Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-Cyclohexyl-3-(2-fluorophenylsulfinyl)-2-methyl-1-benzofuran

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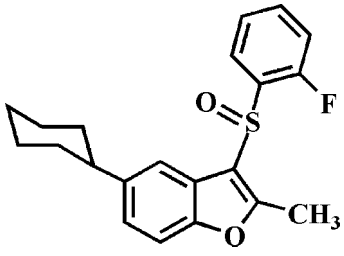
Received 30 April 2013; accepted 1 May 2013

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.116; data-to-parameter ratio = 19.6.

In the title compound, $C_{21}H_{21}FO_2S$, the cyclohexyl ring adopts a chair conformation. The 2-fluorophenyl ring makes a dihedral angle of 88.47 (4)° with the mean plane [r.m.s. deviation = 0.013 (1) Å] of the benzofuran fragment. In the crystal, molecules are linked by weak C—H···O and C—H···π interactions, forming chains propagating along [100]. The crystal structure also exhibits slipped π–π interactions between the furan rings of neighboring molecules [centroid-to-centroid distance = 3.397 (2) Å, interplanar distance = 3.346 (2) Å and slippage = 0.586 (2) Å].

Related literature

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



Experimental

Crystal data

$C_{21}H_{21}FO_2S$
M_r = 356.44
Triclinic, $P\overline{1}$
a = 9.0667 (2) Å
b = 10.3647 (2) Å
c = 10.6838 (2) Å
α = 105.395 (1)°
β = 93.418 (1)°
γ = 110.839 (1)°
V = 891.33 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 173 K
0.30 × 0.22 × 0.21 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.681, T_{max} = 0.746
16785 measured reflections
4455 independent reflections
3495 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.116
S = 1.04
4455 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

*Cg*2 is the centroid of the C2–C7 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2^{i}	0.95	2.60	3.5024 (19)	160
C20—H20···O1^{ii}	0.95	2.53	3.316 (2)	140
C21—H21···O2^{i}	0.95	2.49	3.332 (2)	148
C14—H14*B*···*Cg*2^{iii}	0.99	2.69	3.618 (2)	156
C15—H15*B*···*Cg*2^{iv}	0.98	2.85	3.422 (2)	118

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

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, 2012) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Blue-Bio Industry Regional Innovation Center (grant No. RIC08-06-07) at Dongeui University as an RIC program under the Ministry of Knowledge Economy and Busan city.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2547).

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supporting information

Acta Cryst. (2013). E**69**, o894 [doi:10.1107/S1600536813011902]

5-Cyclohexyl-3-(2-fluorophenylsulfinyl)-2-methyl-1-benzofuran

Hong Dae Choi, Pil Ja Seo and Uk Lee

S1. Comment

As a part of our continuing study of 5-cyclohexyl-2-methyl-1-benzofuran derivatives containing 4-fluorophenylsulfinyl (Choi *et al.*, 2011) and 4-bromophenylsulfinyl (Choi *et al.*, 2012) substituents in 3-position, 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 0.013 (1) Å from the least-squares plane defined by the nine constituent atoms. The cyclohexyl ring has the chair form. The dihedral angle formed by the 2-fluorophenyl ring and the mean plane of the benzofuran fragment is 88.47 (4)°. In the crystal structure (Figs. 2 and 3), molecules are connected by weak C—H···O and C—H···π interactions (Table 1, Cg2 is the centroid of the C2–C7 benzene ring). The crystal packing (Fig. 3) also exhibits slipped π–π interactions between the furan rings of neighbouring molecules, with a Cg1···Cg1^{iv} distance of 3.397 (2) Å and an interplanar distance of 3.346 (2) Å resulting in a slippage of 0.586 (2) Å (Cg1 is the centroid of the C1/C2/C7/O1/C8 furan ring).

S2. Experimental

3-Chloroperoxybenzoic acid (77%, 224 mg, 1.0 mmol) was added in small portions to a stirred solution of 5-cyclohexyl-3-(2-fluorophenylsulfanyl)-2-methyl-1-benzofuran (306 mg, 0.9 mmol) in dichloromethane (40 ml) at 273 K. After being stirred at room temperature for 3 h, 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 (hexane–ethyl acetate, 4:1 v/v) to afford the title compound as a colorless solid [yield 71%, m.p. 424-425 K; R_f = 0.46 (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 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, 1.00 Å for methine, 0.99 Å for methylene and 0.98 Å for methyl H atoms, respectively. U_{iso}(H) = 1.2U_{eq}(C) for aryl, methine and methylene, and 1.5U_{eq}(C) for methyl H atoms. The positions of methyl hydrogens were optimized rotationally.

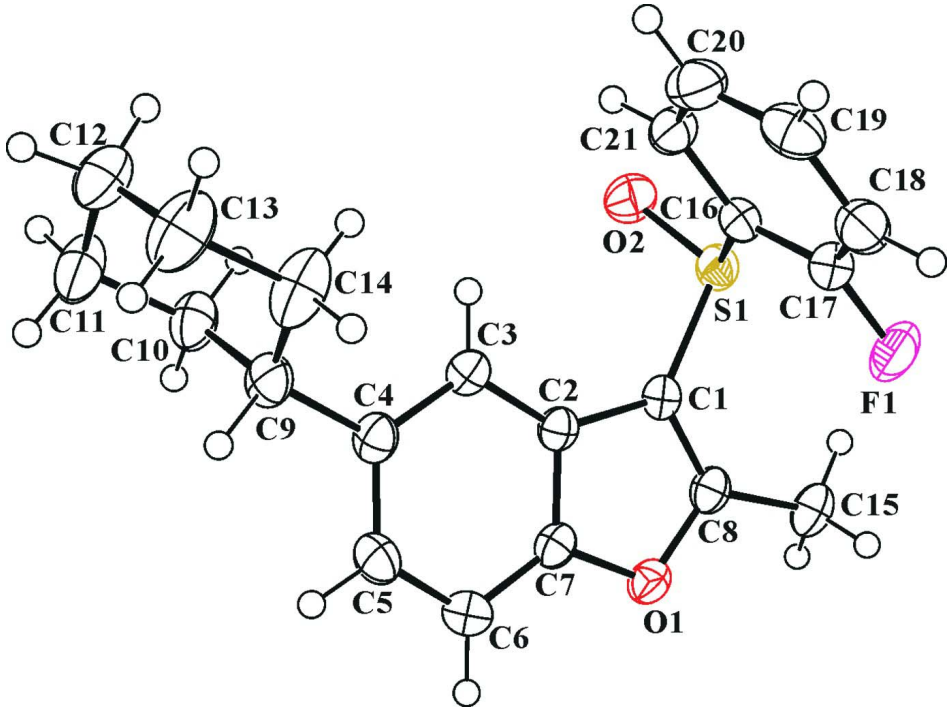

Figure 1

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.

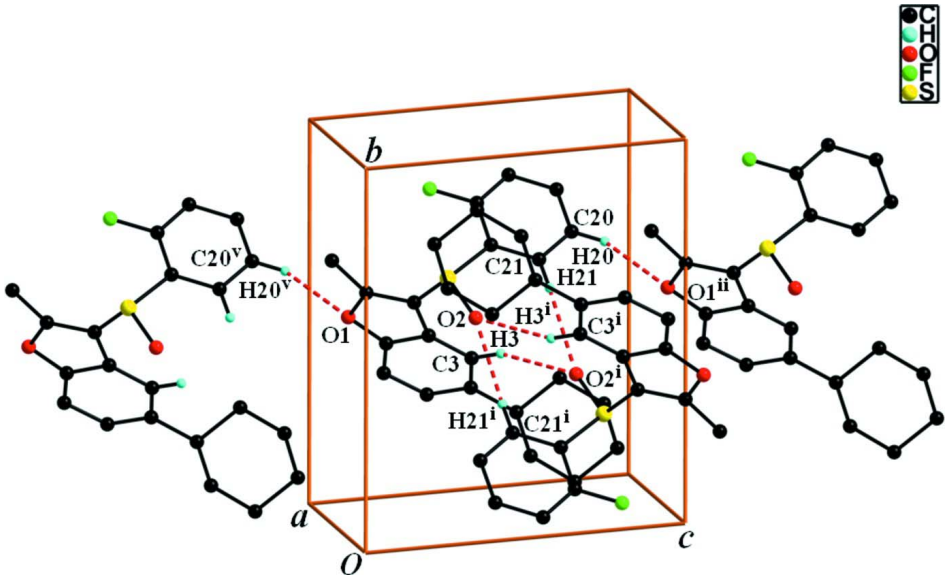

Figure 2

A view of the C—H···O 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* + 2, -*z* + 1; (ii) *x* - 1, *y*, *z*; (v) *x* + 1, *y*, *z*.]

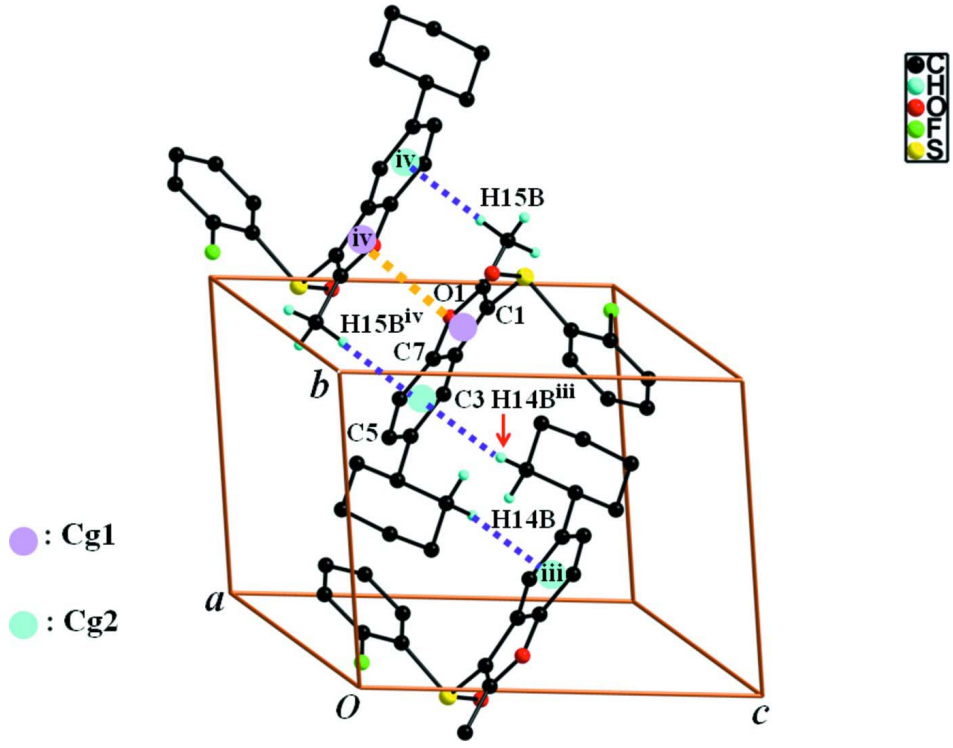

Figure 3

A view of the C—H···π and π–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: (iii) -x + 1, -y + 1, -z + 1; (iv) -x + 2, -y + 2, -z + 1.]

5-Cyclohexyl-3-(2-fluorophenylsulfinyl)-2-methyl-1-benzofuran

Crystal data

$C_{21}H_{21}FO_2S$
M_r = 356.44
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 9.0667 (2) Å
b = 10.3647 (2) Å
c = 10.6838 (2) Å
α = 105.395 (1)°
β = 93.418 (1)°
γ = 110.839 (1)°
V = 891.33 (3) Å^3
Z = 2
F(000) = 376
D_x = 1.328 Mg m^{-3}
Melting point = 424–425 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5827 reflections
θ = 2.5–28.3°
μ = 0.20 mm^{-1}
T = 173 K
Block, colourless
0.30 × 0.22 × 0.21 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} = 0.681, T_{max} = 0.746
16785 measured reflections
4455 independent reflections
3495 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 28.4°, θ_{min} = 2.0°
h = −12→12
k = −13→13
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.116$
$S = 1.04$
4455 reflections
227 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
$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 0.2597P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ 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 $F^2 > 2$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	0.76058 (5)	1.09181 (4)	0.70859 (4)	0.03217 (12)
O1	1.03485 (12)	0.87847 (12)	0.60101 (10)	0.0301 (2)
O2	0.67934 (15)	1.12362 (13)	0.60291 (12)	0.0422 (3)
F1	0.79828 (12)	0.97950 (14)	0.92911 (10)	0.0507 (3)
C1	0.84436 (18)	0.96774 (16)	0.63603 (14)	0.0264 (3)
C2	0.77490 (17)	0.83447 (15)	0.52735 (14)	0.0251 (3)
C3	0.62620 (18)	0.75355 (16)	0.44660 (15)	0.0278 (3)
H3	0.5406	0.7860	0.4560	0.033*
C4	0.60561 (19)	0.62411 (16)	0.35184 (16)	0.0306 (3)
C5	0.7353 (2)	0.58063 (18)	0.33814 (17)	0.0364 (4)
H5	0.7198	0.4925	0.2726	0.044*
C6	0.8845 (2)	0.66036 (18)	0.41581 (17)	0.0351 (4)
H6	0.9717	0.6304	0.4045	0.042*
C7	0.89918 (18)	0.78535 (16)	0.51019 (15)	0.0273 (3)
C8	0.99753 (18)	0.98799 (16)	0.67553 (15)	0.0282 (3)
C9	0.4458 (2)	0.52941 (17)	0.26325 (17)	0.0362 (4)
H9	0.4510	0.4334	0.2193	0.043*
C10	0.4120 (2)	0.5904 (2)	0.15474 (17)	0.0394 (4)
H10A	0.4059	0.6858	0.1949	0.047*
H10B	0.5012	0.6055	0.1039	0.047*
C11	0.2557 (2)	0.4885 (2)	0.06208 (19)	0.0517 (5)
H11A	0.2343	0.5336	−0.0041	0.062*
H11B	0.2662	0.3970	0.0147	0.062*
C12	0.1165 (2)	0.4548 (2)	0.1352 (2)	0.0489 (5)
H12A	0.0959	0.5439	0.1717	0.059*

H12B	0.0194	0.3816	0.0730	0.059*
C13	0.1483 (2)	0.3982 (2)	0.2457 (2)	0.0567 (6)
H13A	0.1532	0.3019	0.2083	0.068*
H13B	0.0590	0.3860	0.2963	0.068*
C14	0.3054 (2)	0.5009 (2)	0.3382 (2)	0.0516 (5)
H14A	0.2964	0.5940	0.3829	0.062*
H14B	0.3254	0.4580	0.4067	0.062*
C15	1.1253 (2)	1.09951 (19)	0.78339 (17)	0.0372 (4)
H15A	1.0949	1.1821	0.8190	0.056*
H15B	1.2256	1.1323	0.7493	0.056*
H15C	1.1401	1.0581	0.8533	0.056*
C16	0.60472 (19)	0.97077 (17)	0.76771 (15)	0.0303 (3)
C17	0.6418 (2)	0.93040 (19)	0.87463 (16)	0.0347 (4)
C18	0.5274 (2)	0.8447 (2)	0.92798 (18)	0.0406 (4)
H18	0.5560	0.8180	1.0014	0.049*
C19	0.3692 (2)	0.79842 (19)	0.87168 (19)	0.0416 (4)
H19	0.2872	0.7398	0.9074	0.050*
C20	0.3288 (2)	0.83647 (19)	0.76392 (19)	0.0427 (4)
H20	0.2194	0.8025	0.7254	0.051*
C21	0.4458 (2)	0.92345 (18)	0.71169 (17)	0.0364 (4)
H21	0.4175	0.9504	0.6383	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0368 (2)	0.0274 (2)	0.0298 (2)	0.01355 (17)	0.00040 (16)	0.00423 (16)
O1	0.0240 (5)	0.0359 (6)	0.0295 (6)	0.0102 (5)	0.0022 (4)	0.0111 (5)
O2	0.0506 (7)	0.0417 (7)	0.0430 (7)	0.0253 (6)	0.0040 (6)	0.0176 (6)
F1	0.0376 (6)	0.0818 (8)	0.0353 (6)	0.0238 (6)	−0.0011 (5)	0.0229 (6)
C1	0.0276 (7)	0.0260 (7)	0.0232 (7)	0.0083 (6)	0.0021 (6)	0.0069 (6)
C2	0.0277 (7)	0.0251 (7)	0.0236 (7)	0.0093 (6)	0.0038 (6)	0.0103 (6)
C3	0.0269 (7)	0.0264 (7)	0.0289 (8)	0.0086 (6)	0.0019 (6)	0.0095 (6)
C4	0.0321 (8)	0.0245 (7)	0.0309 (8)	0.0073 (6)	0.0003 (6)	0.0079 (6)
C5	0.0426 (10)	0.0276 (8)	0.0342 (9)	0.0141 (7)	0.0030 (7)	0.0019 (7)
C6	0.0348 (9)	0.0368 (9)	0.0368 (9)	0.0183 (7)	0.0077 (7)	0.0099 (7)
C7	0.0255 (7)	0.0300 (7)	0.0257 (7)	0.0084 (6)	0.0027 (6)	0.0113 (6)
C8	0.0293 (8)	0.0299 (8)	0.0250 (8)	0.0085 (6)	0.0033 (6)	0.0121 (6)
C9	0.0364 (9)	0.0224 (7)	0.0396 (9)	0.0068 (7)	−0.0048 (7)	0.0019 (7)
C10	0.0337 (9)	0.0483 (10)	0.0296 (9)	0.0080 (8)	0.0040 (7)	0.0126 (8)
C11	0.0410 (11)	0.0669 (13)	0.0342 (10)	0.0092 (10)	−0.0038 (8)	0.0129 (9)
C12	0.0332 (9)	0.0543 (12)	0.0502 (11)	0.0084 (9)	−0.0025 (8)	0.0155 (9)
C13	0.0379 (10)	0.0543 (12)	0.0627 (13)	−0.0061 (9)	−0.0035 (9)	0.0294 (11)
C14	0.0390 (10)	0.0554 (12)	0.0464 (11)	−0.0057 (9)	−0.0023 (8)	0.0284 (10)
C15	0.0306 (8)	0.0394 (9)	0.0329 (9)	0.0057 (7)	−0.0051 (7)	0.0105 (7)
C16	0.0345 (8)	0.0312 (8)	0.0251 (8)	0.0169 (7)	0.0036 (6)	0.0032 (6)
C17	0.0350 (9)	0.0408 (9)	0.0278 (8)	0.0187 (7)	0.0014 (7)	0.0050 (7)
C18	0.0502 (11)	0.0438 (10)	0.0353 (9)	0.0257 (9)	0.0104 (8)	0.0128 (8)
C19	0.0426 (10)	0.0317 (9)	0.0494 (11)	0.0152 (8)	0.0149 (8)	0.0083 (8)

C20	0.0329 (9)	0.0373 (9)	0.0525 (11)	0.0149 (8)	−0.0001 (8)	0.0048 (8)
C21	0.0369 (9)	0.0364 (9)	0.0349 (9)	0.0186 (7)	−0.0021 (7)	0.0053 (7)

Geometric parameters (Å, º)

S1—O2	1.4823 (12)	C11—C12	1.508 (3)
S1—C1	1.7516 (15)	C11—H11A	0.9900
S1—C16	1.7988 (17)	C11—H11B	0.9900
O1—C8	1.3647 (19)	C12—C13	1.506 (3)
O1—C7	1.3790 (18)	C12—H12A	0.9900
F1—C17	1.3569 (19)	C12—H12B	0.9900
C1—C8	1.351 (2)	C13—C14	1.527 (3)
C1—C2	1.447 (2)	C13—H13A	0.9900
C2—C3	1.392 (2)	C13—H13B	0.9900
C2—C7	1.395 (2)	C14—H14A	0.9900
C3—C4	1.392 (2)	C14—H14B	0.9900
C3—H3	0.9500	C15—H15A	0.9800
C4—C5	1.403 (2)	C15—H15B	0.9800
C4—C9	1.513 (2)	C15—H15C	0.9800
C5—C6	1.381 (2)	C16—C17	1.379 (2)
C5—H5	0.9500	C16—C21	1.383 (2)
C6—C7	1.371 (2)	C17—C18	1.368 (3)
C6—H6	0.9500	C18—C19	1.380 (3)
C8—C15	1.479 (2)	C18—H18	0.9500
C9—C10	1.524 (2)	C19—C20	1.382 (3)
C9—C14	1.527 (3)	C19—H19	0.9500
C9—H9	1.0000	C20—C21	1.381 (3)
C10—C11	1.522 (2)	C20—H20	0.9500
C10—H10A	0.9900	C21—H21	0.9500
C10—H10B	0.9900		
O2—S1—C1	108.76 (7)	C10—C11—H11B	109.3
O2—S1—C16	106.28 (8)	H11A—C11—H11B	107.9
C1—S1—C16	97.18 (7)	C13—C12—C11	111.76 (17)
C8—O1—C7	106.55 (11)	C13—C12—H12A	109.3
C8—C1—C2	107.67 (13)	C11—C12—H12A	109.3
C8—C1—S1	122.41 (12)	C13—C12—H12B	109.3
C2—C1—S1	129.89 (11)	C11—C12—H12B	109.3
C3—C2—C7	119.50 (14)	H12A—C12—H12B	107.9
C3—C2—C1	136.36 (14)	C12—C13—C14	111.52 (15)
C7—C2—C1	104.13 (13)	C12—C13—H13A	109.3
C2—C3—C4	118.59 (14)	C14—C13—H13A	109.3
C2—C3—H3	120.7	C12—C13—H13B	109.3
C4—C3—H3	120.7	C14—C13—H13B	109.3
C3—C4—C5	119.45 (15)	H13A—C13—H13B	108.0
C3—C4—C9	121.17 (14)	C9—C14—C13	111.25 (17)
C5—C4—C9	119.38 (14)	C9—C14—H14A	109.4
C6—C5—C4	122.89 (15)	C13—C14—H14A	109.4

C6—C5—H5	118.6	C9—C14—H14B	109.4
C4—C5—H5	118.6	C13—C14—H14B	109.4
C7—C6—C5	116.01 (15)	H14A—C14—H14B	108.0
C7—C6—H6	122.0	C8—C15—H15A	109.5
C5—C6—H6	122.0	C8—C15—H15B	109.5
C6—C7—O1	125.80 (14)	H15A—C15—H15B	109.5
C6—C7—C2	123.52 (15)	C8—C15—H15C	109.5
O1—C7—C2	110.68 (13)	H15A—C15—H15C	109.5
C1—C8—O1	110.97 (13)	H15B—C15—H15C	109.5
C1—C8—C15	132.96 (15)	C17—C16—C21	119.06 (16)
O1—C8—C15	116.03 (13)	C17—C16—S1	120.14 (13)
C4—C9—C10	112.40 (13)	C21—C16—S1	120.71 (13)
C4—C9—C14	113.24 (14)	F1—C17—C18	119.26 (15)
C10—C9—C14	109.31 (14)	F1—C17—C16	118.10 (15)
C4—C9—H9	107.2	C18—C17—C16	122.63 (16)
C10—C9—H9	107.2	C17—C18—C19	117.89 (17)
C14—C9—H9	107.2	C17—C18—H18	121.1
C11—C10—C9	111.29 (15)	C19—C18—H18	121.1
C11—C10—H10A	109.4	C18—C19—C20	120.65 (17)
C9—C10—H10A	109.4	C18—C19—H19	119.7
C11—C10—H10B	109.4	C20—C19—H19	119.7
C9—C10—H10B	109.4	C21—C20—C19	120.64 (17)
H10A—C10—H10B	108.0	C21—C20—H20	119.7
C12—C11—C10	111.80 (16)	C19—C20—H20	119.7
C12—C11—H11A	109.3	C20—C21—C16	119.12 (16)
C10—C11—H11A	109.3	C20—C21—H21	120.4
C12—C11—H11B	109.3	C16—C21—H21	120.4

O2—S1—C1—C8	131.20 (13)	C7—O1—C8—C15	178.13 (12)
C16—S1—C1—C8	−118.85 (14)	C3—C4—C9—C10	75.69 (19)
O2—S1—C1—C2	−46.74 (16)	C5—C4—C9—C10	−104.29 (18)
C16—S1—C1—C2	63.21 (15)	C3—C4—C9—C14	−48.8 (2)
C8—C1—C2—C3	178.69 (16)	C5—C4—C9—C14	131.23 (17)
S1—C1—C2—C3	−3.1 (3)	C4—C9—C10—C11	176.45 (15)
C8—C1—C2—C7	−0.48 (16)	C14—C9—C10—C11	−56.9 (2)
S1—C1—C2—C7	177.70 (12)	C9—C10—C11—C12	55.9 (2)
C7—C2—C3—C4	0.9 (2)	C10—C11—C12—C13	−53.9 (2)
C1—C2—C3—C4	−178.16 (16)	C11—C12—C13—C14	53.8 (3)
C2—C3—C4—C5	−1.5 (2)	C4—C9—C14—C13	−176.82 (15)
C2—C3—C4—C9	178.51 (14)	C10—C9—C14—C13	57.0 (2)
C3—C4—C5—C6	0.5 (3)	C12—C13—C14—C9	−56.0 (2)
C9—C4—C5—C6	−179.48 (15)	O2—S1—C16—C17	−174.67 (12)
C4—C5—C6—C7	1.0 (2)	C1—S1—C16—C17	73.34 (14)
C5—C6—C7—O1	177.69 (14)	O2—S1—C16—C21	1.70 (15)
C5—C6—C7—C2	−1.7 (2)	C1—S1—C16—C21	−110.29 (14)
C8—O1—C7—C6	−179.97 (15)	C21—C16—C17—F1	−179.18 (14)
C8—O1—C7—C2	−0.55 (15)	S1—C16—C17—F1	−2.8 (2)
C3—C2—C7—C6	0.7 (2)	C21—C16—C17—C18	0.1 (2)

C1—C2—C7—C6	−179.93 (14)	S1—C16—C17—C18	176.54 (13)
C3—C2—C7—O1	−178.71 (12)	F1—C17—C18—C19	178.98 (15)
C1—C2—C7—O1	0.63 (16)	C16—C17—C18—C19	−0.3 (3)
C2—C1—C8—O1	0.17 (17)	C17—C18—C19—C20	0.7 (3)
S1—C1—C8—O1	−178.18 (10)	C18—C19—C20—C21	−1.0 (3)
C2—C1—C8—C15	−177.26 (15)	C19—C20—C21—C16	0.8 (3)
S1—C1—C8—C15	4.4 (2)	C17—C16—C21—C20	−0.3 (2)
C7—O1—C8—C1	0.23 (16)	S1—C16—C21—C20	−176.75 (12)

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C2–C7 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O2^{i}	0.95	2.60	3.5024 (19)	160
C20—H20···O1^{ii}	0.95	2.53	3.316 (2)	140
C21—H21···O2^{i}	0.95	2.49	3.332 (2)	148
C14—H14*B*···*Cg2*^{iii}	0.99	2.69	3.618 (2)	156
C15—H15*B*···*Cg2*^{iv}	0.98	2.85	3.422 (2)	118

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