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Ethyl (2-methyl-1-phenylsulfonyl-1*H*-indole-3-carbonyl)acetate

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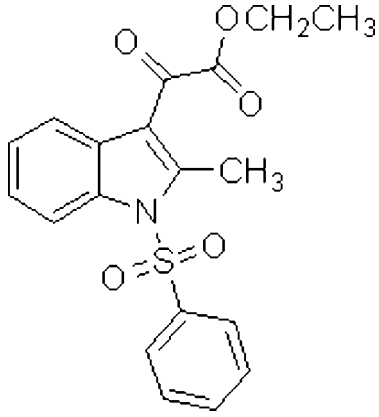
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.050; wR factor = 0.161; data-to-parameter ratio = 25.6.

In the title compound, $C_{19}H_{17}NO_5S$, the phenyl ring forms a dihedral angle of 83.67 (4)° with the indole ring system. The molecular structure is stabilized by weak intramolecular C—H···O interactions and the crystal packing is stabilized by weak intermolecular C—H···O and C—H···π interactions.

Related literature

For releted literature, see: Chai *et al.* (2006); Liu *et al.* (2007); Senthil Kumar *et al.* (2006); Williams *et al.* (1993). A similar compound with a dibromomethyl group has been reported recently (Rinderspacher *et al.*, 2007).



Experimental

Crystal data

$C_{19}H_{17}NO_5S$
M_r = 371.40
Monoclinic, $P2_1/n$
a = 9.6696 (4) Å
b = 13.1526 (5) Å
c = 13.8048 (5) Å
β = 94.898 (1)°
V = 1749.29 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 295 (2) K
0.24 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.929, T_{max} = 0.958
25430 measured reflections
6064 independent reflections
4222 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.161
S = 1.06
6064 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

*Cg*1 is the centroid of the C1–C6 phenyl ring and *Cg*2 is the centroid of the five-membered N1/C7/C8/C9/C14 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O3^{i}	0.93	2.56	3.197 (2)	126
C2—H2···O2	0.93	2.52	2.897 (2)	104
C10—H10···O3	0.93	2.51	3.026 (2)	115
C13—H13···O2	0.93	2.48	3.001 (2)	116
C15—H15*B*···O1	0.96	2.43	2.798 (2)	103
C3—H3···*Cg*1^{ii}	0.93	2.70	3.524	148
C4—H4···*Cg*2^{ii}	0.93	2.90	3.619	135

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2458).

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supplementary materials

Acta Cryst. (2007). E**63**, o3698 [**doi:10.1107/S1600536807037415**]

Ethyl (2-methyl-1-phenylsulfonyl-1*H*-indole-3-carbonyl)acetate

G. Chakkaravarthi, V. Dhayalan, A. K. Mohanakrishnan and V. Manivannan

Comment

Phenylsulfonyl-indole compounds inhibit the HIV-1 RT enzyme *in vitro* and HTLVIIIb viral spread in MT-4 human T-lymphoid cells (Williams *et al.*, 1993). Indole-3-carboxylate derivatives exhibit significant antihepatitis B virus activities (Chai *et al.*, 2006).

The geometric parameters in the title compound (Fig. 1) agree with the reported values of similar structures (Liu *et al.*, 2007; Senthil Kumar *et al.*, 2006). The phenyl ring forms dihedral angle of 83.67 (4)° with the indole ring system. The five- (N1/C7/C8/C9/C14) and six- (C9–C14) membered rings in the indane group are planar, with a dihedral angle of 1.90 (4)° between these rings.

The sum of the bond angles around N1 (359.95°) indicates that N1 is sp^2-hybridized. The torsion angles O2—S1—N1—C14 and O1—S1—N1—C7 [−44.24 (14)° and 9.30 (15)°, respectively] indicate the *syn* conformation of the sulfonyl moiety.

The details of the hydrogen bonding are given in Table 1. The molecular structure is stabilized by weak intramolecular C—H···O interactions and the crystal packing (Fig. 2) is stabilized by weak intermolecular C—H···O interactions and C—H···π interactions involving the C1–C6 (centroid *Cg*1) and N1/C7–C14 (centroid *Cg*2) rings.

A similar compound with dibromomethyl group has been reported (Rinderspacher *et al.*, 2007).

Experimental

To a solution of ethyl 2-(2-methyl-1*H*-indole-3-yl)-2-oxoacetate (10 g, 43.2 mmol) in dry dichloromethane (80 ml) under nitrogen, triethylamine (7.8 ml, 56.2 mmol) followed by dimethyl amino pyridine (0.52 g, 4.2 mmol) were added slowly and stirred at 273 K for 30 min. To this benzenesulfonyl chloride (8.3 ml, 64.9 mmol), dry dichloromethane (10 ml) was slowly added at 273 K for 30 min. Then the reaction mixture was stirred at room temperature and poured over crushed ice and extracted with dichloromethane (3 *x* 20 ml) and dried with sodium sulfate. The solvent was removed under vacuum. Then the crude product was recrystallized from methanol. Single crystals suitable for X-ray analysis were grown by slow evaporation of a methanol solution at room temperature.

Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2Ueq(C) for aromatic C—H, C—H = 0.97 Å and U_{iso}(H) = 1.2Ueq(C) for CH_2 and C—H = 0.96 Å and U_{iso}(H) = 1.5Ueq(C) for CH_3.

Figures

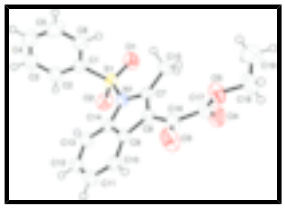

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

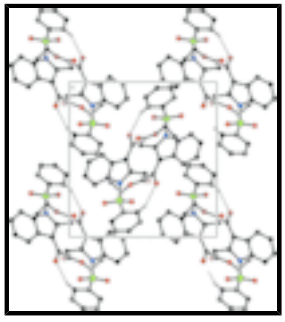

Fig. 2. The packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

Ethyl (2-methyl-1-phenylsulfonyl-1*H*-indole-3-carbonyl)acetate

Crystal data

$C_{19}H_{17}NO_5S$	F_{000} = 776
M_r = 371.40	D_x = 1.410 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 26134 reflections
a = 9.6696 (4) Å	θ = 2.6–29.9º
b = 13.1526 (5) Å	μ = 0.22 mm^{-1}
c = 13.8048 (5) Å	T = 295 (2) K
β = 94.898 (1)º	Block, colourless
V = 1749.29 (12) Å^3	0.24 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker Kappa APEXII diffractometer	6064 independent reflections
Radiation source: fine-focus sealed tube	4222 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.025
T = 295(2) K	θ_{max} = 32.0º
ω and φ scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −14→14
T_{min} = 0.929, T_{max} = 0.958	k = −19→17
25430 measured reflections	l = −20→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.050$	H-atom parameters constrained
$wR(F^2) = 0.161$	$w = 1/[\sigma^2(F_o^2) + (0.0861P)^2 + 0.2836P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
6064 reflections	$\Delta\rho_{max} = 0.64$ e Å^{-3}
237 parameters	$\Delta\rho_{min} = -0.33$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.22318 (4)	0.34233 (3)	0.23436 (3)	0.04290 (12)
O1	0.31603 (13)	0.42516 (11)	0.22844 (9)	0.0597 (3)
O2	0.26854 (14)	0.24114 (10)	0.21807 (9)	0.0583 (3)
O3	0.05279 (16)	0.40881 (12)	0.65463 (10)	0.0754 (5)
O4	0.37370 (15)	0.46654 (12)	0.63655 (13)	0.0749 (4)
O5	0.21527 (16)	0.58575 (10)	0.66369 (11)	0.0693 (4)
N1	0.17082 (13)	0.34280 (9)	0.34772 (9)	0.0388 (3)
C1	0.07099 (16)	0.36573 (12)	0.15947 (10)	0.0417 (3)
C2	0.0143 (2)	0.28885 (14)	0.10043 (15)	0.0578 (4)
H2	0.0542	0.2245	0.1016	0.069*
C3	−0.1034 (2)	0.31005 (19)	0.03940 (17)	0.0715 (6)
H3	−0.1422	0.2597	−0.0018	0.086*
C4	−0.1632 (2)	0.40435 (17)	0.03917 (16)	0.0676 (5)
H4	−0.2431	0.4172	−0.0014	0.081*
C5	−0.1066 (2)	0.47999 (17)	0.09798 (16)	0.0680 (5)
H5	−0.1480	0.5438	0.0972	0.082*
C6	0.0123 (2)	0.46155 (14)	0.15871 (13)	0.0546 (4)
H6	0.0520	0.5128	0.1983	0.066*
C7	0.19316 (14)	0.41714 (11)	0.42039 (10)	0.0371 (3)
C8	0.12836 (14)	0.38506 (11)	0.49973 (10)	0.0364 (3)
C9	0.05878 (14)	0.29003 (10)	0.47616 (10)	0.0357 (3)
C10	−0.01968 (16)	0.22449 (12)	0.52925 (11)	0.0446 (3)
H10	−0.0400	0.2408	0.5920	0.054*
C11	−0.06630 (19)	0.13474 (13)	0.48590 (14)	0.0539 (4)
H11	−0.1192	0.0903	0.5199	0.065*
C12	−0.0356 (2)	0.10986 (14)	0.39263 (14)	0.0564 (4)
H12	−0.0681	0.0487	0.3655	0.068*
C13	0.04189 (19)	0.17325 (13)	0.33887 (12)	0.0500 (4)
H13	0.0624	0.1560	0.2764	0.060*
C14	0.08790 (15)	0.26386 (11)	0.38203 (10)	0.0370 (3)

C15	0.2699 (2)	0.51382 (13)	0.40713 (13)	0.0523 (4)
H15A	0.2545	0.5597	0.4592	0.078*
H15B	0.2373	0.5443	0.3462	0.078*
H15C	0.3674	0.4997	0.4075	0.078*
C16	0.13428 (16)	0.43055 (12)	0.59581 (11)	0.0440 (3)
C17	0.25701 (18)	0.49730 (13)	0.63227 (12)	0.0484 (4)
C18	0.3215 (3)	0.6517 (2)	0.7133 (2)	0.0904 (8)
H18A	0.2796	0.6933	0.7609	0.109*
H18B	0.3928	0.6101	0.7474	0.109*
C19	0.3829 (4)	0.7157 (2)	0.6453 (3)	0.1093 (11)
H19A	0.4346	0.6749	0.6034	0.164*
H19B	0.4440	0.7634	0.6797	0.164*
H19C	0.3113	0.7519	0.6070	0.164*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.03753 (19)	0.0552 (2)	0.03706 (19)	0.00035 (15)	0.00942 (14)	−0.00083 (15)
O1	0.0494 (6)	0.0800 (9)	0.0516 (7)	−0.0196 (6)	0.0145 (5)	0.0025 (6)
O2	0.0546 (7)	0.0659 (8)	0.0556 (7)	0.0185 (6)	0.0124 (6)	−0.0068 (6)
O3	0.0830 (10)	0.0882 (11)	0.0598 (8)	−0.0327 (8)	0.0346 (7)	−0.0305 (7)
O4	0.0513 (8)	0.0735 (10)	0.0966 (12)	0.0002 (7)	−0.0132 (7)	−0.0058 (8)
O5	0.0733 (9)	0.0544 (8)	0.0792 (10)	−0.0107 (6)	0.0011 (7)	−0.0210 (7)
N1	0.0429 (6)	0.0405 (6)	0.0335 (5)	−0.0052 (5)	0.0057 (5)	−0.0013 (5)
C1	0.0420 (7)	0.0498 (8)	0.0342 (6)	0.0002 (6)	0.0075 (5)	−0.0003 (6)
C2	0.0576 (10)	0.0490 (9)	0.0651 (11)	−0.0013 (8)	−0.0049 (8)	−0.0049 (8)
C3	0.0626 (12)	0.0702 (13)	0.0780 (14)	−0.0122 (10)	−0.0152 (10)	−0.0110 (11)
C4	0.0507 (10)	0.0789 (14)	0.0708 (13)	0.0028 (10)	−0.0082 (9)	0.0054 (11)
C5	0.0670 (12)	0.0669 (12)	0.0688 (12)	0.0197 (10)	−0.0020 (10)	0.0006 (10)
C6	0.0629 (11)	0.0533 (10)	0.0470 (9)	0.0080 (8)	0.0011 (8)	−0.0075 (7)
C7	0.0357 (6)	0.0361 (7)	0.0392 (7)	−0.0022 (5)	0.0022 (5)	−0.0003 (5)
C8	0.0362 (6)	0.0362 (6)	0.0368 (6)	−0.0011 (5)	0.0032 (5)	−0.0026 (5)
C9	0.0332 (6)	0.0374 (7)	0.0363 (6)	−0.0025 (5)	0.0018 (5)	−0.0004 (5)
C10	0.0435 (8)	0.0490 (8)	0.0419 (7)	−0.0093 (6)	0.0072 (6)	0.0007 (6)
C11	0.0547 (9)	0.0502 (9)	0.0570 (10)	−0.0180 (7)	0.0062 (8)	0.0049 (7)
C12	0.0657 (11)	0.0451 (9)	0.0575 (10)	−0.0182 (8)	0.0005 (8)	−0.0070 (7)
C13	0.0599 (10)	0.0465 (8)	0.0436 (8)	−0.0096 (7)	0.0049 (7)	−0.0082 (6)
C14	0.0370 (6)	0.0371 (7)	0.0366 (6)	−0.0032 (5)	0.0020 (5)	0.0000 (5)
C15	0.0599 (10)	0.0434 (8)	0.0541 (9)	−0.0150 (7)	0.0090 (8)	0.0007 (7)
C16	0.0465 (8)	0.0431 (8)	0.0429 (7)	−0.0048 (6)	0.0066 (6)	−0.0088 (6)
C17	0.0514 (9)	0.0490 (8)	0.0435 (8)	−0.0063 (7)	−0.0031 (7)	−0.0027 (7)
C18	0.114 (2)	0.0722 (16)	0.0828 (17)	−0.0360 (14)	−0.0062 (15)	−0.0201 (12)
C19	0.109 (2)	0.0856 (19)	0.127 (3)	−0.0298 (17)	−0.028 (2)	0.0274 (17)

Geometric parameters (Å, °)

S1—O1	1.4185 (13)	C8—C9	1.4433 (19)
S1—O2	1.4251 (13)	C8—C16	1.452 (2)
S1—N1	1.6854 (12)	C9—C14	1.3960 (19)

S1—C1	1.7520 (16)	C9—C10	1.3967 (19)
O3—C16	1.2130 (19)	C10—C11	1.382 (2)
O4—C17	1.195 (2)	C10—H10	0.9300
O5—C17	1.317 (2)	C11—C12	1.385 (3)
O5—C18	1.468 (3)	C11—H11	0.9300
N1—C7	1.4042 (18)	C12—C13	1.379 (2)
N1—C14	1.4178 (18)	C12—H12	0.9300
C1—C6	1.382 (2)	C13—C14	1.389 (2)
C1—C2	1.382 (2)	C13—H13	0.9300
C2—C3	1.385 (3)	C15—H15A	0.9600
C2—H2	0.9300	C15—H15B	0.9600
C3—C4	1.368 (3)	C15—H15C	0.9600
C3—H3	0.9300	C16—C17	1.527 (2)
C4—C5	1.368 (3)	C18—C19	1.427 (4)
C4—H4	0.9300	C18—H18A	0.9700
C5—C6	1.385 (3)	C18—H18B	0.9700
C5—H5	0.9300	C19—H19A	0.9600
C6—H6	0.9300	C19—H19B	0.9600
C7—C8	1.3738 (19)	C19—H19C	0.9600
C7—C15	1.492 (2)		
O1—S1—O2	120.22 (8)	C11—C10—H10	120.9
O1—S1—N1	107.01 (7)	C9—C10—H10	120.9
O2—S1—N1	105.72 (7)	C10—C11—C12	121.10 (15)
O1—S1—C1	109.57 (8)	C10—C11—H11	119.4
O2—S1—C1	108.98 (8)	C12—C11—H11	119.4
N1—S1—C1	104.09 (6)	C13—C12—C11	121.79 (16)
C17—O5—C18	116.98 (19)	C13—C12—H12	119.1
C7—N1—C14	109.15 (11)	C11—C12—H12	119.1
C7—N1—S1	128.74 (10)	C12—C13—C14	117.18 (15)
C14—N1—S1	122.06 (10)	C12—C13—H13	121.4
C6—C1—C2	121.39 (16)	C14—C13—H13	121.4
C6—C1—S1	119.23 (13)	C13—C14—C9	121.89 (13)
C2—C1—S1	119.36 (13)	C13—C14—N1	130.91 (13)
C1—C2—C3	118.37 (18)	C9—C14—N1	107.17 (12)
C1—C2—H2	120.8	C7—C15—H15A	109.5
C3—C2—H2	120.8	C7—C15—H15B	109.5
C4—C3—C2	120.57 (19)	H15A—C15—H15B	109.5
C4—C3—H3	119.7	C7—C15—H15C	109.5
C2—C3—H3	119.7	H15A—C15—H15C	109.5
C3—C4—C5	120.70 (19)	H15B—C15—H15C	109.5
C3—C4—H4	119.7	O3—C16—C8	122.50 (15)
C5—C4—H4	119.7	O3—C16—C17	116.49 (14)
C4—C5—C6	120.06 (19)	C8—C16—C17	120.47 (13)
C4—C5—H5	120.0	O4—C17—O5	126.67 (17)
C6—C5—H5	120.0	O4—C17—C16	121.70 (16)
C1—C6—C5	118.90 (17)	O5—C17—C16	111.42 (15)
C1—C6—H6	120.6	C19—C18—O5	110.8 (2)
C5—C6—H6	120.6	C19—C18—H18A	109.5
C8—C7—N1	107.63 (12)	O5—C18—H18A	109.5

C8—C7—C15	128.71 (14)	C19—C18—H18B	109.5
N1—C7—C15	123.62 (13)	O5—C18—H18B	109.5
C7—C8—C9	108.77 (12)	H18A—C18—H18B	108.1
C7—C8—C16	128.08 (13)	C18—C19—H19A	109.5
C9—C8—C16	122.96 (13)	C18—C19—H19B	109.5
C14—C9—C10	119.87 (13)	H19A—C19—H19B	109.5
C14—C9—C8	107.22 (12)	C18—C19—H19C	109.5
C10—C9—C8	132.83 (13)	H19A—C19—H19C	109.5
C11—C10—C9	118.15 (15)	H19B—C19—H19C	109.5
O1—S1—N1—C7	9.30 (15)	C16—C8—C9—C14	−173.10 (14)
O2—S1—N1—C7	138.55 (13)	C7—C8—C9—C10	178.99 (16)
C1—S1—N1—C7	−106.67 (14)	C16—C8—C9—C10	3.6 (3)
O1—S1—N1—C14	−173.50 (12)	C14—C9—C10—C11	0.0 (2)
O2—S1—N1—C14	−44.24 (14)	C8—C9—C10—C11	−176.40 (16)
C1—S1—N1—C14	70.53 (13)	C9—C10—C11—C12	0.4 (3)
O1—S1—C1—C6	−42.83 (15)	C10—C11—C12—C13	−0.3 (3)
O2—S1—C1—C6	−176.23 (13)	C11—C12—C13—C14	−0.2 (3)
N1—S1—C1—C6	71.33 (14)	C12—C13—C14—C9	0.6 (3)
O1—S1—C1—C2	135.39 (14)	C12—C13—C14—N1	178.30 (16)
O2—S1—C1—C2	1.99 (16)	C10—C9—C14—C13	−0.5 (2)
N1—S1—C1—C2	−110.45 (14)	C8—C9—C14—C13	176.71 (15)
C6—C1—C2—C3	0.3 (3)	C10—C9—C14—N1	−178.69 (13)
S1—C1—C2—C3	−177.86 (16)	C8—C9—C14—N1	−1.45 (16)
C1—C2—C3—C4	−1.2 (3)	C7—N1—C14—C13	−177.75 (16)
C2—C3—C4—C5	1.1 (4)	S1—N1—C14—C13	4.6 (2)
C3—C4—C5—C6	−0.1 (4)	C7—N1—C14—C9	0.18 (16)
C2—C1—C6—C5	0.7 (3)	S1—N1—C14—C9	−177.51 (10)
S1—C1—C6—C5	178.83 (15)	C7—C8—C16—O3	165.01 (17)
C4—C5—C6—C1	−0.8 (3)	C9—C8—C16—O3	−20.6 (3)
C14—N1—C7—C8	1.23 (16)	C7—C8—C16—C17	−23.7 (2)
S1—N1—C7—C8	178.72 (11)	C9—C8—C16—C17	150.71 (15)
C14—N1—C7—C15	−176.61 (14)	C18—O5—C17—O4	−3.1 (3)
S1—N1—C7—C15	0.9 (2)	C18—O5—C17—C16	171.70 (18)
N1—C7—C8—C9	−2.13 (16)	O3—C16—C17—O4	114.6 (2)
C15—C7—C8—C9	175.57 (15)	C8—C16—C17—O4	−57.2 (2)
N1—C7—C8—C16	172.93 (14)	O3—C16—C17—O5	−60.5 (2)
C15—C7—C8—C16	−9.4 (3)	C8—C16—C17—O5	127.69 (16)
C7—C8—C9—C14	2.26 (16)	C17—O5—C18—C19	89.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O3^{i}	0.93	2.56	3.197 (2)	126
C2—H2···O2	0.93	2.52	2.897 (2)	104
C10—H10···O3	0.93	2.51	3.026 (2)	115
C13—H13···O2	0.93	2.48	3.001 (2)	116
C15—H15B···O1	0.96	2.43	2.798 (2)	103
C3—H3···Cg1^{ii}	0.93	2.70	3.524	148

C4—H4···Cg2^{ii}	0.93	2.90	3.619	135

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

Fig. 1

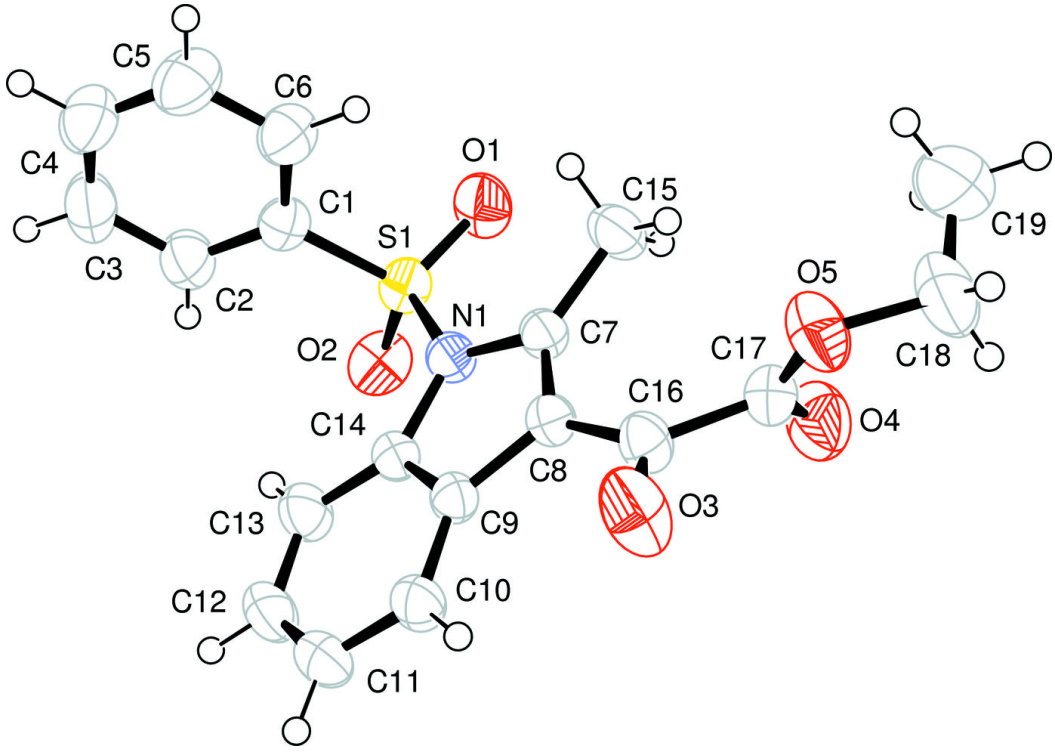

Fig. 2