

2-(4-Fluorophenyl)-3-methylsulfinyl-5-phenyl-1-benzofuran

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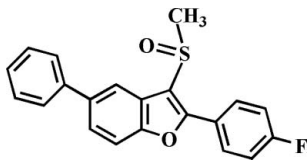
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.032; wR factor = 0.086; data-to-parameter ratio = 14.1.

In the title molecule, $\text{C}_{21}\text{H}_{15}\text{FO}_2\text{S}$, the O atom and the methyl group of the methylsulfinyl substituent are situated on the opposite sides of the plane through the benzofuran fragment. The benzofuran ring plane makes dihedral angles of 28.63 (6) and 31.55 (5)° with the 4-fluorophenyl and phenyl rings, respectively. Weak C—H...F and C—H...O hydrogen bonds and intermolecular C—H... π interactions are present in the crystal structure. The title crystal was refined as an inversion twin with a 0.39 (7):0.61 (7) domain ratio.

Related literature

For the crystal structures of similar 3-alkylsulfanyl-2-(4-fluorophenyl)-5-phenyl-1-benzofuran derivatives, see: Choi *et al.* (2009, 2010). For the pharmacological activity of benzofuran compounds, see: Aslam *et al.* (2006); Galal *et al.* (2009); Khan *et al.* (2005). For natural products with benzofuran rings, see: Akgul & Anil (2003); Soekamto *et al.* (2003). For hydrogen bonding, see: Desiraju & Steiner (1999).



Experimental

Crystal data

| | |
|---|-----------------------------------|
| $\text{C}_{21}\text{H}_{15}\text{FO}_2\text{S}$ | $V = 813.6$ (2) Å ³ |
| $M_r = 350.39$ | $Z = 2$ |
| Monoclinic, $P2_1$ | Mo $K\alpha$ radiation |
| $a = 10.148$ (2) Å | $\mu = 0.22$ mm ⁻¹ |
| $b = 7.117$ (1) Å | $T = 173$ K |
| $c = 11.991$ (2) Å | $0.40 \times 0.40 \times 0.25$ mm |
| $\beta = 110.047$ (2)° | |

Data collection

| | |
|--|--|
| Bruker SMART APEXII CCD diffractometer | 4812 measured reflections |
| Absorption correction: multi-scan (SADABS; Bruker, 2009) | 3226 independent reflections |
| $T_{\min} = 0.917$, $T_{\max} = 0.947$ | 3065 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.019$ |

Refinement

| | |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.032$ | H-atom parameters constrained |
| $wR(F^2) = 0.086$ | $\Delta\rho_{\text{max}} = 0.31$ e Å ⁻³ |
| $S = 1.06$ | $\Delta\rho_{\text{min}} = -0.21$ e Å ⁻³ |
| 3226 reflections | Absolute structure: Flack (1983), |
| 228 parameters | 1308 Friedel pairs |
| 1 restraint | Flack parameter: 0.39 (7) |

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 and Cg2 are the centroids of the C15–C20 (5-phenyl) and the C9–14 (4-fluorophenyl) rings, respectively.

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------------|-------|-------------|-------------|---------------|
| C18—H18...O2 ⁱ | 0.93 | 2.61 | 3.301 (3) | 131 |
| C21—H21A...O2 ⁱⁱ | 0.96 | 2.63 | 3.375 (3) | 135 |
| C21—H21B...F ⁱⁱⁱ | 0.96 | 2.55 | 3.478 (3) | 164 |
| C10—H10...Cg1 ^{iv} | 0.93 | 2.86 | 3.450 (2) | 122 |
| C13—H13...Cg2 ⁱⁱⁱ | 0.93 | 2.81 | 3.417 (2) | 124 |

Symmetry codes: (i) $-x, y - \frac{1}{2}, -z + 1$; (ii) $-x + 1, y - \frac{1}{2}, -z + 2$; (iii) $-x + 2, y - \frac{1}{2}, -z + 2$; (iv) $-x + 1, y + \frac{1}{2}, -z + 1$.

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 (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: FB2185).

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supporting information

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2-(4-Fluorophenyl)-3-methylsulfinyl-5-phenyl-1-benzofuran**Hong Dae Choi, Pil Ja Seo, Byeng Wha Son and Uk Lee****S1. Comment**

The compounds with the benzofuran skeleton show significant pharmacological activities such as fungicide (Aslam *et al.*, 2006), antitumor and antiviral (Galal *et al.*, 2009) and antimicrobial (Khan *et al.*, 2005) properties. These compounds are common in Nature (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our ongoing studies of the effect of the side chain substituents on the solid state structures of 3-alkylsulfanyl-2-(4-fluorophenyl)-5-phenyl-1-benzofuran analogues (Choi *et al.*, 2009, 2010), we report the title crystal structure. The title molecule is depicted in Fig. 1.

The benzofuran ring is essentially planar, with a mean deviation of 0.006 (2) Å from the least-squares plane defined by the nine constituent atoms. In the molecule, the benzofuran plane makes dihedral angles of 28.63 (6) and 31.55 (5)° with the 4-fluorophenyl ring and the phenyl ring, respectively. The molecular packing (Fig. 2) is stabilized by an intermolecular C—H···F hydrogen bond between the methyl H atom and the fluorine (Tab. 1). There are also C—H···O interactions (Tab. 1 and Fig. 2) with geometrical parameters that are on the limit of their acceptance as true weak C—H···O hydrogen bonds (Desiraju & Steiner, 1999). The molecular packing (Fig. 3) is further stabilized by two intermolecular C—H··· π -electron ring interactions: The first one between the 4-fluorophenyl H atom and the 5-phenyl ring, and the second one between the 4-fluorophenyl H atom and 4-fluorophenyl ring (Tab. 1).

S2. Experimental

77% 3-chloroperoxybenzoic acid (224 mg, 1.0 mmol) was added in small portions to a stirred solution of 2-(4-fluorophenyl)-3-methylsulfanyl-5-phenyl-1-benzofuran (301 mg, 0.9 mmol) in dichloromethane (30 ml) at 273 K. After having been stirred at room temperature for 4h, the mixture was washed with saturated sodium hydrogencarbonate solution and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated at reduced pressure. The residue was purified by column chromatography (silica gel, hexane–ethyl acetate, 1:1 v/v) to afford the title compound as a colourless solid [yield 80%, m.p. 506–507 K; R_f = 0.59 (hexane–ethyl acetate, 1:1 v/v)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title compound in chloroform at room temperature. The average crystal size was approximately 1.0 × 1.0 × 0.5 mm. (The measured crystal was cut from the larger one.) The crystals are colourless and soluble in polar solvents.

S3. Refinement

All the H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å for the aryl H atoms and 0.96 Å for the methyl H atoms, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for the aryl H atoms and $1.5U_{\text{eq}}(\text{C})$ for the methyl H atoms. 1308 Friedel pairs have been used in the refinement.

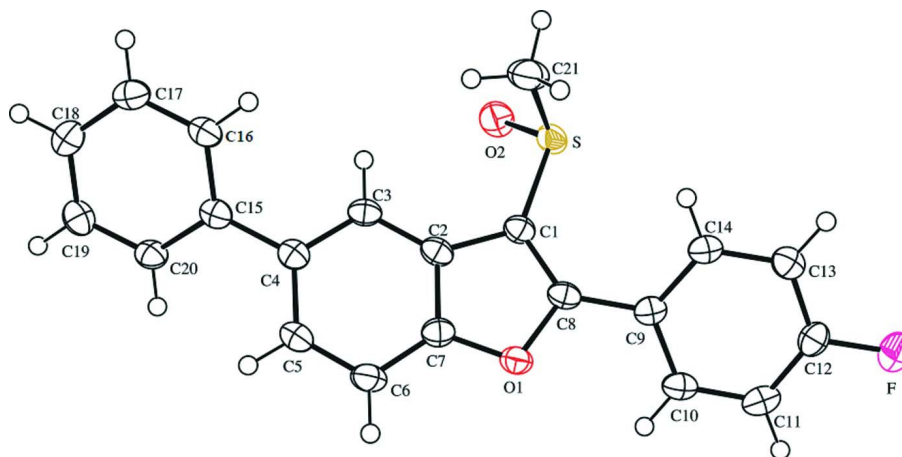


Figure 1

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

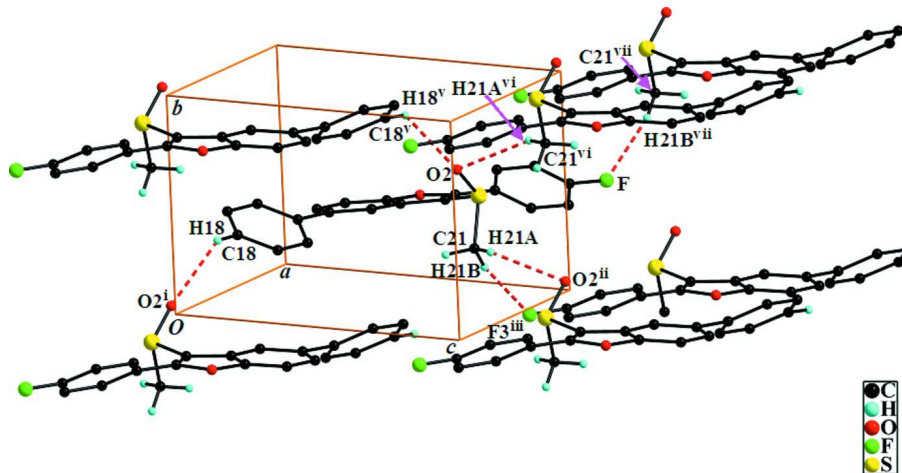


Figure 2

C—H...F and C—H...O interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (i) $-x, y-1/2, -z+1$; (ii) $-x+1, y-1/2, -z+2$; (iii) $-x+2, y-1/2, -z+2$; (v) $-x, y+1/2, -z+1$; (vi) $-x+1, y+1/2, -z+2$; (vii) $-x+2, y+1/2, -z+2$.]

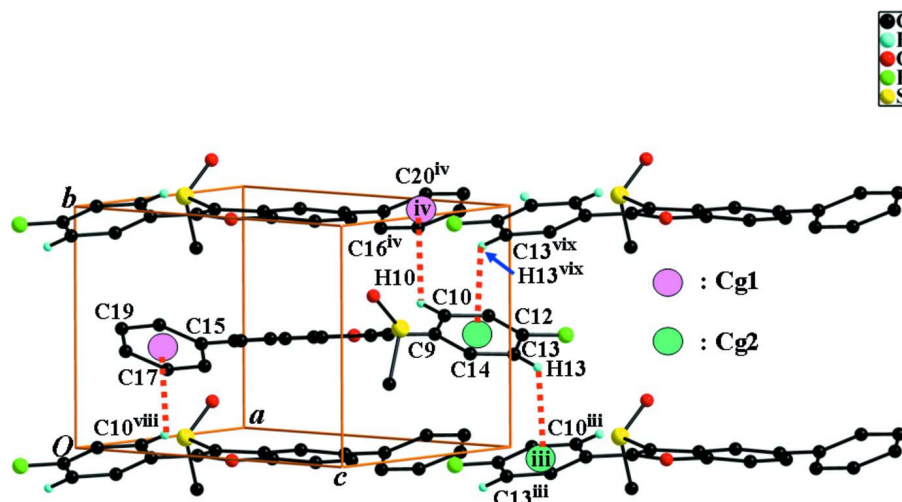


Figure 3

C—H... π -electron ring interactions (dotted lines) in the crystal structure of the title compound. Cg denotes the ring centroids. [Symmetry codes: (iii) $-x+2, y-1/2, -z+2$; (iv) $-x+1, y+1/2, -z+1$; (viii) $-x+1, y-1/2, -z+1$; (ix) $-x+2, y+1/2, -z+2$.]

2-(4-Fluorophenyl)-3-methylsulfinyl-5-phenyl-1-benzofuran

Crystal data

$C_{21}H_{15}FO_2S$

$M_r = 350.39$

Monoclinic, $P2_1$

Hall symbol: $P\ 2y_b$

$a = 10.148\ (2)\ \text{\AA}$

$b = 7.117\ (1)\ \text{\AA}$

$c = 11.991\ (2)\ \text{\AA}$

$\beta = 110.047\ (2)^\circ$

$V = 813.6\ (2)\ \text{\AA}^3$

$Z = 2$

$F(000) = 364$

$D_x = 1.430\ \text{Mg m}^{-3}$

Melting point = 506–507 K

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3710 reflections

$\theta = 2.3\text{--}28.3^\circ$

$\mu = 0.22\ \text{mm}^{-1}$

$T = 173\ \text{K}$

Block, colourless

$0.40 \times 0.40 \times 0.25\ \text{mm}$

Data collection

Bruker SMART APEXII CCD
diffractometer

Radiation source: rotating anode

Graphite multilayer monochromator

Detector resolution: $10.0\ \text{pixels mm}^{-1}$

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2009)

$T_{\min} = 0.917, T_{\max} = 0.947$

4812 measured reflections

3226 independent reflections

3065 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$

$\theta_{\max} = 27.0^\circ, \theta_{\min} = 1.8^\circ$

$h = -8 \rightarrow 12$

$k = -9 \rightarrow 8$

$l = -15 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.086$

$S = 1.06$

3226 reflections

228 parameters

1 restraint

59 constraints

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

$$w = 1/[\sigma^2(F_o^2) + (0.0516P)^2 + 0.1094P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 0.31 \text{ e } \text{Å}^{-3}$$

$$\Delta\rho_{\min} = -0.21 \text{ e } \text{Å}^{-3}$$

Absolute structure: Flack (1983), 1308 Friedel pairs

Absolute structure parameter: 0.39 (7)

Special details

Experimental. The measured sample has been cut from the larger crystal. The crystals, both the grown ones as well as the cut one, have not been examined under the polarization microscope.

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 $F^2 > 2\sigma(F^2)$ 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. The diffractions 1 0 0 and 0 0 1 as well as their equivalents have been excluded from the refinement because their respective intensities significantly differed from the calculated ones.

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

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|-------------|--------------|----------------------------------|
| S | 0.55747 (5) | 0.51643 (8) | 0.86742 (4) | 0.03009 (13) |
| F | 1.26845 (12) | 0.4440 (2) | 1.03910 (11) | 0.0425 (3) |
| O1 | 0.70363 (13) | 0.4548 (2) | 0.60162 (10) | 0.0280 (3) |
| O2 | 0.44274 (15) | 0.6590 (2) | 0.83904 (13) | 0.0398 (4) |
| C1 | 0.59124 (17) | 0.4753 (3) | 0.73449 (15) | 0.0251 (4) |
| C2 | 0.48587 (19) | 0.4671 (3) | 0.61728 (15) | 0.0257 (4) |
| C3 | 0.33954 (18) | 0.4703 (3) | 0.57251 (15) | 0.0256 (4) |
| H3 | 0.2883 | 0.4810 | 0.6234 | 0.031* |
| C4 | 0.27128 (18) | 0.4572 (3) | 0.44981 (15) | 0.0255 (4) |
| C5 | 0.35234 (19) | 0.4441 (3) | 0.37470 (16) | 0.0286 (4) |
| H5 | 0.3061 | 0.4352 | 0.2932 | 0.034* |
| C6 | 0.4975 (2) | 0.4439 (3) | 0.41758 (16) | 0.0317 (4) |
| H6 | 0.5495 | 0.4366 | 0.3672 | 0.038* |
| C7 | 0.56102 (19) | 0.4553 (3) | 0.53979 (16) | 0.0264 (4) |
| C8 | 0.71883 (19) | 0.4670 (3) | 0.72036 (15) | 0.0255 (4) |
| C9 | 0.86341 (18) | 0.4633 (3) | 0.80353 (15) | 0.0242 (4) |
| C10 | 0.97478 (18) | 0.5278 (3) | 0.76948 (16) | 0.0278 (4) |
| H10 | 0.9566 | 0.5745 | 0.6932 | 0.033* |
| C11 | 1.11179 (18) | 0.5224 (3) | 0.84845 (17) | 0.0317 (4) |
| H11 | 1.1857 | 0.5663 | 0.8265 | 0.038* |
| C12 | 1.13528 (19) | 0.4503 (3) | 0.96030 (17) | 0.0291 (4) |
| C13 | 1.0289 (2) | 0.3813 (3) | 0.99652 (17) | 0.0288 (4) |
| H13 | 1.0484 | 0.3314 | 1.0722 | 0.035* |
| C14 | 0.89299 (19) | 0.3886 (3) | 0.91741 (16) | 0.0268 (4) |
| H14 | 0.8201 | 0.3432 | 0.9402 | 0.032* |
| C15 | 0.11547 (19) | 0.4540 (3) | 0.39950 (15) | 0.0250 (4) |
| C16 | 0.0356 (2) | 0.3732 (3) | 0.46221 (16) | 0.0281 (4) |
| H16 | 0.0806 | 0.3231 | 0.5373 | 0.034* |

| | | | | |
|------|---------------|------------|--------------|------------|
| C17 | -0.1097 (2) | 0.3669 (3) | 0.41369 (17) | 0.0313 (4) |
| H17 | -0.1610 | 0.3139 | 0.4568 | 0.038* |
| C18 | -0.1788 (2) | 0.4392 (3) | 0.30148 (18) | 0.0323 (4) |
| H18 | -0.2760 | 0.4326 | 0.2686 | 0.039* |
| C19 | -0.10197 (19) | 0.5216 (3) | 0.23840 (16) | 0.0315 (4) |
| H19 | -0.1478 | 0.5718 | 0.1635 | 0.038* |
| C20 | 0.04378 (18) | 0.5288 (3) | 0.28756 (15) | 0.0277 (4) |
| H20 | 0.0944 | 0.5848 | 0.2448 | 0.033* |
| C21 | 0.4775 (2) | 0.2943 (4) | 0.8756 (2) | 0.0421 (6) |
| H21A | 0.4490 | 0.2925 | 0.9441 | 0.063* |
| H21B | 0.5438 | 0.1952 | 0.8817 | 0.063* |
| H21C | 0.3970 | 0.2765 | 0.8053 | 0.063* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|--------------|-------------|--------------|--------------|
| S | 0.0302 (2) | 0.0398 (3) | 0.02136 (19) | 0.0062 (2) | 0.01031 (15) | -0.0019 (2) |
| F | 0.0287 (6) | 0.0505 (8) | 0.0447 (7) | -0.0009 (6) | 0.0080 (5) | 0.0011 (6) |
| O1 | 0.0297 (7) | 0.0328 (7) | 0.0243 (6) | 0.0016 (6) | 0.0128 (5) | 0.0010 (6) |
| O2 | 0.0390 (8) | 0.0470 (10) | 0.0350 (8) | 0.0117 (7) | 0.0148 (7) | -0.0033 (7) |
| C1 | 0.0285 (9) | 0.0257 (11) | 0.0232 (8) | 0.0025 (7) | 0.0116 (7) | -0.0012 (7) |
| C2 | 0.0336 (9) | 0.0226 (10) | 0.0228 (8) | 0.0019 (7) | 0.0120 (7) | 0.0007 (7) |
| C3 | 0.0306 (9) | 0.0244 (11) | 0.0253 (8) | 0.0003 (7) | 0.0142 (7) | -0.0004 (7) |
| C4 | 0.0306 (9) | 0.0213 (9) | 0.0250 (8) | -0.0008 (8) | 0.0100 (7) | 0.0015 (8) |
| C5 | 0.0361 (10) | 0.0289 (10) | 0.0224 (8) | -0.0012 (8) | 0.0122 (7) | -0.0009 (8) |
| C6 | 0.0364 (10) | 0.0369 (11) | 0.0269 (9) | 0.0023 (9) | 0.0173 (8) | 0.0011 (9) |
| C7 | 0.0292 (9) | 0.0247 (9) | 0.0285 (9) | 0.0011 (8) | 0.0140 (7) | 0.0003 (8) |
| C8 | 0.0322 (9) | 0.0220 (10) | 0.0253 (8) | 0.0005 (7) | 0.0135 (7) | 0.0017 (7) |
| C9 | 0.0264 (9) | 0.0198 (9) | 0.0289 (8) | 0.0020 (7) | 0.0129 (7) | -0.0005 (8) |
| C10 | 0.0346 (9) | 0.0241 (9) | 0.0304 (8) | 0.0022 (9) | 0.0184 (7) | 0.0027 (9) |
| C11 | 0.0311 (9) | 0.0265 (10) | 0.0439 (10) | -0.0006 (9) | 0.0211 (8) | -0.0002 (10) |
| C12 | 0.0249 (9) | 0.0264 (10) | 0.0354 (9) | 0.0025 (8) | 0.0094 (7) | -0.0021 (9) |
| C13 | 0.0337 (11) | 0.0249 (10) | 0.0289 (9) | 0.0027 (8) | 0.0121 (8) | 0.0015 (8) |
| C14 | 0.0292 (10) | 0.0242 (10) | 0.0310 (9) | 0.0007 (7) | 0.0154 (8) | 0.0016 (8) |
| C15 | 0.0330 (9) | 0.0196 (9) | 0.0237 (8) | -0.0035 (8) | 0.0114 (7) | -0.0042 (8) |
| C16 | 0.0374 (11) | 0.0254 (10) | 0.0234 (8) | -0.0021 (8) | 0.0126 (8) | -0.0002 (8) |
| C17 | 0.0352 (10) | 0.0285 (11) | 0.0351 (10) | -0.0046 (8) | 0.0183 (8) | -0.0027 (9) |
| C18 | 0.0265 (9) | 0.0319 (11) | 0.0385 (10) | -0.0017 (8) | 0.0108 (8) | -0.0040 (9) |
| C19 | 0.0358 (9) | 0.0270 (10) | 0.0288 (8) | 0.0016 (9) | 0.0073 (7) | 0.0011 (9) |
| C20 | 0.0342 (9) | 0.0234 (9) | 0.0273 (8) | -0.0040 (9) | 0.0130 (7) | 0.0017 (9) |
| C21 | 0.0451 (13) | 0.0481 (15) | 0.0405 (12) | 0.0055 (11) | 0.0242 (10) | 0.0131 (11) |

Geometric parameters (Å, °)

| | | | |
|-------|-------------|---------|-----------|
| S—O2 | 1.4931 (16) | C10—H10 | 0.9300 |
| S—C1 | 1.7660 (17) | C11—C12 | 1.379 (3) |
| S—C21 | 1.795 (2) | C11—H11 | 0.9300 |
| F—C12 | 1.359 (2) | C12—C13 | 1.385 (3) |

| | | | |
|------------|-------------|-------------|-------------|
| O1—C8 | 1.381 (2) | C13—C14 | 1.381 (3) |
| O1—C7 | 1.382 (2) | C13—H13 | 0.9300 |
| C1—C8 | 1.364 (2) | C14—H14 | 0.9300 |
| C1—C2 | 1.446 (2) | C15—C20 | 1.395 (3) |
| C2—C7 | 1.392 (2) | C15—C16 | 1.404 (3) |
| C2—C3 | 1.395 (2) | C16—C17 | 1.388 (3) |
| C3—C4 | 1.398 (2) | C16—H16 | 0.9300 |
| C3—H3 | 0.9300 | C17—C18 | 1.386 (3) |
| C4—C5 | 1.416 (2) | C17—H17 | 0.9300 |
| C4—C15 | 1.487 (2) | C18—C19 | 1.388 (3) |
| C5—C6 | 1.383 (3) | C18—H18 | 0.9300 |
| C5—H5 | 0.9300 | C19—C20 | 1.393 (2) |
| C6—C7 | 1.386 (3) | C19—H19 | 0.9300 |
| C6—H6 | 0.9300 | C20—H20 | 0.9300 |
| C8—C9 | 1.464 (2) | C21—H21A | 0.9600 |
| C9—C14 | 1.399 (2) | C21—H21B | 0.9600 |
| C9—C10 | 1.404 (2) | C21—H21C | 0.9600 |
| C10—C11 | 1.389 (2) | | |
| O2—S—C1 | 106.52 (9) | C12—C11—H11 | 120.9 |
| O2—S—C21 | 106.22 (10) | C10—C11—H11 | 120.9 |
| C1—S—C21 | 97.72 (10) | F—C12—C11 | 119.20 (16) |
| C8—O1—C7 | 106.22 (13) | F—C12—C13 | 117.85 (18) |
| C8—C1—C2 | 107.14 (15) | C11—C12—C13 | 122.95 (18) |
| C8—C1—S | 127.27 (14) | C14—C13—C12 | 118.27 (18) |
| C2—C1—S | 125.19 (13) | C14—C13—H13 | 120.9 |
| C7—C2—C3 | 119.90 (16) | C12—C13—H13 | 120.9 |
| C7—C2—C1 | 105.03 (15) | C13—C14—C9 | 120.97 (17) |
| C3—C2—C1 | 135.07 (16) | C13—C14—H14 | 119.5 |
| C2—C3—C4 | 118.80 (15) | C9—C14—H14 | 119.5 |
| C2—C3—H3 | 120.6 | C20—C15—C16 | 117.73 (17) |
| C4—C3—H3 | 120.6 | C20—C15—C4 | 121.06 (15) |
| C3—C4—C5 | 119.18 (16) | C16—C15—C4 | 121.20 (16) |
| C3—C4—C15 | 120.16 (15) | C17—C16—C15 | 120.94 (18) |
| C5—C4—C15 | 120.66 (16) | C17—C16—H16 | 119.5 |
| C6—C5—C4 | 122.70 (17) | C15—C16—H16 | 119.5 |
| C6—C5—H5 | 118.7 | C18—C17—C16 | 120.43 (18) |
| C4—C5—H5 | 118.7 | C18—C17—H17 | 119.8 |
| C5—C6—C7 | 116.31 (16) | C16—C17—H17 | 119.8 |
| C5—C6—H6 | 121.8 | C17—C18—C19 | 119.61 (18) |
| C7—C6—H6 | 121.8 | C17—C18—H18 | 120.2 |
| O1—C7—C6 | 126.11 (16) | C19—C18—H18 | 120.2 |
| O1—C7—C2 | 110.78 (15) | C18—C19—C20 | 119.88 (17) |
| C6—C7—C2 | 123.10 (17) | C18—C19—H19 | 120.1 |
| C1—C8—O1 | 110.83 (15) | C20—C19—H19 | 120.1 |
| C1—C8—C9 | 133.51 (16) | C19—C20—C15 | 121.40 (17) |
| O1—C8—C9 | 115.64 (14) | C19—C20—H20 | 119.3 |
| C14—C9—C10 | 118.91 (16) | C15—C20—H20 | 119.3 |

| | | | |
|--------------|--------------|-----------------|--------------|
| C14—C9—C8 | 120.10 (15) | S—C21—H21A | 109.5 |
| C10—C9—C8 | 120.96 (16) | S—C21—H21B | 109.5 |
| C11—C10—C9 | 120.69 (17) | H21A—C21—H21B | 109.5 |
| C11—C10—H10 | 119.7 | S—C21—H21C | 109.5 |
| C9—C10—H10 | 119.7 | H21A—C21—H21C | 109.5 |
| C12—C11—C10 | 118.19 (16) | H21B—C21—H21C | 109.5 |
| O2—S—C1—C8 | 133.81 (19) | C7—O1—C8—C9 | 178.29 (16) |
| C21—S—C1—C8 | -116.67 (19) | C1—C8—C9—C14 | 27.8 (3) |
| O2—S—C1—C2 | -38.02 (19) | O1—C8—C9—C14 | -150.11 (18) |
| C21—S—C1—C2 | 71.50 (18) | C1—C8—C9—C10 | -154.5 (2) |
| C8—C1—C2—C7 | -0.3 (2) | O1—C8—C9—C10 | 27.6 (3) |
| S—C1—C2—C7 | 172.91 (16) | C14—C9—C10—C11 | -1.7 (3) |
| C8—C1—C2—C3 | -179.7 (2) | C8—C9—C10—C11 | -179.48 (19) |
| S—C1—C2—C3 | -6.5 (3) | C9—C10—C11—C12 | 0.7 (3) |
| C7—C2—C3—C4 | 1.4 (3) | C10—C11—C12—F | -179.86 (19) |
| C1—C2—C3—C4 | -179.3 (2) | C10—C11—C12—C13 | 0.8 (3) |
| C2—C3—C4—C5 | -1.0 (3) | F—C12—C13—C14 | 179.42 (18) |
| C2—C3—C4—C15 | 178.04 (17) | C11—C12—C13—C14 | -1.2 (3) |
| C3—C4—C5—C6 | -0.1 (3) | C12—C13—C14—C9 | 0.1 (3) |
| C15—C4—C5—C6 | -179.11 (19) | C10—C9—C14—C13 | 1.3 (3) |
| C4—C5—C6—C7 | 0.7 (3) | C8—C9—C14—C13 | 179.05 (18) |
| C8—O1—C7—C6 | -179.6 (2) | C3—C4—C15—C20 | 149.0 (2) |
| C8—O1—C7—C2 | -0.1 (2) | C5—C4—C15—C20 | -32.0 (3) |
| C5—C6—C7—O1 | 179.1 (2) | C3—C4—C15—C16 | -31.9 (3) |
| C5—C6—C7—C2 | -0.3 (3) | C5—C4—C15—C16 | 147.1 (2) |
| C3—C2—C7—O1 | 179.75 (16) | C20—C15—C16—C17 | 0.5 (3) |
| C1—C2—C7—O1 | 0.3 (2) | C4—C15—C16—C17 | -178.57 (19) |
| C3—C2—C7—C6 | -0.8 (3) | C15—C16—C17—C18 | 0.6 (3) |
| C1—C2—C7—C6 | 179.71 (19) | C16—C17—C18—C19 | -1.3 (3) |
| C2—C1—C8—O1 | 0.2 (2) | C17—C18—C19—C20 | 0.8 (3) |
| S—C1—C8—O1 | -172.79 (14) | C18—C19—C20—C15 | 0.3 (3) |
| C2—C1—C8—C9 | -177.7 (2) | C16—C15—C20—C19 | -1.0 (3) |
| S—C1—C8—C9 | 9.2 (3) | C4—C15—C20—C19 | 178.14 (19) |
| C7—O1—C8—C1 | -0.1 (2) | | |

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1 and Cg2 are the centroids of the C15—C20 (5-phenyl) and the C9—14 (4-fluorophenyl) rings, respectively.

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------------------------|-------|-------------|-------------|---------------|
| C18—H18 \cdots O2 ⁱ | 0.93 | 2.61 | 3.301 (3) | 131 |
| C21—H21A \cdots O2 ⁱⁱ | 0.96 | 2.63 | 3.375 (3) | 135 |
| C21—H21B \cdots F ⁱⁱⁱ | 0.96 | 2.55 | 3.478 (3) | 164 |
| C10—H10 \cdots Cg1 ^{iv} | 0.93 | 2.86 | 3.450 (2) | 122 |
| C13—H13 \cdots Cg2 ⁱⁱⁱ | 0.93 | 2.81 | 3.417 (2) | 124 |

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