



Crystal structure of 5-chloro-2-(2-fluorophenyl)-3-methylsulfinyl-1-benzofuran

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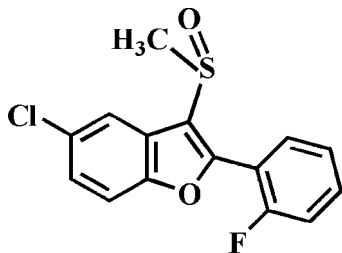
In the title compound, C₁₅H₁₀ClFO₂S, the dihedral angle between the mean planes of the benzofuran ring [r.m.s. deviation = 0.007 (1) Å] and the 2-fluorophenyl ring is 32.53 (5)°. In the crystal, molecules related by inversion are paired into dimers *via* two different C—H···O hydrogen bonds. Further, Cl···O halogen bonds [3.114 (1) Å], and F···π [F-to-furan-centroid distance = 3.109 (1) Å] and S···F [3.1984 (9) Å] interactions link these into a three-dimensional network.

Keywords: crystal structure; benzofuran; 2-fluorophenyl; C—H···O hydrogen bonds; F···π and S···F contacts.

CCDC reference: 1414408

1. Related literature

For the pharmacological properties of benzofuran compounds, see: Aslam *et al.* (2009); Galal *et al.* (2009); Howlett *et al.* (1999); Wahab Khan *et al.* (2005); Ono *et al.* (2002). For a related structure, see: Choi & Lee (2014). For further synthetic details, see: Choi *et al.* (1999). For a review of halogen bonding, see: Politzer *et al.* (2007).



2. Experimental

2.1. Crystal data

C ₁₅ H ₁₀ ClFO ₂ S	$\gamma = 112.373 (1)^\circ$
$M_r = 308.74$	$V = 652.97 (2) \text{ \AA}^3$
Triclinic, $P\bar{1}$	$Z = 2$
$a = 7.9626 (1) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 8.3518 (1) \text{ \AA}$	$\mu = 0.46 \text{ mm}^{-1}$
$c = 10.7127 (2) \text{ \AA}$	$T = 173 \text{ K}$
$\alpha = 92.758 (1)^\circ$	$0.45 \times 0.36 \times 0.32 \text{ mm}$
$\beta = 95.509 (1)^\circ$	

2.2. Data collection

Bruker SMART APEXII CCD diffractometer	12250 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2009)	3263 independent reflections
$T_{\min} = 0.690$, $T_{\max} = 0.746$	3030 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.023$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$	183 parameters
$wR(F^2) = 0.081$	H-atom parameters constrained
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.34 \text{ e \AA}^{-3}$
3263 reflections	$\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C6—H6···O1 ⁱ	0.95	2.53	3.4756 (16)	176
C14—H14···O2 ⁱⁱ	0.95	2.44	3.3591 (17)	163

Symmetry codes: (i) $-x + 2, -y + 1, -z$; (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: SHELXL2014 (Sheldrick, 2015); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012) and DIAMOND (Brandenburg, 1998); software used to prepare material for publication: SHELXL2014.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: FY2120).

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supporting information

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Crystal structure of 5-chloro-2-(2-fluorophenyl)-3-methylsulfinyl-1-benzofuran

Hong Dae Choi and Uk Lee

S1. Comment

Many compounds involving a benzofuran ring show significant pharmacological properties, such as antibacterial, antifungal, antitumor, antiviral and antimicrobial activities (Aslam *et al.* 2009; Galal *et al.*, 2009; Wahab Khan *et al.*, 2005), and are potential inhibitors of β -amyloid aggregation (Howlett *et al.*, 1999; Ono *et al.*, 2002). As a part of our continuing project on benzofuran derivatives (Choi & Lee, 2014), 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 0.007 (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 0.007 (1) Å from the least-squares plane defined by the six constituent atoms. The dihedral angle formed by the benzofuran ring and the 2-fluorophenyl ring is 32.53 (5)°. In the crystal structure (Fig. 2), molecules related by inversion are paired into dimers *via* two different C–H...O hydrogen bonds (Table 1), and a Cl...O halogen bond between the chlorine and the oxygen of the S=O unit [C11...O2ⁱⁱⁱ = 3.114 (1) Å, C4–C11...O2ⁱⁱⁱ = 171.16 (5)°] (Politzer *et al.*, 2007), F1...Cg^v [3.109 (1) Å] (Cg is the centroid of the C1/C2/C7/O1/C8 furan ring) and S1...F1^{iv} [3.1984 (9) Å] interactions, forming a three-dimensional network. [Symmetry codes: (i) $-x + 2, -y + 1, -z$; (ii) $-x + 1, -y + 1, -z$; (iii) $-x + 1, -y + 1, -z + 1$; (iv) $-x, -y, -z$; (v) $-x + 1, -y, -z$.]

S2. Experimental

The starting material 5-chloro-2-(2-fluorophenyl)-3-methylsulfonyl-1-benzofuran was prepared by a literature method (Choi *et al.*, 1999). 3-Chloroperoxybenzoic acid (77%, 224 mg, 1.0 mmol) was added in small portions to a stirred solution of 5-chloro-2-(2-fluorophenyl)-3-methylsulfonyl-1-benzofuran (263 mg, 0.9 mmol) in dichloromethane (25 ml) at 273 K. After being stirred at room temperature for 8h, the mixture was washed with saturated sodium bicarbonate solution (2 × 10 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, 1:2 v/v) to afford the title compound as a colorless solid [yield 68% (188 mg); m.p. 431–432 K; R_f = 0.55 (hexane-ethyl acetate, 1:2 v/v)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title compound (18 mg) in ethyl acetate (20 ml) 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 and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aryl and $1.5U_{\text{eq}}(\text{C})$ for methyl H atoms. The positions of methyl hydrogens were optimized using the *SHELXL-2014/7* command AFIX 137 (Sheldrick, 2015).

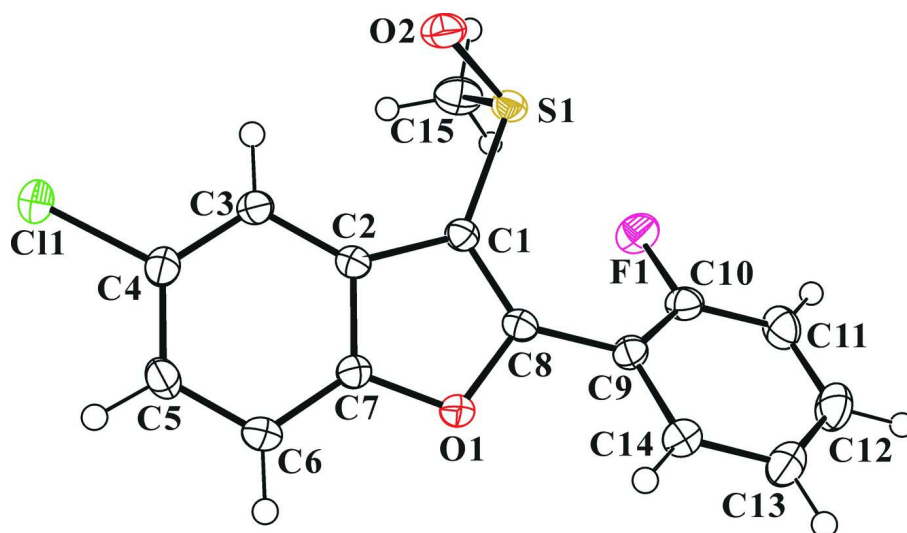


Figure 1

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.

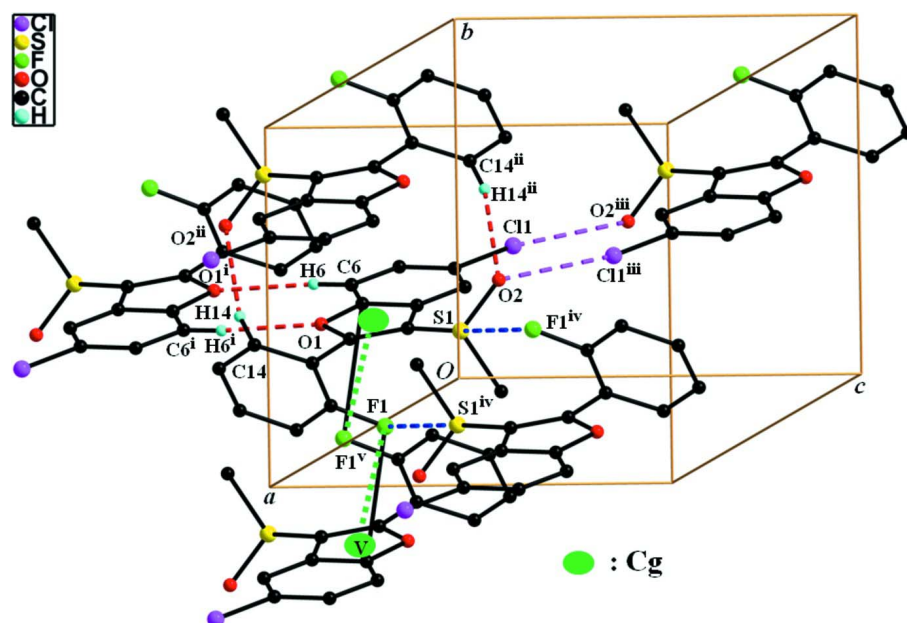


Figure 2

A view of the C–H...O, Cl...O, F... π and S...F interactions (dotted lines) in the crystal structure of the title compound. H atoms not participating in hydrogen-bonding were omitted for clarity. [Symmetry codes: (i) $-x + 2, -y + 1, -z$; (ii) $-x + 1, -y + 1, -z$; (iii) $-x + 1, -y + 1, -z + 1$; (iv) $-x, -y, -z$; (v) $-x + 1, -y, -z$.]

5-Chloro-2-(2-fluorophenyl)-3-methylsulfinyl-1-benzofuran

Crystal data

$C_{15}H_{10}ClFO_2S$

$M_r = 308.74$

Triclinic, $P\bar{1}$

$a = 7.9626 (1) \text{ \AA}$

$b = 8.3518 (1) \text{ \AA}$

$c = 10.7127 (2) \text{ \AA}$

$\alpha = 92.758 (1)^\circ$
 $\beta = 95.509 (1)^\circ$
 $\gamma = 112.373 (1)^\circ$
 $V = 652.97 (2) \text{ \AA}^3$
 $Z = 2$
 $F(000) = 316$
 $D_x = 1.570 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 6796 reflections
 $\theta = 2.7\text{--}28.4^\circ$
 $\mu = 0.46 \text{ mm}^{-1}$
 $T = 173 \text{ K}$
 Block, colourless
 $0.45 \times 0.36 \times 0.32 \text{ mm}$

Data collection

Bruker SMART APEXII CCD
 diffractometer
 Radiation source: rotating anode
 Detector resolution: $10.0 \text{ pixels mm}^{-1}$
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2009)
 $T_{\min} = 0.690$, $T_{\max} = 0.746$

12250 measured reflections
 3263 independent reflections
 3030 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$
 $\theta_{\max} = 28.4^\circ$, $\theta_{\min} = 1.9^\circ$
 $h = -10 \rightarrow 10$
 $k = -11 \rightarrow 11$
 $l = -14 \rightarrow 14$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.081$
 $S = 1.05$
 3263 reflections
 183 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
 $w = 1/[\sigma^2(F_o^2) + (0.0399P)^2 + 0.2911P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.34 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.26 \text{ e \AA}^{-3}$
 Extinction correction: SHELXL2014 (Sheldrick,
 2015), $F_c^* = kF_c[1 + 0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$
 Extinction coefficient: $0.042 (3)$

Special details

Experimental. $^1\text{H NMR}$ (δ p.p.m., CDCl_3 , 400 Hz): 8.21 (d, $J = 2.04 \text{ Hz}$, 1H), 7.66-7.71 (m, 1H), 7.50-7.57 (m, 2H), 7.32-7.41 (m, 2H), 7.21-7.26 (m, 1H), 3.15 (s, 3H).

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.80773 (5)	0.60679 (5)	0.52105 (3)	0.03134 (11)
S1	0.20658 (4)	0.19225 (4)	0.10339 (3)	0.02090 (10)
F1	0.22939 (12)	-0.06448 (11)	-0.07604 (8)	0.0324 (2)
O1	0.70194 (12)	0.36314 (12)	-0.00857 (8)	0.02229 (19)
O2	0.18502 (13)	0.32691 (13)	0.18956 (10)	0.0283 (2)
C1	0.44206 (16)	0.27158 (16)	0.08330 (11)	0.0198 (2)
C2	0.58981 (17)	0.37914 (16)	0.17693 (11)	0.0198 (2)
C3	0.60633 (18)	0.43369 (17)	0.30452 (12)	0.0220 (3)
H3	0.5032	0.4009	0.3498	0.026*
C4	0.77958 (18)	0.53749 (17)	0.36158 (12)	0.0231 (3)

C5	0.93409 (18)	0.58960 (18)	0.29751 (13)	0.0258 (3)
H5	1.0502	0.6620	0.3411	0.031*
C6	0.91896 (18)	0.53654 (18)	0.17133 (13)	0.0255 (3)
H6	1.0220	0.5701	0.1260	0.031*
C7	0.74560 (17)	0.43207 (16)	0.11491 (12)	0.0208 (2)
C8	0.51654 (17)	0.26585 (16)	-0.02553 (12)	0.0201 (2)
C9	0.44641 (17)	0.17903 (16)	-0.15243 (12)	0.0210 (2)
C10	0.30426 (18)	0.01690 (17)	-0.17542 (13)	0.0242 (3)
C11	0.2375 (2)	-0.06907 (19)	-0.29337 (14)	0.0304 (3)
H11	0.1390	-0.1796	-0.3049	0.036*
C12	0.3186 (2)	0.0106 (2)	-0.39495 (14)	0.0341 (3)
H12	0.2744	-0.0450	-0.4778	0.041*
C13	0.4640 (2)	0.1712 (2)	-0.37641 (13)	0.0311 (3)
H13	0.5198	0.2238	-0.4466	0.037*
C14	0.52834 (19)	0.25528 (17)	-0.25675 (12)	0.0244 (3)
H14	0.6282	0.3649	-0.2451	0.029*
C15	0.2029 (2)	0.02115 (19)	0.20017 (15)	0.0323 (3)
H15A	0.2950	0.0697	0.2741	0.048*
H15B	0.2302	-0.0665	0.1516	0.048*
H15C	0.0814	-0.0330	0.2276	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.02955 (19)	0.0403 (2)	0.02092 (16)	0.01176 (15)	-0.00124 (12)	-0.00425 (13)
S1	0.01618 (16)	0.02104 (16)	0.02386 (16)	0.00518 (12)	0.00408 (11)	0.00099 (11)
F1	0.0333 (5)	0.0245 (4)	0.0318 (4)	0.0018 (3)	0.0101 (4)	0.0004 (3)
O1	0.0179 (4)	0.0253 (4)	0.0208 (4)	0.0049 (4)	0.0045 (3)	0.0002 (3)
O2	0.0243 (5)	0.0265 (5)	0.0342 (5)	0.0092 (4)	0.0093 (4)	-0.0024 (4)
C1	0.0168 (6)	0.0198 (6)	0.0214 (6)	0.0054 (4)	0.0033 (4)	0.0016 (4)
C2	0.0176 (6)	0.0194 (6)	0.0223 (6)	0.0068 (4)	0.0031 (4)	0.0021 (4)
C3	0.0211 (6)	0.0247 (6)	0.0212 (6)	0.0095 (5)	0.0042 (5)	0.0024 (5)
C4	0.0245 (6)	0.0250 (6)	0.0199 (6)	0.0102 (5)	0.0007 (5)	0.0000 (5)
C5	0.0191 (6)	0.0268 (6)	0.0270 (6)	0.0054 (5)	-0.0012 (5)	-0.0009 (5)
C6	0.0185 (6)	0.0280 (7)	0.0274 (6)	0.0056 (5)	0.0054 (5)	0.0017 (5)
C7	0.0200 (6)	0.0216 (6)	0.0201 (5)	0.0069 (5)	0.0041 (4)	0.0014 (4)
C8	0.0174 (6)	0.0188 (5)	0.0232 (6)	0.0057 (4)	0.0032 (4)	0.0022 (4)
C9	0.0213 (6)	0.0221 (6)	0.0213 (6)	0.0104 (5)	0.0028 (5)	-0.0004 (4)
C10	0.0230 (6)	0.0235 (6)	0.0265 (6)	0.0092 (5)	0.0051 (5)	0.0009 (5)
C11	0.0286 (7)	0.0263 (7)	0.0319 (7)	0.0083 (6)	-0.0015 (6)	-0.0066 (5)
C12	0.0409 (9)	0.0368 (8)	0.0247 (7)	0.0177 (7)	-0.0020 (6)	-0.0067 (6)
C13	0.0395 (8)	0.0347 (7)	0.0221 (6)	0.0176 (6)	0.0047 (6)	0.0025 (5)
C14	0.0259 (6)	0.0244 (6)	0.0240 (6)	0.0106 (5)	0.0048 (5)	0.0027 (5)
C15	0.0310 (7)	0.0285 (7)	0.0386 (8)	0.0097 (6)	0.0134 (6)	0.0126 (6)

Geometric parameters (Å, °)

C11—C4	1.7425 (13)	C6—C7	1.3800 (18)
S1—O2	1.4913 (10)	C6—H6	0.9500
S1—C1	1.7739 (12)	C8—C9	1.4618 (17)
S1—C15	1.7983 (14)	C9—C10	1.3867 (18)
F1—C10	1.3542 (15)	C9—C14	1.4043 (18)
O1—C7	1.3741 (15)	C10—C11	1.3740 (19)
O1—C8	1.3762 (15)	C11—C12	1.386 (2)
C1—C8	1.3647 (17)	C11—H11	0.9500
C1—C2	1.4420 (17)	C12—C13	1.388 (2)
C2—C7	1.3945 (17)	C12—H12	0.9500
C2—C3	1.3976 (17)	C13—C14	1.3830 (19)
C3—C4	1.3802 (18)	C13—H13	0.9500
C3—H3	0.9500	C14—H14	0.9500
C4—C5	1.3990 (19)	C15—H15A	0.9800
C5—C6	1.3815 (19)	C15—H15B	0.9800
C5—H5	0.9500	C15—H15C	0.9800
O2—S1—C1	105.84 (6)	C1—C8—C9	135.10 (12)
O2—S1—C15	105.10 (7)	O1—C8—C9	114.01 (10)
C1—S1—C15	97.80 (6)	C10—C9—C14	117.07 (12)
C7—O1—C8	106.59 (9)	C10—C9—C8	122.54 (12)
C8—C1—C2	106.80 (11)	C14—C9—C8	120.32 (12)
C8—C1—S1	127.53 (10)	F1—C10—C11	117.65 (12)
C2—C1—S1	125.04 (9)	F1—C10—C9	118.49 (12)
C7—C2—C3	119.16 (11)	C11—C10—C9	123.83 (13)
C7—C2—C1	105.31 (11)	C10—C11—C12	117.90 (14)
C3—C2—C1	135.52 (12)	C10—C11—H11	121.1
C4—C3—C2	116.81 (12)	C12—C11—H11	121.0
C4—C3—H3	121.6	C11—C12—C13	120.39 (13)
C2—C3—H3	121.6	C11—C12—H12	119.8
C3—C4—C5	123.12 (12)	C13—C12—H12	119.8
C3—C4—C11	118.55 (10)	C14—C13—C12	120.60 (13)
C5—C4—C11	118.33 (10)	C14—C13—H13	119.7
C6—C5—C4	120.45 (12)	C12—C13—H13	119.7
C6—C5—H5	119.8	C13—C14—C9	120.18 (13)
C4—C5—H5	119.8	C13—C14—H14	119.9
C7—C6—C5	116.19 (12)	C9—C14—H14	119.9
C7—C6—H6	121.9	S1—C15—H15A	109.5
C5—C6—H6	121.9	S1—C15—H15B	109.5
O1—C7—C6	125.31 (11)	H15A—C15—H15B	109.5
O1—C7—C2	110.42 (11)	S1—C15—H15C	109.5
C6—C7—C2	124.26 (12)	H15A—C15—H15C	109.5
C1—C8—O1	110.87 (11)	H15B—C15—H15C	109.5
O2—S1—C1—C8	-138.17 (12)	C1—C2—C7—C6	-179.34 (12)
C15—S1—C1—C8	113.63 (13)	C2—C1—C8—O1	-0.33 (14)

O2—S1—C1—C2	31.48 (12)	S1—C1—C8—O1	170.83 (9)
C15—S1—C1—C2	-76.71 (12)	C2—C1—C8—C9	178.19 (13)
C8—C1—C2—C7	0.43 (14)	S1—C1—C8—C9	-10.6 (2)
S1—C1—C2—C7	-171.01 (9)	C7—O1—C8—C1	0.10 (14)
C8—C1—C2—C3	-178.84 (14)	C7—O1—C8—C9	-178.76 (10)
S1—C1—C2—C3	9.7 (2)	C1—C8—C9—C10	-33.0 (2)
C7—C2—C3—C4	-0.38 (18)	O1—C8—C9—C10	145.51 (12)
C1—C2—C3—C4	178.82 (13)	C1—C8—C9—C14	150.06 (15)
C2—C3—C4—C5	0.61 (19)	O1—C8—C9—C14	-31.45 (17)
C2—C3—C4—C11	-179.26 (9)	C14—C9—C10—F1	176.27 (11)
C3—C4—C5—C6	-0.5 (2)	C8—C9—C10—F1	-0.78 (19)
C11—C4—C5—C6	179.35 (11)	C14—C9—C10—C11	-1.8 (2)
C4—C5—C6—C7	0.2 (2)	C8—C9—C10—C11	-178.88 (13)
C8—O1—C7—C6	179.14 (12)	F1—C10—C11—C12	-177.47 (13)
C8—O1—C7—C2	0.19 (14)	C9—C10—C11—C12	0.6 (2)
C5—C6—C7—O1	-178.76 (12)	C10—C11—C12—C13	0.8 (2)
C5—C6—C7—C2	0.0 (2)	C11—C12—C13—C14	-1.0 (2)
C3—C2—C7—O1	179.03 (11)	C12—C13—C14—C9	-0.2 (2)
C1—C2—C7—O1	-0.39 (14)	C10—C9—C14—C13	1.59 (19)
C3—C2—C7—C6	0.1 (2)	C8—C9—C14—C13	178.71 (12)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C6—H6...O1 ⁱ	0.95	2.53	3.4756 (16)	176
C14—H14...O2 ⁱⁱ	0.95	2.44	3.3591 (17)	163

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