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Crystal structure of 2-ethyl-3-(4-fluorophenylsulfonyl)-5,7-dimethyl-1-benzofuran

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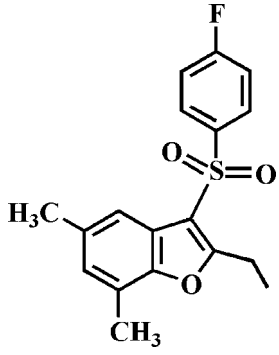
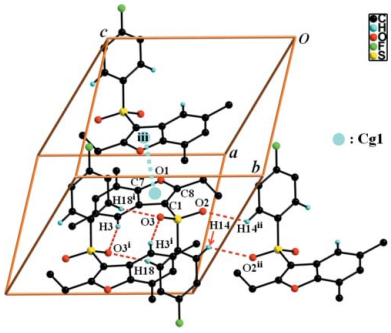
In the title compound, $C_{18}H_{17}FO_3S$, the dihedral angle between the plane of the benzofuran ring [r.m.s. deviation = 0.006 (1) Å] and that of the 4-fluorophenyl ring [r.m.s. deviation = 0.004 (1) Å] is 82.45 (4)°. In the crystal, molecules are linked *via* three different pairs of C—H···O hydrogen bonds, forming chains along [001] and enclosing two $R_2^2(10)$ and one $R_2^2(12)$ ring motifs. The chains are further linked by π–π interactions [inter-centroid distance = 3.566 (1) Å] between the furan rings of inversion-related molecules, forming a two-dimensional network lying parallel to (100).

1. Chemical Context

Substituted benzofurans show important pharmacological properties such as antibacterial and antifungal, antitumour and antiviral, and antimicrobial activities (Aslam *et al.* 2009; Galal *et al.*, 2009; Khan *et al.*, 2005), and are potential inhibitors of β-amyloid aggregation (Howlett *et al.*, 1999; Ono *et al.*, 2002). These benzofuran compounds occur in a great number of natural products (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our ongoing project concerning 2-alkyl-3-(phenylsulfonyl)-5,7-dimethyl-1-benzofuran derivatives, we report herein on the synthesis and crystal structure of the title compound.





2. Structural commentary

In the title molecule, Fig. 1, the benzofuran unit (O1/C1–C8) is essentially planar, with a mean deviation of 0.006 (1) Å from the mean plane defined by the nine constituent atoms. The 4-fluorophenyl ring (C13–C18) is inclined to the benzofuran ring by 82.45 (4)°.

3. Supramolecular features

In the crystal, molecules are linked *via* three different pairs of C—H···O hydrogen bonds, forming chains along [001] and

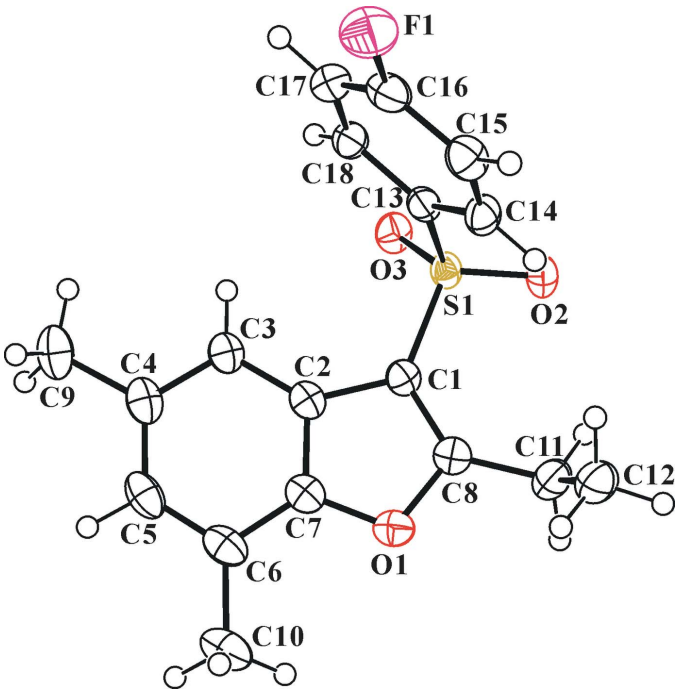


Figure 1
The molecular structure of the title molecule, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

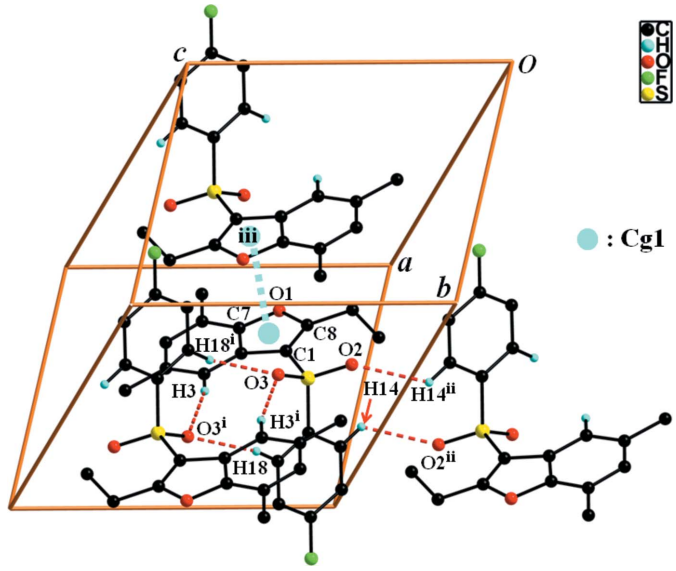


Figure 2
A view of the C—H···O and π–π interactions (dotted lines) in the crystal structure of the title compound [see Table 1 for details; H atoms not involved in hydrogen bonding have been omitted for clarity; symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $-x+1, -y+2, -z$; (iii) $-x+1, -y+1, -z+1$].

enclosing two $R_2^2(10)$ and one $R_2^2(12)$ ring motifs (Fig. 2 and Table 1). The chains are further linked by π–π interactions between the furan rings of inversion-related molecules, forming a two-dimensional network lying parallel to (100) [illustrated in Fig. 2; $Cg1\cdots Cg1^{i}$ = 3.566 (1), interplanar distance = 3.553 (1); slippage = 0.305 Å; $Cg1$ is the centroid of the C1/C2/C7/O1/C8 furan ring; symmetry code: (i) $-x+1, -y+1, -z+1$].

4. Database survey

A search of the Cambridge Structural Database (Version 5.35, last update May 2014; Allen, 2002) for 3-(phenylsulfonyl)-benzofuran gave 65 hits. Six of these involve 5,7-dimethyl-3-(phenylsulfonyl)benzofuran derivatives. They include the 2-methyl derivative of the title compound, 2-methyl-3-(4-fluorophenylsulfonyl)-5,7-dimethyl-1-benzofuran (Choi *et al.*, 2010). In these six compounds, the dihedral angle between the phenylsulfonyl ring and the benzofuran ring varies from *ca.* 72.68° in the 2-methyl derivative mentioned above, to 87.61° in 2-methyl-3-(2-fluorophenylsulfonyl)-5,7-dimethyl-1-benzofuran (Choi *et al.*, 2014). The same angle in the title compound is 82.45 (4)°.

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O3^{i}	0.95	2.55	3.4804 (18)	167
C14—H14···O2^{ii}	0.95	2.49	3.1211 (17)	124
C18—H18···O3^{i}	0.95	2.36	3.2742 (17)	160

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{17}FO_3S$
M_r	332.38
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	173
a, b, c (Å)	8.8756 (2), 9.3917 (2), 11.0284 (2)
α, β, γ (°)	65.735 (1), 80.735 (1), 71.145 (1)
V (Å^3)	792.68 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.23
Crystal size (mm)	0.39 × 0.33 × 0.30
Data collection	
Diffractometer	Bruker *SMART* APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.918, 0.936
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14813, 3934, 3489
R_{int}	0.025
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.108, 1.07
No. of reflections	3934
No. of parameters	211
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.44

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97* and *SHELXL2014* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 1998) and *PLATON* (Spek, 2009).

5. Synthesis and crystallization

The starting material 2-ethyl-3-(4-fluorophenylsulfanyl)-5,7-dimethyl-1-benzofuran was prepared by a literature method (Choi *et al.* 1999). 3-Chloroperoxybenzoic acid (77%, 448 mg, 2.0 mmol) was added in small portions to a stirred solution of 2-ethyl-3-(4-fluorophenylsulfanyl)-5,7-dimethyl-1-benzofuran (270 mg, 0.9 mmol) in dichloromethane (35 ml) at 273 K. After being stirred at room temperature for 8h, the mixture was washed with saturated sodium bicarbonate solution (2 × 15 ml) 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 colourless solid [yield 61% (236 mg); m.p. 416–417 K; R_f = 0.63 (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 (21 mg) in acetone (15 ml) at room temperature. ^{1}H NMR (δ p.p.m., $CDCl_3$, 400 Hz): 7.99–8.04 (*m*, 2H), 7.47 (*s*, 1H), 7.14–7.19 (*m*, 2H), 6.93 (*s*, 1H), 3.22 (*q*, *J* = 7.52 Hz, 2H), 2.43 (*s*, 3H), 2.41 (*s*, 3H), 1.36 (*t*, *J* = 7.54 Hz, 3H).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were positioned geometrically and refined as riding atoms: C—H = 0.95 Å for aryl, 0.99 Å for methylene and 0.98 Å for methyl H atoms, respectively, with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and = 1.2U_{eq}(C) for other H atoms.

Acknowledgements

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Crystal structure of 2-ethyl-3-(4-fluorophenylsulfonyl)-5,7-dimethyl-1-benzofuran

Hong Dae Choi and Uk Lee

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

2-Ethyl-3-(4-fluorophenylsulfonyl)-5,7-dimethyl-1-benzofuran

Crystal data

$C_{18}H_{17}FO_3S$
M_r = 332.38
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.8756 (2) Å
b = 9.3917 (2) Å
c = 11.0284 (2) Å
α = 65.735 (1)°
β = 80.735 (1)°
γ = 71.145 (1)°
V = 792.68 (3) Å^3
Z = 2
$F(000)$ = 348
D_x = 1.393 Mg m^{-3}
Melting point = 417–416 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6147 reflections
θ = 2.4–28.2°
μ = 0.23 mm^{-1}
T = 173 K
Block, colourless
0.39 × 0.33 × 0.30 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} = 0.918, T_{max} = 0.936
14813 measured reflections
3934 independent reflections
3489 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 28.4°, θ_{min} = 2.0°
h = −11→11
k = −12→12
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.108
S = 1.07
3934 reflections
211 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

$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.2229P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ 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	0.47686 (4)	0.90767 (4)	0.29373 (3)	0.02612 (11)
F1	0.95796 (13)	1.25062 (13)	0.04333 (11)	0.0519 (3)
O1	0.69433 (12)	0.44317 (12)	0.38093 (10)	0.0329 (2)
O2	0.37720 (12)	0.93598 (13)	0.19098 (10)	0.0339 (2)
O3	0.40523 (12)	0.95254 (13)	0.40432 (10)	0.0331 (2)
C1	0.58429 (16)	0.70342 (16)	0.35637 (13)	0.0268 (3)
C2	0.68621 (15)	0.62616 (16)	0.46953 (13)	0.0274 (3)
C3	0.72804 (16)	0.67484 (18)	0.55984 (13)	0.0300 (3)
H3	0.6840	0.7834	0.5555	0.036*
C4	0.83619 (17)	0.5600 (2)	0.65658 (14)	0.0343 (3)
C5	0.89864 (17)	0.40020 (19)	0.66131 (15)	0.0374 (3)
H5	0.9724	0.3241	0.7282	0.045*
C6	0.85859 (17)	0.34717 (18)	0.57367 (15)	0.0352 (3)
C7	0.75119 (16)	0.46619 (17)	0.47913 (14)	0.0304 (3)
C8	0.59290 (16)	0.58923 (17)	0.30738 (14)	0.0296 (3)
C9	0.8875 (2)	0.6073 (2)	0.75486 (16)	0.0472 (4)
H9A	0.8299	0.7212	0.7398	0.071*
H9B	1.0023	0.5946	0.7432	0.071*
H9C	0.8636	0.5370	0.8456	0.071*
C10	0.9270 (2)	0.17627 (19)	0.57832 (19)	0.0461 (4)
H10A	0.8523	0.1503	0.5397	0.069*
H10B	0.9449	0.0998	0.6710	0.069*
H10C	1.0284	0.1673	0.5273	0.069*
C11	0.52011 (18)	0.58876 (19)	0.19537 (15)	0.0364 (3)
H11A	0.4181	0.6764	0.1747	0.044*
H11B	0.4962	0.4836	0.2233	0.044*
C12	0.6270 (2)	0.6136 (2)	0.06985 (16)	0.0425 (4)
H12A	0.6419	0.7225	0.0361	0.064*
H12B	0.5772	0.6031	0.0020	0.064*
H12C	0.7307	0.5311	0.0907	0.064*
C13	0.62269 (16)	1.01143 (16)	0.21923 (13)	0.0261 (3)
C14	0.68862 (17)	1.01386 (17)	0.09555 (13)	0.0306 (3)

H14	0.6562	0.9596	0.0527	0.037*
C15	0.80202 (18)	1.09615 (19)	0.03520 (14)	0.0348 (3)
H15	0.8485	1.0998	−0.0495	0.042*
C16	0.84549 (18)	1.17233 (17)	0.10114 (15)	0.0349 (3)
C17	0.7805 (2)	1.17300 (18)	0.22324 (15)	0.0363 (3)
H17	0.8130	1.2283	0.2650	0.044*
C18	0.66666 (17)	1.09115 (17)	0.28363 (14)	0.0307 (3)
H18	0.6194	1.0895	0.3677	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02580 (17)	0.02980 (17)	0.02171 (17)	−0.00369 (12)	−0.00149 (12)	−0.01186 (13)
F1	0.0532 (6)	0.0496 (6)	0.0541 (6)	−0.0289 (5)	0.0052 (5)	−0.0128 (5)
O1	0.0315 (5)	0.0285 (5)	0.0380 (5)	−0.0076 (4)	0.0000 (4)	−0.0131 (4)
O2	0.0317 (5)	0.0415 (6)	0.0287 (5)	−0.0063 (4)	−0.0073 (4)	−0.0145 (4)
O3	0.0316 (5)	0.0399 (5)	0.0275 (5)	−0.0046 (4)	0.0029 (4)	−0.0185 (4)
C1	0.0262 (6)	0.0289 (6)	0.0241 (6)	−0.0070 (5)	0.0012 (5)	−0.0104 (5)
C2	0.0243 (6)	0.0301 (6)	0.0240 (6)	−0.0092 (5)	0.0027 (5)	−0.0069 (5)
C3	0.0280 (6)	0.0354 (7)	0.0243 (6)	−0.0101 (5)	0.0016 (5)	−0.0092 (5)
C4	0.0288 (7)	0.0445 (8)	0.0244 (6)	−0.0135 (6)	0.0014 (5)	−0.0067 (6)
C5	0.0288 (7)	0.0398 (8)	0.0293 (7)	−0.0094 (6)	−0.0023 (6)	0.0008 (6)
C6	0.0271 (7)	0.0299 (7)	0.0371 (8)	−0.0084 (5)	0.0021 (6)	−0.0028 (6)
C7	0.0265 (6)	0.0307 (7)	0.0303 (7)	−0.0100 (5)	0.0028 (5)	−0.0081 (5)
C8	0.0266 (6)	0.0313 (6)	0.0306 (7)	−0.0084 (5)	0.0018 (5)	−0.0124 (6)
C9	0.0453 (9)	0.0623 (11)	0.0312 (8)	−0.0132 (8)	−0.0081 (7)	−0.0144 (8)
C10	0.0366 (8)	0.0301 (7)	0.0568 (10)	−0.0065 (6)	−0.0028 (7)	−0.0042 (7)
C11	0.0357 (7)	0.0402 (8)	0.0403 (8)	−0.0100 (6)	−0.0021 (6)	−0.0226 (7)
C12	0.0564 (10)	0.0399 (8)	0.0350 (8)	−0.0134 (7)	−0.0004 (7)	−0.0187 (7)
C13	0.0284 (6)	0.0242 (6)	0.0225 (6)	−0.0029 (5)	−0.0030 (5)	−0.0086 (5)
C14	0.0339 (7)	0.0341 (7)	0.0252 (6)	−0.0077 (6)	−0.0014 (5)	−0.0139 (6)
C15	0.0358 (7)	0.0366 (7)	0.0279 (7)	−0.0081 (6)	0.0023 (6)	−0.0114 (6)
C16	0.0339 (7)	0.0274 (6)	0.0368 (8)	−0.0090 (6)	−0.0029 (6)	−0.0052 (6)
C17	0.0464 (8)	0.0290 (7)	0.0359 (8)	−0.0101 (6)	−0.0072 (6)	−0.0133 (6)
C18	0.0382 (7)	0.0281 (6)	0.0253 (6)	−0.0055 (5)	−0.0033 (5)	−0.0121 (5)

Geometric parameters (Å, º)

S1—O2	1.4353 (10)	C9—H9B	0.9800
S1—O3	1.4383 (10)	C9—H9C	0.9800
S1—C1	1.7341 (14)	C10—H10A	0.9800
S1—C13	1.7648 (14)	C10—H10B	0.9800
F1—C16	1.3520 (17)	C10—H10C	0.9800
O1—C8	1.3684 (17)	C11—C12	1.525 (2)
O1—C7	1.3833 (18)	C11—H11A	0.9900
C1—C8	1.3630 (19)	C11—H11B	0.9900
C1—C2	1.4482 (18)	C12—H12A	0.9800
C2—C7	1.3892 (19)	C12—H12B	0.9800

C2—C3	1.3935 (19)	C12—H12C	0.9800
C3—C4	1.392 (2)	C13—C14	1.3891 (18)
C3—H3	0.9500	C13—C18	1.3901 (19)
C4—C5	1.403 (2)	C14—C15	1.385 (2)
C4—C9	1.505 (2)	C14—H14	0.9500
C5—C6	1.389 (2)	C15—C16	1.373 (2)
C5—H5	0.9500	C15—H15	0.9500
C6—C7	1.385 (2)	C16—C17	1.379 (2)
C6—C10	1.503 (2)	C17—C18	1.385 (2)
C8—C11	1.485 (2)	C17—H17	0.9500
C9—H9A	0.9800	C18—H18	0.9500

O2—S1—O3	119.08 (6)	C6—C10—H10A	109.5
O2—S1—C1	108.98 (6)	C6—C10—H10B	109.5
O3—S1—C1	108.06 (6)	H10A—C10—H10B	109.5
O2—S1—C13	108.05 (6)	C6—C10—H10C	109.5
O3—S1—C13	107.27 (6)	H10A—C10—H10C	109.5
C1—S1—C13	104.43 (6)	H10B—C10—H10C	109.5
C8—O1—C7	107.20 (11)	C8—C11—C12	113.00 (13)
C8—C1—C2	108.02 (12)	C8—C11—H11A	109.0
C8—C1—S1	127.10 (11)	C12—C11—H11A	109.0
C2—C1—S1	124.84 (10)	C8—C11—H11B	109.0
C7—C2—C3	119.68 (13)	C12—C11—H11B	109.0
C7—C2—C1	104.35 (12)	H11A—C11—H11B	107.8
C3—C2—C1	135.96 (13)	C11—C12—H12A	109.5
C4—C3—C2	118.14 (14)	C11—C12—H12B	109.5
C4—C3—H3	120.9	H12A—C12—H12B	109.5
C2—C3—H3	120.9	C11—C12—H12C	109.5
C3—C4—C5	119.77 (15)	H12A—C12—H12C	109.5
C3—C4—C9	120.17 (15)	H12B—C12—H12C	109.5
C5—C4—C9	120.05 (14)	C14—C13—C18	121.55 (13)
C6—C5—C4	123.62 (14)	C14—C13—S1	118.74 (10)
C6—C5—H5	118.2	C18—C13—S1	119.70 (10)
C4—C5—H5	118.2	C15—C14—C13	119.42 (13)
C7—C6—C5	114.32 (14)	C15—C14—H14	120.3
C7—C6—C10	122.25 (15)	C13—C14—H14	120.3
C5—C6—C10	123.43 (14)	C16—C15—C14	118.19 (13)
O1—C7—C6	125.00 (14)	C16—C15—H15	120.9
O1—C7—C2	110.53 (12)	C14—C15—H15	120.9
C6—C7—C2	124.47 (14)	F1—C16—C15	118.29 (14)
C1—C8—O1	109.89 (12)	F1—C16—C17	118.31 (14)
C1—C8—C11	135.05 (13)	C15—C16—C17	123.41 (14)
O1—C8—C11	115.06 (12)	C16—C17—C18	118.51 (13)
C4—C9—H9A	109.5	C16—C17—H17	120.7
C4—C9—H9B	109.5	C18—C17—H17	120.7
H9A—C9—H9B	109.5	C17—C18—C13	118.92 (13)
C4—C9—H9C	109.5	C17—C18—H18	120.5
H9A—C9—H9C	109.5	C13—C18—H18	120.5

H9B—C9—H9C	109.5		
O2—S1—C1—C8	8.30 (15)	C3—C2—C7—C6	−0.5 (2)
O3—S1—C1—C8	139.05 (12)	C1—C2—C7—C6	179.20 (13)
C13—S1—C1—C8	−106.97 (13)	C2—C1—C8—O1	−0.30 (15)
O2—S1—C1—C2	−173.96 (10)	S1—C1—C8—O1	177.75 (9)
O3—S1—C1—C2	−43.20 (13)	C2—C1—C8—C11	−179.77 (15)
C13—S1—C1—C2	70.78 (12)	S1—C1—C8—C11	−1.7 (2)
C8—C1—C2—C7	0.46 (14)	C7—O1—C8—C1	0.01 (15)
S1—C1—C2—C7	−177.64 (10)	C7—O1—C8—C11	179.60 (11)
C8—C1—C2—C3	−179.96 (15)	C1—C8—C11—C12	95.6 (2)
S1—C1—C2—C3	1.9 (2)	O1—C8—C11—C12	−83.88 (16)
C7—C2—C3—C4	0.70 (19)	O2—S1—C13—C14	−38.40 (12)
C1—C2—C3—C4	−178.83 (14)	O3—S1—C13—C14	−167.95 (10)
C2—C3—C4—C5	−0.4 (2)	C1—S1—C13—C14	77.52 (12)
C2—C3—C4—C9	178.89 (13)	O2—S1—C13—C18	140.33 (11)
C3—C4—C5—C6	−0.1 (2)	O3—S1—C13—C18	10.79 (13)
C9—C4—C5—C6	−179.43 (14)	C1—S1—C13—C18	−103.75 (12)
C4—C5—C6—C7	0.4 (2)	C18—C13—C14—C15	0.6 (2)
C4—C5—C6—C10	179.40 (14)	S1—C13—C14—C15	179.36 (11)
C8—O1—C7—C6	−179.37 (13)	C13—C14—C15—C16	0.2 (2)
C8—O1—C7—C2	0.30 (15)	C14—C15—C16—F1	179.00 (13)
C5—C6—C7—O1	179.55 (12)	C14—C15—C16—C17	−1.0 (2)
C10—C6—C7—O1	0.5 (2)	F1—C16—C17—C18	−179.19 (13)
C5—C6—C7—C2	−0.1 (2)	C15—C16—C17—C18	0.8 (2)
C10—C6—C7—C2	−179.13 (13)	C16—C17—C18—C13	0.1 (2)
C3—C2—C7—O1	179.87 (11)	C14—C13—C18—C17	−0.8 (2)
C1—C2—C7—O1	−0.47 (14)	S1—C13—C18—C17	−179.53 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O3^{i}	0.95	2.55	3.4804 (18)	167
C14—H14···O2^{ii}	0.95	2.49	3.1211 (17)	124
C18—H18···O3^{i}	0.95	2.36	3.2742 (17)	160

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