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5-Cyclohexyl-2-methyl-3-phenylsulfonyl-1-benzofuran

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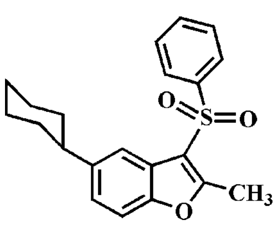
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.108; data-to-parameter ratio = 17.2.

In the title compound, $C_{21}H_{22}O_3S$, the cyclohexyl ring adopts a chair conformation. The phenyl ring makes a dihedral angle of 78.07 (5)° with the mean plane of the benzofuran fragment. In the crystal, molecules are linked through weak intermolecular C—H⋯O hydrogen bonds and C—H⋯π interactions.

Related literature

For the biological activity of benzofuran compounds, see: Aslam *et al.* (2009); Galal *et al.* (2009); Khan *et al.* (2005). For natural products with benzofuran moieties, see: Akgul & Anil (2003); Soekamto *et al.* (2003). For structural studies of related 3-arylsulfonyl-5-cyclohexyl-2-methyl-1-benzofuran derivatives, see: Choi *et al.* (2011*a*,*b*).



Experimental

Crystal data

$C_{21}H_{22}O_3S$
M_r = 354.45
Triclinic, $P\bar{1}$
a = 9.0424 (2) Å
b = 10.1585 (3) Å
c = 10.3451 (3) Å
α = 90.689 (2)°
β = 109.470 (1)°
γ = 95.634 (2)°
V = 890.59 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 173 K
0.34 × 0.23 × 0.18 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.682, T_{max} = 0.746
15432 measured reflections
3899 independent reflections
3309 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.108
S = 1.05
3899 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

Cg is the centroid of the C1/C2/C7/O1/C8 furan ring.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C21—H21⋯O3^{i}	0.95	2.39	3.284 (2)	157
C11—H11B⋯Cg^{ii}	0.99	2.81	3.632 (2)	142

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

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* (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: LD2013).

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supplementary materials

Acta Cryst. (2011). E**67**, o1496 [doi:10.1107/S1600536811018903]

5-Cyclohexyl-2-methyl-3-phenylsulfonyl-1-benzofuran

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Comment

Recently, compounds involving a benzofuran moiety have attracted much attention owing to their valuable pharmacological properties such as antibacterial, antifungal, antitumor, antiviral, and antimicrobial activities (Aslam *et al.*, 2009, Galal *et al.*, 2009, Khan *et al.*, 2005). These compounds occur in a wide range of natural products (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our ongoing program of stydying substituent effect on solid state structures of analogues of 3-arylsulfonyl-5-cyclohexyl-2-methyl-1-benzofuran (Choi *et al.*, 2011*a,b*), we report herein crystal structure of the title compound.

In the title molecule (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.005 (1) Å from the least-squares plane defined by the nine constituent atoms. The cyclohexyl ring is in the chair form. The phenyl ring makes a dihedral angle of 78.07 (5)° with the mean plane of the benzofuran ring. The crystal packing (Fig. 2) is stabilized by weak intermolecular C—H···O hydrogen bonds between a phenyl H atom and the O atom of the sulfonyl group (Table; C21—H21···O3^{i}). The crystal packing (Fig. 2) is further stabilized by intermolecular C—H···π interactions between a cyclohexyl H atom and the furan ring (Table 1; C11—H11B···Cg^{ii}, Cg is the centroid of the C1/C2/C7/O1/C8 furan ring),

Experimental

77% 3-chloroperoxybenzoic acid (493 mg, 2.2 mmol) was added in small portions to a stirred solution of 5-cyclohexyl-2-methyl-3-phenylsulfanyl-1-benzofuran (354 mg, 1.1 mmol) in dichloromethane (40 mL) at 273 K. After being stirred at room temperature for 8h, 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. 430–431 K; R_f = 0.48 (hexane–ethyl acetate, 4:1 v/v)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of benzene solution of the title compound at room temperature.

Refinement

All H atoms were placed 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, methylene, and 1.5U_{eq}(C) for methyl H atoms. Positions of H atoms of the methyl group were optimized rotationally using AFIX 137 instruction.

Figures

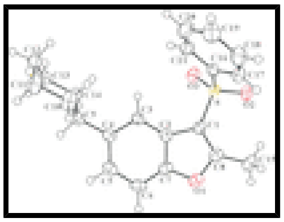

Fig. 1. The molecular structure of the title compound with atom numbering scheme. Displacement ellipsoids are drawn at 50% probability level. H atoms are represented as small spheres of arbitrary radius.

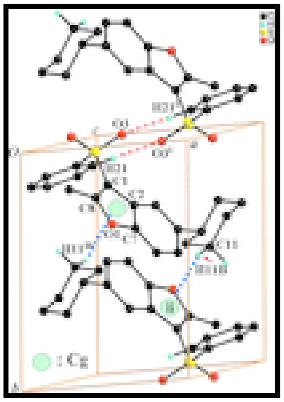

Fig. 2. A view of the C—H···O and C—H···π interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (i) -*x* + 1, -*y*, - *z* + 1; (ii) - *x* + 1, - *y* + 1, -*z* + 1; (iii) - *x* + 1, - *y* + 1, - *z* + 1.]

5-Cyclohexyl-2-methyl-3-phenylsulfonyl-1-benzofuran

Crystal data

$C_{21}H_{22}O_3S$	$Z = 2$
$M_r = 354.45$	$F(000) = 376$
Triclinic, $P\overline{1}$	$D_x = 1.322$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 9.0424$ (2) Å	Cell parameters from 6655 reflections
$b = 10.1585$ (3) Å	$\theta = 2.4$–$27.1°$
$c = 10.3451$ (3) Å	$\mu = 0.20$ mm^{-1}
$\alpha = 90.689$ (2)°	$T = 173$ K
$\beta = 109.470$ (1)°	Block, colourless
$\gamma = 95.634$ (2)°	0.34 × 0.23 × 0.18 mm
$V = 890.59$ (4) Å^3	

Data collection

Bruker SMART APEXII CCD diffractometer	3899 independent reflections
Radiation source: rotating anode	3309 reflections with $I > 2\sigma(I)$
graphite multilayer	$R_{int} = 0.031$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 27.0°$, $\theta_{min} = 2.0°$
φ and ω scans	$h = -11 \rightarrow 11$
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)	$k = -11 \rightarrow 12$

T_{min} = 0.682, T_{max} = 0.746	$l = -13 \rightarrow 13$
15432 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.041$	Hydrogen site location: difference Fourier map
$wR(F^2) = 0.108$	H-atom parameters constrained
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 0.3567P]$ where $P = (F_o^2 + 2F_c^2)/3$
3899 reflections	$(\Delta/\sigma)_{max} < 0.001$
227 parameters	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
0 restraints	$\Delta\rho_{min}$ = −0.45 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 > 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}
S1	0.35282 (4)	0.02944 (4)	0.20427 (4)	0.02763 (12)
O1	0.52551 (14)	0.33013 (12)	0.04563 (12)	0.0356 (3)
O2	0.26982 (14)	−0.04640 (12)	0.07882 (12)	0.0372 (3)
O3	0.46616 (13)	−0.03055 (11)	0.31344 (12)	0.0353 (3)
C1	0.44833 (18)	0.17184 (16)	0.16487 (16)	0.0280 (3)
C2	0.55947 (17)	0.26784 (15)	0.26329 (16)	0.0273 (3)
C3	0.62369 (17)	0.28344 (15)	0.40582 (16)	0.0273 (3)
H3	0.5958	0.2194	0.4622	0.033*
C4	0.72944 (18)	0.39460 (16)	0.46415 (17)	0.0293 (3)
C5	0.7685 (2)	0.48740 (17)	0.37830 (19)	0.0357 (4)
H5	0.8407	0.5629	0.4190	0.043*
C6	0.7061 (2)	0.47346 (18)	0.23670 (19)	0.0381 (4)
H6	0.7334	0.5370	0.1796	0.046*
C7	0.60245 (19)	0.36255 (17)	0.18333 (17)	0.0314 (4)
C8	0.43211 (19)	0.21380 (17)	0.03673 (17)	0.0318 (4)
C9	0.79944 (18)	0.41842 (16)	0.61788 (17)	0.0302 (3)
H9	0.8891	0.4900	0.6367	0.036*

C10	0.6804 (2)	0.4677 (2)	0.67798 (19)	0.0441 (5)
H10A	0.6430	0.5497	0.6335	0.053*
H10B	0.5881	0.4001	0.6582	0.053*
C11	0.7530 (2)	0.4957 (2)	0.83250 (19)	0.0461 (5)
H11A	0.8386	0.5695	0.8518	0.055*
H11B	0.6717	0.5232	0.8686	0.055*
C12	0.8189 (2)	0.37507 (19)	0.90467 (18)	0.0385 (4)
H12A	0.7314	0.3045	0.8942	0.046*
H12B	0.8710	0.3980	1.0039	0.046*
C13	0.9367 (2)	0.32409 (17)	0.84674 (17)	0.0349 (4)
H13A	0.9716	0.2415	0.8912	0.042*
H13B	1.0305	0.3903	0.8678	0.042*
C14	0.8662 (2)	0.29686 (17)	0.69219 (17)	0.0332 (4)
H14A	0.7810	0.2227	0.6720	0.040*
H14B	0.9486	0.2697	0.6572	0.040*
C15	0.3387 (2)	0.1631 (2)	−0.10457 (17)	0.0412 (4)
H15A	0.3062	0.0683	−0.1041	0.062*
H15B	0.4030	0.1771	−0.1639	0.062*
H15C	0.2449	0.2104	−0.1393	0.062*
C16	0.21258 (18)	0.08522 (15)	0.27032 (16)	0.0269 (3)
C17	0.06959 (19)	0.11585 (17)	0.17967 (17)	0.0347 (4)
H17	0.0482	0.1080	0.0834	0.042*
C18	−0.0408 (2)	0.1578 (2)	0.2310 (2)	0.0434 (4)
H18	−0.1388	0.1796	0.1700	0.052*
C19	−0.0097 (2)	0.1683 (2)	0.3705 (2)	0.0471 (5)
H19	−0.0865	0.1968	0.4055	0.057*
C20	0.1332 (2)	0.1373 (2)	0.45998 (19)	0.0464 (5)
H20	0.1539	0.1449	0.5562	0.056*
C21	0.2459 (2)	0.09552 (18)	0.41083 (17)	0.0355 (4)
H21	0.3441	0.0743	0.4721	0.043*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0291 (2)	0.0271 (2)	0.0247 (2)	0.00455 (15)	0.00598 (15)	0.00047 (15)
O1	0.0392 (6)	0.0417 (7)	0.0311 (6)	0.0062 (5)	0.0180 (5)	0.0068 (5)
O2	0.0424 (7)	0.0356 (6)	0.0303 (6)	0.0008 (5)	0.0090 (5)	−0.0063 (5)
O3	0.0351 (6)	0.0344 (6)	0.0345 (6)	0.0113 (5)	0.0068 (5)	0.0066 (5)
C1	0.0274 (7)	0.0318 (8)	0.0266 (8)	0.0068 (6)	0.0105 (6)	0.0020 (6)
C2	0.0225 (7)	0.0299 (8)	0.0316 (8)	0.0057 (6)	0.0111 (6)	0.0023 (6)
C3	0.0240 (7)	0.0280 (8)	0.0309 (8)	0.0036 (6)	0.0105 (6)	0.0035 (6)
C4	0.0234 (7)	0.0290 (8)	0.0353 (9)	0.0045 (6)	0.0092 (6)	0.0024 (7)
C5	0.0299 (8)	0.0321 (9)	0.0456 (10)	0.0000 (7)	0.0143 (7)	0.0032 (7)
C6	0.0369 (9)	0.0382 (10)	0.0447 (10)	0.0015 (7)	0.0212 (8)	0.0105 (8)
C7	0.0295 (8)	0.0377 (9)	0.0317 (8)	0.0076 (7)	0.0154 (7)	0.0059 (7)
C8	0.0316 (8)	0.0370 (9)	0.0314 (8)	0.0104 (7)	0.0145 (7)	0.0037 (7)
C9	0.0254 (7)	0.0271 (8)	0.0348 (9)	0.0003 (6)	0.0067 (6)	−0.0012 (6)
C10	0.0369 (9)	0.0514 (11)	0.0402 (10)	0.0184 (8)	0.0045 (8)	−0.0088 (8)

C11	0.0431 (10)	0.0510 (12)	0.0413 (10)	0.0178 (9)	0.0073 (8)	−0.0128 (9)
C12	0.0351 (9)	0.0454 (10)	0.0340 (9)	−0.0002 (8)	0.0121 (7)	−0.0078 (8)
C13	0.0326 (8)	0.0365 (9)	0.0349 (9)	0.0074 (7)	0.0096 (7)	0.0015 (7)
C14	0.0356 (8)	0.0330 (9)	0.0332 (9)	0.0091 (7)	0.0131 (7)	0.0006 (7)
C15	0.0493 (10)	0.0493 (11)	0.0268 (9)	0.0113 (9)	0.0133 (8)	0.0026 (8)
C16	0.0272 (7)	0.0249 (7)	0.0273 (8)	0.0008 (6)	0.0077 (6)	0.0024 (6)
C17	0.0333 (8)	0.0392 (9)	0.0279 (8)	0.0057 (7)	0.0047 (7)	0.0026 (7)
C18	0.0315 (9)	0.0501 (11)	0.0448 (11)	0.0116 (8)	0.0060 (8)	−0.0006 (9)
C19	0.0386 (10)	0.0572 (12)	0.0495 (12)	0.0076 (9)	0.0196 (9)	−0.0071 (9)
C20	0.0472 (11)	0.0631 (13)	0.0305 (9)	0.0069 (9)	0.0151 (8)	−0.0052 (9)
C21	0.0340 (9)	0.0424 (10)	0.0269 (8)	0.0041 (7)	0.0058 (7)	0.0013 (7)

Geometric parameters (Å, °)

S1—O2	1.4333 (12)	C11—C12	1.510 (3)
S1—O3	1.4370 (11)	C11—H11A	0.9900
S1—C1	1.7344 (16)	C11—H11B	0.9900
S1—C16	1.7622 (16)	C12—C13	1.513 (2)
O1—C8	1.367 (2)	C12—H12A	0.9900
O1—C7	1.380 (2)	C12—H12B	0.9900
C1—C8	1.363 (2)	C13—C14	1.521 (2)
C1—C2	1.449 (2)	C13—H13A	0.9900
C2—C7	1.386 (2)	C13—H13B	0.9900
C2—C3	1.394 (2)	C14—H14A	0.9900
C3—C4	1.393 (2)	C14—H14B	0.9900
C3—H3	0.9500	C15—H15A	0.9800
C4—C5	1.402 (2)	C15—H15B	0.9800
C4—C9	1.509 (2)	C15—H15C	0.9800
C5—C6	1.383 (3)	C16—C21	1.383 (2)
C5—H5	0.9500	C16—C17	1.388 (2)
C6—C7	1.373 (2)	C17—C18	1.375 (3)
C6—H6	0.9500	C17—H17	0.9500
C8—C15	1.479 (2)	C18—C19	1.376 (3)
C9—C14	1.530 (2)	C18—H18	0.9500
C9—C10	1.530 (2)	C19—C20	1.384 (3)
C9—H9	1.0000	C19—H19	0.9500
C10—C11	1.523 (2)	C20—C21	1.379 (3)
C10—H10A	0.9900	C20—H20	0.9500
C10—H10B	0.9900	C21—H21	0.9500
O2—S1—O3	119.24 (7)	C12—C11—H11B	109.3
O2—S1—C1	108.08 (8)	C10—C11—H11B	109.3
O3—S1—C1	107.73 (7)	H11A—C11—H11B	108.0
O2—S1—C16	108.19 (7)	C11—C12—C13	111.29 (15)
O3—S1—C16	107.58 (7)	C11—C12—H12A	109.4
C1—S1—C16	105.18 (7)	C13—C12—H12A	109.4
C8—O1—C7	107.18 (12)	C11—C12—H12B	109.4
C8—C1—C2	107.85 (14)	C13—C12—H12B	109.4
C8—C1—S1	126.38 (13)	H12A—C12—H12B	108.0
C2—C1—S1	125.77 (12)	C12—C13—C14	111.59 (14)

C7—C2—C3	119.42 (15)	C12—C13—H13A	109.3
C7—C2—C1	104.35 (14)	C14—C13—H13A	109.3
C3—C2—C1	136.23 (15)	C12—C13—H13B	109.3
C4—C3—C2	118.86 (15)	C14—C13—H13B	109.3
C4—C3—H3	120.6	H13A—C13—H13B	108.0
C2—C3—H3	120.6	C13—C14—C9	111.94 (14)
C3—C4—C5	119.30 (15)	C13—C14—H14A	109.2
C3—C4—C9	121.16 (14)	C9—C14—H14A	109.2
C5—C4—C9	119.53 (15)	C13—C14—H14B	109.2
C6—C5—C4	122.64 (16)	C9—C14—H14B	109.2
C6—C5—H5	118.7	H14A—C14—H14B	107.9
C4—C5—H5	118.7	C8—C15—H15A	109.5
C7—C6—C5	116.24 (16)	C8—C15—H15B	109.5
C7—C6—H6	121.9	H15A—C15—H15B	109.5
C5—C6—H6	121.9	C8—C15—H15C	109.5
C6—C7—O1	125.78 (15)	H15A—C15—H15C	109.5
C6—C7—C2	123.55 (16)	H15B—C15—H15C	109.5
O1—C7—C2	110.67 (14)	C21—C16—C17	121.39 (16)
C1—C8—O1	109.95 (15)	C21—C16—S1	119.54 (12)
C1—C8—C15	134.96 (17)	C17—C16—S1	119.06 (13)
O1—C8—C15	115.09 (14)	C18—C17—C16	119.13 (16)
C4—C9—C14	113.14 (13)	C18—C17—H17	120.4
C4—C9—C10	111.63 (13)	C16—C17—H17	120.4
C14—C9—C10	109.87 (14)	C17—C18—C19	120.22 (16)
C4—C9—H9	107.3	C17—C18—H18	119.9
C14—C9—H9	107.3	C19—C18—H18	119.9
C10—C9—H9	107.3	C18—C19—C20	120.16 (18)
C11—C10—C9	111.47 (14)	C18—C19—H19	119.9
C11—C10—H10A	109.3	C20—C19—H19	119.9
C9—C10—H10A	109.3	C21—C20—C19	120.64 (17)
C11—C10—H10B	109.3	C21—C20—H20	119.7
C9—C10—H10B	109.3	C19—C20—H20	119.7
H10A—C10—H10B	108.0	C20—C21—C16	118.46 (16)
C12—C11—C10	111.40 (15)	C20—C21—H21	120.8
C12—C11—H11A	109.3	C16—C21—H21	120.8
C10—C11—H11A	109.3		

O2—S1—C1—C8	7.74 (17)	C7—O1—C8—C1	−0.16 (17)
O3—S1—C1—C8	137.82 (14)	C7—O1—C8—C15	179.66 (13)
C16—S1—C1—C8	−107.65 (15)	C3—C4—C9—C14	48.8 (2)
O2—S1—C1—C2	−172.58 (12)	C5—C4—C9—C14	−132.76 (16)
O3—S1—C1—C2	−42.50 (15)	C3—C4—C9—C10	−75.79 (19)
C16—S1—C1—C2	72.03 (14)	C5—C4—C9—C10	102.70 (18)
C8—C1—C2—C7	−0.12 (17)	C4—C9—C10—C11	−178.26 (15)
S1—C1—C2—C7	−179.85 (12)	C14—C9—C10—C11	55.4 (2)
C8—C1—C2—C3	179.19 (17)	C9—C10—C11—C12	−56.4 (2)
S1—C1—C2—C3	−0.5 (3)	C10—C11—C12—C13	55.5 (2)
C7—C2—C3—C4	0.2 (2)	C11—C12—C13—C14	−54.8 (2)
C1—C2—C3—C4	−179.04 (16)	C12—C13—C14—C9	55.05 (19)
C2—C3—C4—C5	−0.1 (2)	C4—C9—C14—C13	179.67 (13)

C2—C3—C4—C9	178.41 (13)	C10—C9—C14—C13	−54.83 (18)
C3—C4—C5—C6	0.0 (2)	O2—S1—C16—C21	145.40 (14)
C9—C4—C5—C6	−178.53 (15)	O3—S1—C16—C21	15.35 (15)
C4—C5—C6—C7	0.0 (3)	C1—S1—C16—C21	−99.29 (14)
C5—C6—C7—O1	179.21 (15)	O2—S1—C16—C17	−33.55 (15)
C5—C6—C7—C2	0.2 (3)	O3—S1—C16—C17	−163.60 (13)
C8—O1—C7—C6	−179.08 (16)	C1—S1—C16—C17	81.76 (14)
C8—O1—C7—C2	0.08 (17)	C21—C16—C17—C18	0.2 (3)
C3—C2—C7—C6	−0.3 (2)	S1—C16—C17—C18	179.18 (14)
C1—C2—C7—C6	179.20 (15)	C16—C17—C18—C19	−0.4 (3)
C3—C2—C7—O1	−179.43 (13)	C17—C18—C19—C20	0.3 (3)
C1—C2—C7—O1	0.03 (17)	C18—C19—C20—C21	−0.1 (3)
C2—C1—C8—O1	0.18 (18)	C19—C20—C21—C16	−0.1 (3)
S1—C1—C8—O1	179.90 (11)	C17—C16—C21—C20	0.0 (3)
C2—C1—C8—C15	−179.60 (18)	S1—C16—C21—C20	−178.94 (14)
S1—C1—C8—C15	0.1 (3)		

Hydrogen-bond geometry (Å, °)

Cg is the centroid of the C1/C2/C7/O1/C8 furan ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C21—H21···O3^{i}	0.95	2.39	3.284 (2)	157
C11—H11B···Cg^{ii}	0.99	2.81	3.632 (2)	142

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

Fig. 1

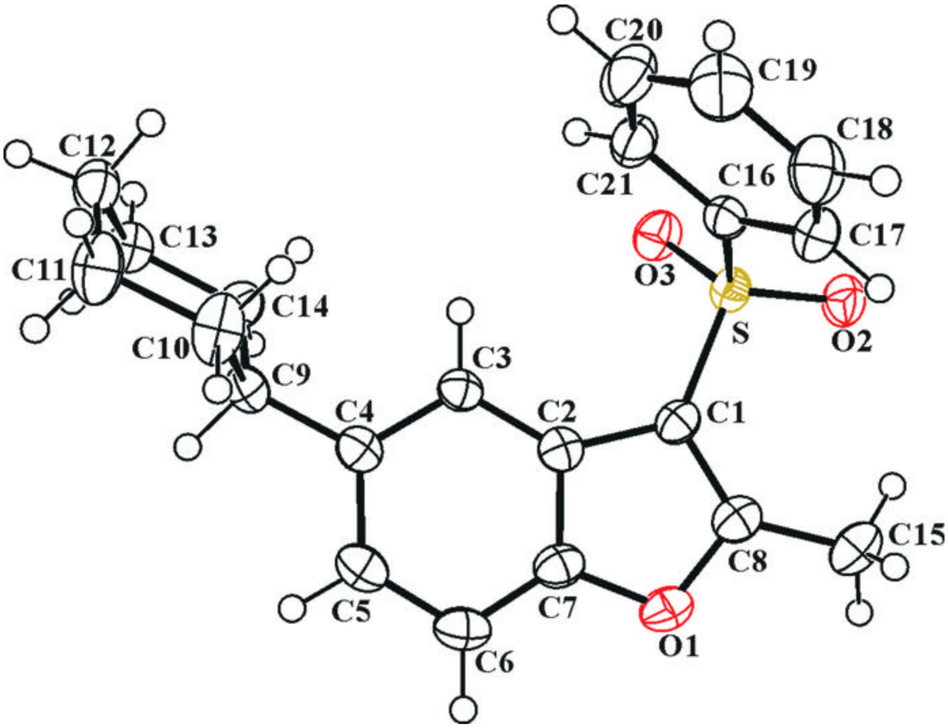
C20
C19
C12
C18
C21
C16
C13
C17
C11
O3
C14
S
O2
C10
C3
C9
C1
C4
C2
C15
C8
C5
C7
O1
C6

Fig. 2