6—C7—O1	−178.51 (13)
C1—S1—C12—C17	−58.41 (13)	C10—C6—C7—O1	0.4 (2)
C13—C12—C17—F1	179.51 (13)	C5—C6—C7—C2	−0.3 (2)
S1—C12—C17—F1	1.30 (19)	C10—C6—C7—C2	178.56 (13)
C13—C12—C17—C16	0.2 (2)	C3—C2—C7—O1	179.19 (12)
S1—C12—C17—C16	−178.05 (12)	C1—C2—C7—O1	0.22 (15)
O3—S1—C1—C8	−7.65 (16)	C3—C2—C7—C6	0.8 (2)
O2—S1—C1—C8	−138.77 (14)	C1—C2—C7—C6	−178.20 (13)
C12—S1—C1—C8	108.69 (14)	C2—C1—C8—O1	−1.05 (16)
O3—S1—C1—C2	177.27 (12)	S1—C1—C8—O1	−176.80 (10)
O2—S1—C1—C2	46.15 (14)	C2—C1—C8—C11	177.56 (16)
C12—S1—C1—C2	−66.39 (13)	S1—C1—C8—C11	1.8 (3)
C8—C1—C2—C7	0.50 (16)	C7—O1—C8—C1	1.17 (15)
S1—C1—C2—C7	176.40 (11)	C7—O1—C8—C11	−177.74 (12)
C8—C1—C2—C3	−178.21 (16)	C17—C12—C13—C14	−0.2 (2)
S1—C1—C2—C3	−2.3 (2)	S1—C12—C13—C14	178.09 (12)
C7—C2—C3—C4	−0.6 (2)	C12—C13—C14—C15	−0.5 (2)
C1—C2—C3—C4	177.95 (15)	C13—C14—C15—C16	1.3 (2)
C2—C3—C4—C5	0.1 (2)	F1—C17—C16—C15	−178.80 (14)
C2—C3—C4—C9	−178.71 (14)	C12—C17—C16—C15	0.6 (2)
C3—C4—C5—C6	0.4 (2)	C14—C15—C16—C17	−1.3 (2)
C9—C4—C5—C6	179.20 (14)		

Hydrogen-bond geometry (Å, º)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···O2^{i}	0.95	2.58	3.462 (2)	155
C9—H9*C*···*Cg*1^{ii}	0.98	2.79	3.612 (2)	142

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