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

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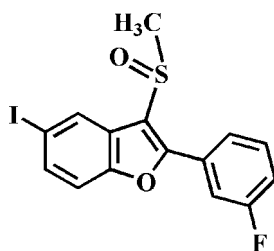
In the title compound, $C_{15}H_{10}FIO_2S$, the dihedral angle between the planes of the benzofuran ring system [r.m.s. deviation = 0.015 (2) Å] and the 3-fluorophenyl ring is 29.63 (7)°. In the crystal, molecules are linked into inversion dimers along the $b$-axis direction by two different pairs of C—H⋯O hydrogen bonds and I⋯O [3.228 (1) Å] contacts.

Keywords: crystal structure; benzofuran; 3-fluorophenyl; C—H⋯O hydrogen bonds; I⋯O contacts.

CCDC reference: 1029138

## 1. Related literature

For a related structure and background to benzofuran derivatives, 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

$C_{15}H_{10}FIO_2S$

$M_r = 400.19$

Triclinic, $P\bar{1}$
$a = 8.1348 (3)$ Å
$b = 8.6378 (3)$ Å
$c = 10.8350 (4)$ Å
$\alpha = 86.063 (1)°$
$\beta = 82.088 (1)°$
$\gamma = 66.408 (1)°$
$V = 690.99 (4)$ Å$^3$
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 2.48$ mm$^{-1}$
$T = 173$ K
$0.45 \times 0.28 \times 0.11$ mm

### 2.2. Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2009)
$T_{min} = 0.496$, $T_{max} = 0.746$
12585 measured reflections
3450 independent reflections
3226 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.054$
$S = 1.05$
3450 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.71$ e Å$^{-3}$
$\Delta\rho_{min} = -0.59$ e Å$^{-3}$

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

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| C6—H6⋯O1$^i$ | 0.95 | 2.57 | 3.520 (2) | 177 |
| C11—H11⋯O2$^{ii}$ | 0.95 | 2.55 | 3.372 (2) | 145 |

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

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.

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# supporting information

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

**Hong Dae Choi and Uk Lee**

### S1. Comment

As part of our continuing program for benzofuran derivatives (Choi & Lee, 2014), we report herein on the crystal structure of the title compound.

In the title molecule (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.015 (2) Å from the least-squares plane defined by the nine constituent atoms. The 3-fluorophenyl ring is essentially planar, with a mean deviation of 0.002 (1) Å from the least-squares plane defined by the six constituent atoms. The dihedral angle formed by the benzofuran ring and the 3-fluorophenyl ring is 29.63 (7)°. In the crystal structure (Fig. 2), molecules are linked into inversion-related dimers along *b*-axis direction by two different pairs of C—H⋯O hydrogen bonds (Table 1) and I⋯O halogen-bondings (Politzer *et al.*, 2007) between the iodine and the O atom of the sulfinyl group [I1⋯O2$^{iii}$ = 3.228 (2) Å, C4—I1⋯O2$^{iii}$ = 162.99 (6)°, symmetry code: (iii) - *x* + 1, - *y* + 2, - *z* + 2],

### S2. Experimental

The starting material 2-(3-fluorophenyl)-5-iodo-3-methylsulfanyl-1-benzofuran was prepared by 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 2-(3-fluorophenyl)-5-iodo-3-methylsulfanyl-1-benzofuran (346 mg, 0.9 mmol) in dichloromethane (30 ml) at 273 K. After being stirred at room temperature for 8h, the mixture was washed with saturated sodium bicarbonate solution (2 X 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 73% (263 mg); m.p. 453–454 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 (26 mg) in ethyl acetate (25 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, respectively. $U_{iso}$ (H) = 1.2$U_{eq}$ (C) for aryl and 1.5$U_{eq}$ (C)) for methyl H atoms. The positions of methyl hydrogens were optimized using the SHELXL-97's command AFIX 137 (Sheldrick, 2008).
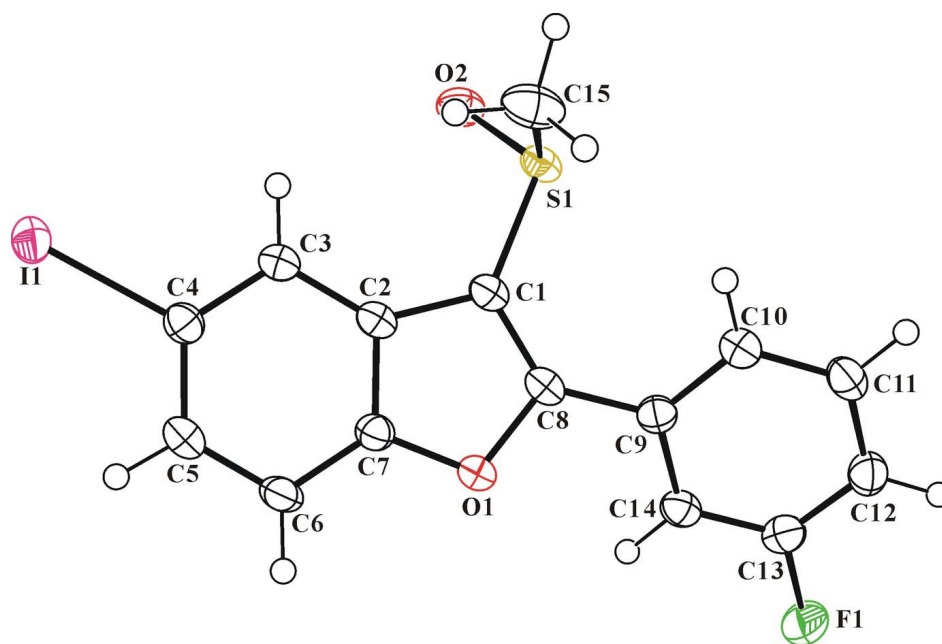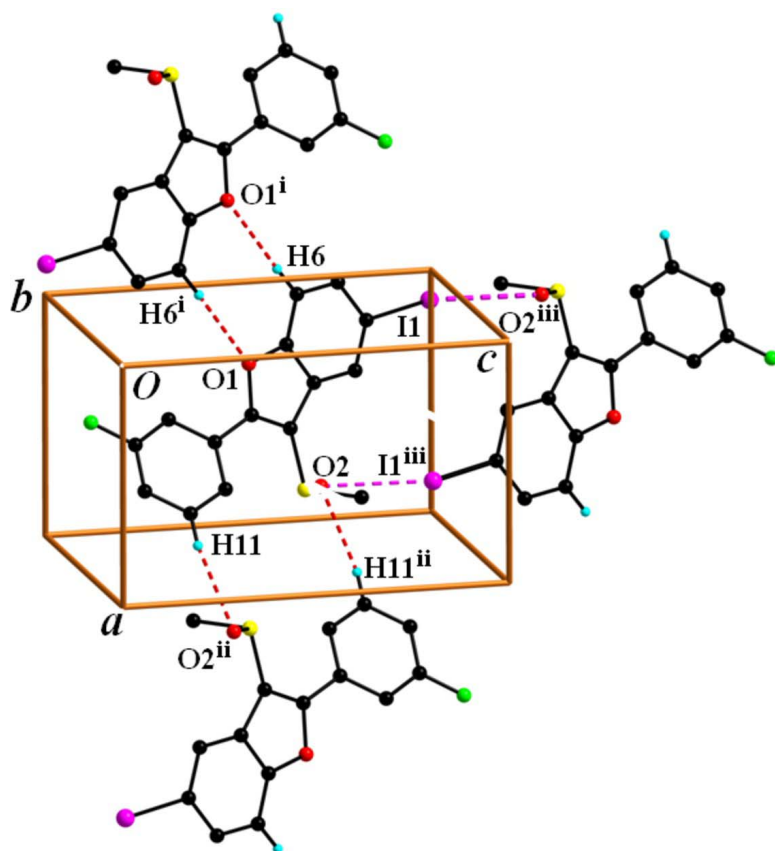
**Figure 1**

The molecular structure of the title 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 I···O 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*, -*y* + 2, -*z* + 1; (ii) -*x* + 2, -*y* + 1, -*z*; (iii) -*x* + 1, -*y* + 2, -*z* + 2.]

## 2-(3-Fluorophenyl)-5-iodo-3-methylsulfinyl-1-benzofuran

*Crystal data*

| | |
|---|---|
| $C_{15}H_{10}FIO_2S$ | $Z = 2$ |
| $M_r = 400.19$ | $F(000) = 388$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.923$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Melting point = 454–453 K |
| $a = 8.1348$ (3) Å | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $b = 8.6378$ (3) Å | Cell parameters from 8421 reflections |
| $c = 10.8350$ (4) Å | $\theta = 2.6$–28.4° |
| $\alpha = 86.063$ (1)° | $\mu = 2.48$ mm$^{-1}$ |
| $\beta = 82.088$ (1)° | $T = 173$ K |
| $\gamma = 66.408$ (1)° | Block, colourless |
| $V = 690.99$ (4) Å$^3$ | 0.45 × 0.28 × 0.11 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD diffractometer | Detector resolution: 10.0 pixels mm$^{-1}$ |
| Radiation source: rotating anode | $\varphi$ and $\omega$ scans |
| Graphite multilayer monochromator | Absorption correction: multi-scan (*SADABS*; Bruker, 2009) |

$T_{min} = 0.496$, $T_{max} = 0.746$  
12585 measured reflections  
3450 independent reflections  
3226 reflections with $I > 2\sigma(I)$  
$R_{int} = 0.028$

$\theta_{max} = 28.4°$, $\theta_{min} = 1.9°$  
$h = -10 \rightarrow 10$  
$k = -11 \rightarrow 11$  
$l = -14 \rightarrow 14$

*Refinement*

Refinement on $F^2$  
Least-squares matrix: full  
$R[F^2 > 2\sigma(F^2)] = 0.021$  
$wR(F^2) = 0.054$  
$S = 1.05$  
3450 reflections  
182 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  
$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2 + 0.2506P]$  
where $P = (F_o^2 + 2F_c^2)/3$  
$(\Delta/\sigma)_{max} = 0.002$  
$\Delta\rho_{max} = 0.71$ e Å$^{-3}$  
$\Delta\rho_{min} = -0.59$ e Å$^{-3}$

*Special details*

**Experimental**. $^1$H NMR ($\delta$ p.p.m., CDCl$_3$, 400 Hz): 8.59 (s, 1H), 7.70 (dd, $J$ =8.56 and 1.72 Hz, 1H), 7.46-7.62 (m, 3H), 7.36 (d, $J$ =8.88 Hz, 1H), 6.16-7.22 (m, 1H), 3.11 (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.

**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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| I1 | 0.171392 (16) | 1.149394 (16) | 1.025925 (12) | 0.03179 (6) |
| S1 | 0.78329 (6) | 0.70139 (6) | 0.61226 (5) | 0.02565 (10) |
| F1 | 0.44813 (19) | 0.69674 (18) | 0.05731 (12) | 0.0428 (3) |
| O1 | 0.29753 (17) | 0.86217 (16) | 0.49979 (13) | 0.0257 (3) |
| O2 | 0.81435 (19) | 0.83024 (18) | 0.67958 (15) | 0.0322 (3) |
| C1 | 0.5521 (2) | 0.7849 (2) | 0.59123 (18) | 0.0236 (4) |
| C2 | 0.4042 (2) | 0.8963 (2) | 0.67518 (18) | 0.0229 (3) |
| C3 | 0.3844 (2) | 0.9583 (2) | 0.79446 (18) | 0.0245 (4) |
| H3 | 0.4851 | 0.9312 | 0.8393 | 0.029* |
| C4 | 0.2108 (2) | 1.0612 (2) | 0.84450 (18) | 0.0252 (4) |
| C5 | 0.0602 (3) | 1.1041 (2) | 0.77957 (19) | 0.0279 (4) |
| H5 | −0.0560 | 1.1753 | 0.8173 | 0.033* |
| C6 | 0.0793 (3) | 1.0437 (2) | 0.6614 (2) | 0.0280 (4) |
| H6 | −0.0209 | 1.0718 | 0.6158 | 0.034* |
| C7 | 0.2528 (2) | 0.9398 (2) | 0.61297 (18) | 0.0240 (4) |
| C8 | 0.4815 (2) | 0.7686 (2) | 0.48808 (18) | 0.0239 (4) |
| C9 | 0.5539 (2) | 0.6727 (2) | 0.37323 (18) | 0.0246 (4) |
| C10 | 0.7027 (3) | 0.5184 (2) | 0.36961 (19) | 0.0284 (4) |

| | | | |
|---|---|---|---|
| H10 | 0.7611 | 0.4757 | 0.4422 | 0.034* |
| C11 | 0.7657 (3) | 0.4272 (3) | 0.2604 (2) | 0.0298 (4) |
| H11 | 0.8680 | 0.3228 | 0.2583 | 0.036* |
| C12 | 0.6806 (3) | 0.4872 (3) | 0.1544 (2) | 0.0310 (4) |
| H12 | 0.7223 | 0.4250 | 0.0794 | 0.037* |
| C14 | 0.4675 (3) | 0.7348 (2) | 0.26611 (18) | 0.0259 (4) |
| H14 | 0.3661 | 0.8396 | 0.2666 | 0.031* |
| C13 | 0.5339 (3) | 0.6395 (3) | 0.16068 (19) | 0.0296 (4) |
| C15 | 0.7795 (3) | 0.5423 (3) | 0.7268 (2) | 0.0399 (5) |
| H15A | 0.8990 | 0.4863 | 0.7554 | 0.060* |
| H15B | 0.7483 | 0.4587 | 0.6898 | 0.060* |
| H15C | 0.6893 | 0.5949 | 0.7976 | 0.060* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| I1 | 0.02741 (8) | 0.03722 (9) | 0.02882 (8) | −0.01142 (6) | 0.00213 (5) | −0.00751 (6) |
| S1 | 0.01711 (19) | 0.0255 (2) | 0.0331 (2) | −0.00688 (17) | −0.00367 (17) | −0.00041 (18) |
| F1 | 0.0462 (8) | 0.0463 (8) | 0.0316 (7) | −0.0101 (6) | −0.0147 (6) | −0.0038 (6) |
| O1 | 0.0192 (6) | 0.0277 (7) | 0.0269 (7) | −0.0050 (5) | −0.0048 (5) | −0.0025 (5) |
| O2 | 0.0279 (7) | 0.0310 (7) | 0.0421 (8) | −0.0142 (6) | −0.0108 (6) | 0.0011 (6) |
| C1 | 0.0189 (8) | 0.0222 (8) | 0.0287 (9) | −0.0072 (7) | −0.0034 (7) | 0.0005 (7) |
| C2 | 0.0187 (8) | 0.0212 (8) | 0.0283 (9) | −0.0078 (7) | −0.0032 (7) | 0.0020 (7) |
| C3 | 0.0205 (8) | 0.0259 (9) | 0.0272 (9) | −0.0089 (7) | −0.0043 (7) | 0.0010 (7) |
| C4 | 0.0232 (8) | 0.0245 (9) | 0.0279 (9) | −0.0100 (7) | −0.0014 (7) | −0.0001 (7) |
| C5 | 0.0204 (8) | 0.0254 (9) | 0.0341 (10) | −0.0059 (7) | −0.0007 (7) | −0.0007 (8) |
| C6 | 0.0184 (8) | 0.0292 (9) | 0.0340 (10) | −0.0059 (7) | −0.0063 (7) | 0.0000 (8) |
| C7 | 0.0218 (8) | 0.0235 (8) | 0.0254 (9) | −0.0074 (7) | −0.0045 (7) | 0.0004 (7) |
| C8 | 0.0181 (8) | 0.0215 (8) | 0.0295 (9) | −0.0060 (7) | −0.0019 (7) | 0.0019 (7) |
| C9 | 0.0228 (8) | 0.0258 (9) | 0.0280 (9) | −0.0127 (7) | −0.0025 (7) | −0.0013 (7) |
| C10 | 0.0248 (9) | 0.0283 (9) | 0.0305 (10) | −0.0085 (7) | −0.0042 (7) | −0.0010 (8) |
| C11 | 0.0225 (9) | 0.0270 (9) | 0.0363 (11) | −0.0066 (7) | −0.0002 (8) | −0.0030 (8) |
| C12 | 0.0284 (9) | 0.0331 (10) | 0.0318 (10) | −0.0128 (8) | 0.0008 (8) | −0.0076 (8) |
| C14 | 0.0224 (8) | 0.0254 (9) | 0.0307 (9) | −0.0101 (7) | −0.0043 (7) | 0.0009 (7) |
| C13 | 0.0291 (9) | 0.0342 (10) | 0.0283 (10) | −0.0148 (8) | −0.0061 (8) | 0.0000 (8) |
| C15 | 0.0357 (11) | 0.0310 (11) | 0.0560 (14) | −0.0147 (9) | −0.0186 (10) | 0.0156 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| I1—C4 | 2.0937 (19) | C6—C7 | 1.385 (3) |
| I1—O2$^i$ | 3.2282 (16) | C6—H6 | 0.9500 |
| S1—O2 | 1.4906 (15) | C8—C9 | 1.460 (3) |
| S1—C1 | 1.7660 (18) | C9—C10 | 1.396 (3) |
| S1—C15 | 1.794 (2) | C9—C14 | 1.402 (3) |
| F1—C13 | 1.360 (2) | C10—C11 | 1.386 (3) |
| O1—C7 | 1.371 (2) | C10—H10 | 0.9500 |
| O1—C8 | 1.380 (2) | C11—C12 | 1.385 (3) |
| C1—C8 | 1.364 (3) | C11—H11 | 0.9500 |

| | | | |
|---|---|---|---|
| C1—C2 | 1.447 (2) | C12—C13 | 1.376 (3) |
| C2—C7 | 1.392 (3) | C12—H12 | 0.9500 |
| C2—C3 | 1.397 (3) | C14—C13 | 1.370 (3) |
| C3—C4 | 1.389 (2) | C14—H14 | 0.9500 |
| C3—H3 | 0.9500 | C15—H15A | 0.9800 |
| C4—C5 | 1.404 (3) | C15—H15B | 0.9800 |
| C5—C6 | 1.382 (3) | C15—H15C | 0.9800 |
| C5—H5 | 0.9500 | | |
| | | | |
| C4—I1—O2ⁱ | 162.99 (6) | C1—C8—C9 | 135.08 (17) |
| O2—S1—C1 | 107.27 (8) | O1—C8—C9 | 114.36 (16) |
| O2—S1—C15 | 105.59 (11) | C10—C9—C14 | 119.72 (18) |
| C1—S1—C15 | 97.77 (10) | C10—C9—C8 | 121.22 (18) |
| C7—O1—C8 | 106.51 (14) | C14—C9—C8 | 119.02 (17) |
| C8—C1—C2 | 107.22 (16) | C11—C10—C9 | 120.19 (19) |
| C8—C1—S1 | 126.32 (14) | C11—C10—H10 | 119.9 |
| C2—C1—S1 | 126.23 (14) | C9—C10—H10 | 119.9 |
| C7—C2—C3 | 119.44 (16) | C12—C11—C10 | 120.41 (19) |
| C7—C2—C1 | 104.72 (16) | C12—C11—H11 | 119.8 |
| C3—C2—C1 | 135.82 (17) | C10—C11—H11 | 119.8 |
| C4—C3—C2 | 116.96 (17) | C13—C12—C11 | 118.20 (18) |
| C4—C3—H3 | 121.5 | C13—C12—H12 | 120.9 |
| C2—C3—H3 | 121.5 | C11—C12—H12 | 120.9 |
| C3—C4—C5 | 122.53 (18) | C13—C14—C9 | 117.96 (18) |
| C3—C4—I1 | 118.63 (14) | C13—C14—H14 | 121.0 |
| C5—C4—I1 | 118.81 (13) | C9—C14—H14 | 121.0 |
| C6—C5—C4 | 120.71 (17) | F1—C13—C14 | 118.31 (18) |
| C6—C5—H5 | 119.6 | F1—C13—C12 | 118.15 (18) |
| C4—C5—H5 | 119.6 | C14—C13—C12 | 123.5 (2) |
| C5—C6—C7 | 116.21 (18) | S1—C15—H15A | 109.5 |
| C5—C6—H6 | 121.9 | S1—C15—H15B | 109.5 |
| C7—C6—H6 | 121.9 | H15A—C15—H15B | 109.5 |
| O1—C7—C6 | 124.79 (17) | S1—C15—H15C | 109.5 |
| O1—C7—C2 | 111.03 (15) | H15A—C15—H15C | 109.5 |
| C6—C7—C2 | 124.15 (18) | H15B—C15—H15C | 109.5 |
| C1—C8—O1 | 110.51 (16) | | |
| | | | |
| O2—S1—C1—C8 | 141.12 (17) | C3—C2—C7—C6 | 0.5 (3) |
| C15—S1—C1—C8 | −109.83 (19) | C1—C2—C7—C6 | 178.84 (18) |
| O2—S1—C1—C2 | −32.64 (19) | C2—C1—C8—O1 | 0.0 (2) |
| C15—S1—C1—C2 | 76.41 (18) | S1—C1—C8—O1 | −174.78 (13) |
| C8—C1—C2—C7 | −0.4 (2) | C2—C1—C8—C9 | −177.5 (2) |
| S1—C1—C2—C7 | 174.33 (15) | S1—C1—C8—C9 | 7.7 (3) |
| C8—C1—C2—C3 | 177.6 (2) | C7—O1—C8—C1 | 0.5 (2) |
| S1—C1—C2—C3 | −7.7 (3) | C7—O1—C8—C9 | 178.56 (16) |
| C7—C2—C3—C4 | 0.2 (3) | C1—C8—C9—C10 | 29.0 (3) |
| C1—C2—C3—C4 | −177.6 (2) | O1—C8—C9—C10 | −148.40 (17) |
| C2—C3—C4—C5 | −0.6 (3) | C1—C8—C9—C14 | −153.2 (2) |

| | | | |
|---|---|---|---|
| C2—C3—C4—I1 | 177.44 (13) | O1—C8—C9—C14 | 29.3 (2) |
| O2<sup>i</sup>—I1—C4—C3 | −46.0 (3) | C14—C9—C10—C11 | 0.4 (3) |
| O2<sup>i</sup>—I1—C4—C5 | 132.10 (18) | C8—C9—C10—C11 | 178.10 (18) |
| C3—C4—C5—C6 | 0.3 (3) | C9—C10—C11—C12 | −0.7 (3) |
| I1—C4—C5—C6 | −177.70 (15) | C10—C11—C12—C13 | 0.5 (3) |
| C4—C5—C6—C7 | 0.3 (3) | C10—C9—C14—C13 | 0.1 (3) |
| C8—O1—C7—C6 | −178.87 (18) | C8—C9—C14—C13 | −177.66 (17) |
| C8—O1—C7—C2 | −0.8 (2) | C9—C14—C13—F1 | 178.38 (17) |
| C5—C6—C7—O1 | 177.14 (18) | C9—C14—C13—C12 | −0.3 (3) |
| C5—C6—C7—C2 | −0.7 (3) | C11—C12—C13—F1 | −178.69 (18) |
| C3—C2—C7—O1 | −177.65 (16) | C11—C12—C13—C14 | 0.0 (3) |
| C1—C2—C7—O1 | 0.7 (2) | | |

Symmetry code: (i) −*x*+1, −*y*+2, −*z*+2.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C6—H6···O1<sup>ii</sup> | 0.95 | 2.57 | 3.520 (2) | 177 |
| C11—H11···O2<sup>iii</sup> | 0.95 | 2.55 | 3.372 (2) | 145 |

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