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Ethyl 2-(bromomethyl)-5-methoxy-1-phenylsulfonyl-1*H*-indole-3-carboxylate

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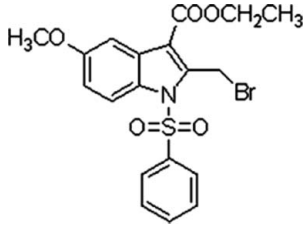
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.045; wR factor = 0.127; data-to-parameter ratio = 24.3.

In the title compound, $C_{19}H_{18}BrNO_5S$, the plane of the phenyl ring forms a dihedral angle of 76.99 (6)° with the indole ring system. The Br atom is disordered over two positions, with site-occupancy factors of 0.833 (14) and 0.167 (14). The molecular structure is stabilized by weak intramolecular C—H···O interactions and the crystal packing is stabilized by weak intermolecular C—H···O interactions.

Related literature

For biological activity, see: Nieto *et al.* (2005); Yang *et al.* (2002). For the structures of closely related compounds, see: Chakkaravarthi *et al.* (2007, 2008).



Experimental

Crystal data

$C_{19}H_{18}BrNO_5S$
M_r = 452.31
Triclinic, $P\overline{1}$
a = 8.9988 (3) Å
b = 9.2343 (2) Å
c = 11.6068 (3) Å
α = 82.524 (1)°
β = 87.666 (2)°
γ = 84.942 (3)°
V = 952.16 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.30 mm^{-1}
T = 295 (2) K
0.20 × 0.20 × 0.16 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.593, T_{max} = 0.692
25160 measured reflections
6169 independent reflections
4163 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.127
S = 1.03
6169 reflections
254 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.89 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O1^{i}	0.93	2.56	3.472 (3)	165
C2—H2···O5^{ii}	0.93	2.60	3.235 (3)	126
C6—H6···O2	0.93	2.54	2.908 (4)	104
C10—H10···O4	0.93	2.37	2.892 (3)	116
C13—H13···O1	0.93	2.28	2.863 (3)	120
C15—H15*A*···O5	0.97	2.31	2.911 (4)	119
C15—H15*D*···O2	0.97	2.16	2.895 (4)	131

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); 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: RK2082).

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supplementary materials

Acta Cryst. (2008). E**64**, o732 [**doi:10.1107/S1600536808007319**]

Ethyl 2-(bromomethyl)-5-methoxy-1-phenylsulfonyl-1*H*-indole-3-carboxylate

G. Chakkaravarthi, R. Sureshbabu, A. K. Mohanakrishnan and V. Manivannan

Comment

In continuation of our studies of benzenesulfonamide derivatives, which are known to exhibit anti–bacterial (Nieto *et al.*, 2005) anti–tumour (Yang *et al.*, 2002) activities, we report the crystal structure of the title compound (**I**). The geometric parameters of the molecule of **I** (Fig. 1) agree well with the reported structures (Chakkaravarthi *et al.*, 2007; Chakkaravarthi *et al.*, 2008).

The plane of the phenyl ring forms a dihedral angle of 76.99 (6)° with the indole ring system. The N1—S1—C1 plane is orthogonal to indole ring (dihedral angle 88.70 (7)°) and makes 75.97 (9)° with the phenyl ring. The plane of indole ring is almost coplanar (dihedral angle 2.66 (7)°) with the ester group and makes 6.33 (18)° with the methoxy group.

The torsion angles O2–S1–N1–C7 and O1–S1–N1–C14 [-30.0 (2)° and 27.3 (2)°, respectively] indicate *syn*–conformation of the sulfonyl moiety. The Br1 atom is disordered over two positions with the site occupancy factors of 0.833 (14) and 0.167 (14). The molecular packing is stabilized by weak intramolecular C—H···O interactions and the crystal packing of **I** (Fig. 2) is stabilized by weak intermolecular C—H···O interactions (see Table).

Experimental

Ethyl 2-(methyl)-5-methoxy-1-(phenylsulfonyl)-1*H*-indole-3-carboxylate (1g, 2.2 mmol), *N*–bromo succinimide (0.4 g, 2.3 mmol), azo–bis–isobutyronitrile (50 mg) were dissolved in 50 ml of carbon tetrachloride. Refluxed on a waterbath for 2hr. Cooled to room temperature. Succinimide was filtered off over sodium sulfate. Filtrate was evaporated under reduced pressure. Product was recrystallized from methanol. Yield: 78%.

Refinement

The 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. The site occupancy factors for disordered Br atom is refined as Br1= 0.833 (14) and Br1A = 0.167 (14) during anisotropic refinement. The C15—Br1A distance was restrained to 1.91 (10) Å. The anisotropic displacement parameters of Br1 and Br1A were set equal by the command EADP and the anisotropic thermal parameters of C4, C5, C15 and Br1A atoms were restrained with DELU in the final cycles of refinement (Sheldrick, 2008).

Figures

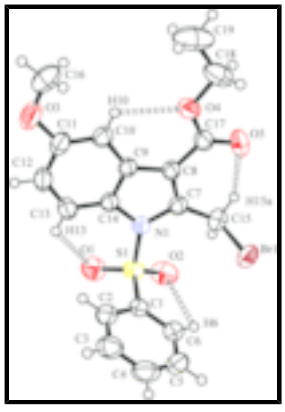


Fig. 1. The molecular structure of **I**, with atom labeling scheme. Displacement ellipsoids are drawn at 50% probability level. H atoms are presented as a small spheres of arbitrary radius. Only major fragment for disordered Br1 and C15 are drawn. Intramolecular H–bonds are shown as dashed lines.

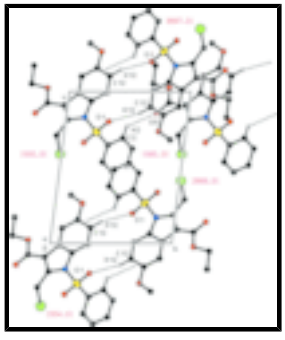


Fig. 2. The packing of **I**, viewed down the *a* axis. Intermolecular H–bonds are shown as dashed lines H atoms not involving hydrogen bonding have been omitted for clarity. [Symmetry codes: (i) -*x*+1, -*y*+1, -*z*+2; (ii) *x*, *y*+1, *z*].

Ethyl 2-(bromomethyl)-5-methoxy-1-phenylsulfonyl-1*H*-indole-3-carboxylate

Crystal data

$C_{19}H_{18}BrNO_5S$	$Z = 2$
$M_r = 452.31$	$F_{000} = 460$
Triclinic, $P\overline{1}$	$D_x = 1.578$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.9988$ (3) Å	Cell parameters from 8207 reflections
$b = 9.2343$ (2) Å	$\theta = 2.2$–$27.5°$
$c = 11.6068$ (3) Å	$\mu = 2.30$ mm^{-1}
$\alpha = 82.524$ (1)°	$T = 295$ (2) K
$\beta = 87.666$ (2)°	Block, colourless
$\gamma = 84.942$ (3)°	0.20 × 0.20 × 0.16 mm
$V = 952.16$ (5) Å^3	

Data collection

Bruker Kappa APEXII diffractometer	6169 independent reflections
Radiation source: Fine–focus sealed tube	4163 reflections with $I > 2\sigma(I)$
Monochromator: Graphite	$R_{int} = 0.027$

T = 295(2) K

ω and φ scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

T_{min} = 0.593, T_{max} = 0.692

25160 measured reflections

θ_{max} = 31.2º

θ_{min} = 1.8º

h = −13→13

k = −13→13

l = −16→16

Refinement

Refinement on F^2

Least-squares matrix: Full

$R[F^2 > 2\sigma(F^2)]$ = 0.044

$wR(F^2)$ = 0.127

S = 1.04

6169 reflections

254 parameters

3 restraints

Primary atom site location: Direct

Secondary atom site location: Difmap

Hydrogen site location: Geom

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 0.4811P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max}$ = 0.68 e Å^{-3}

$\Delta\rho_{min}$ = −0.89 e Å^{-3}

Extinction correction: None

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	0.2859 (3)	−0.0105 (2)	0.5880 (3)	0.0695 (4)	0.833 (14)
Br1A	0.2613 (8)	0.0063 (7)	0.6105 (7)	0.0695 (4)	0.167 (14)
S1	0.53695 (6)	0.26331 (6)	0.73409 (5)	0.04656 (14)	
O1	0.6066 (2)	0.3534 (2)	0.80232 (18)	0.0623 (5)	
O2	0.6249 (2)	0.1714 (2)	0.66452 (19)	0.0688 (6)	
O3	0.1927 (3)	0.2237 (2)	1.26357 (17)	0.0714 (6)	
O4	0.1493 (2)	−0.18350 (18)	1.02343 (16)	0.0551 (4)	
O5	0.2440 (3)	−0.2589 (2)	0.8592 (2)	0.0783 (6)	
N1	0.4384 (2)	0.15286 (19)	0.82973 (15)	0.0410 (4)	
C1	0.4041 (2)	0.3722 (2)	0.64784 (18)	0.0407 (4)	
C2	0.3253 (3)	0.4881 (3)	0.6931 (2)	0.0499 (5)	
H2	0.3405	0.5062	0.7686	0.060*	
C3	0.2243 (3)	0.5759 (3)	0.6245 (3)	0.0627 (7)	
H3	0.1703	0.6545	0.6537	0.075*	
C4	0.2020 (4)	0.5490 (3)	0.5135 (3)	0.0690 (7)	
H4	0.1321	0.6085	0.4682	0.083*	
C5	0.2818 (4)	0.4352 (3)	0.4690 (2)	0.0693 (7)	
H5	0.2663	0.4178	0.3935	0.083*	
C6	0.3860 (3)	0.3453 (3)	0.5360 (2)	0.0561 (6)	
H6	0.4422	0.2688	0.5058	0.067*	
C7	0.3878 (2)	0.0171 (2)	0.81460 (18)	0.0412 (4)	
C8	0.3026 (2)	−0.0297 (2)	0.90984 (18)	0.0393 (4)	
C9	0.2973 (2)	0.0781 (2)	0.98934 (17)	0.0380 (4)	
C10	0.2300 (3)	0.0839 (3)	1.10015 (19)	0.0452 (5)	

H10	0.1742	0.0093	1.1353	0.054*	
C11	0.2498 (3)	0.2044 (3)	1.1549 (2)	0.0510 (5)	
C12	0.3333 (3)	0.3160 (3)	1.1024 (2)	0.0555 (6)	
H12	0.3444	0.3958	1.1417	0.067*	
C13	0.3993 (3)	0.3117 (3)	0.9951 (2)	0.0516 (5)	
H13	0.4547	0.3871	0.9607	0.062*	
C14	0.3808 (2)	0.1902 (2)	0.93842 (18)	0.0399 (4)	
C15	0.4242 (3)	−0.0591 (3)	0.7108 (2)	0.0560 (5)	
H15A	0.4287	−0.1640	0.7346	0.067*	0.833 (14)
H15B	0.5226	−0.0356	0.6808	0.067*	0.833 (14)
H15C	0.4302	−0.1646	0.7312	0.067*	0.167 (14)
H15D	0.5176	−0.0306	0.6736	0.067*	0.167 (14)
C16	0.0958 (4)	0.1221 (4)	1.3175 (3)	0.0719 (8)	
H16A	0.0109	0.1221	1.2700	0.108*	
H16B	0.0630	0.1487	1.3922	0.108*	
H16C	0.1474	0.0259	1.3271	0.108*	
C17	0.2311 (3)	−0.1686 (2)	0.9262 (2)	0.0470 (5)	
C18	0.0781 (3)	−0.3188 (3)	1.0520 (3)	0.0738 (9)	
H18A	0.1507	−0.4023	1.0488	0.089*	
H18B	0.0008	−0.3243	0.9972	0.089*	
C19	0.0120 (4)	−0.3191 (5)	1.1716 (4)	0.1037 (15)	
H19A	0.0896	−0.3150	1.2252	0.156*	
H19B	−0.0375	−0.4070	1.1930	0.156*	
H19C	−0.0589	−0.2354	1.1739	0.156*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0960 (5)	0.0791 (4)	0.0381 (5)	−0.0300 (4)	−0.0142 (5)	−0.0064 (4)
Br1A	0.0960 (5)	0.0791 (4)	0.0381 (5)	−0.0300 (4)	−0.0142 (5)	−0.0064 (4)
S1	0.0417 (3)	0.0457 (3)	0.0503 (3)	−0.0032 (2)	0.0003 (2)	0.0003 (2)
O1	0.0509 (10)	0.0655 (11)	0.0719 (12)	−0.0198 (8)	−0.0153 (8)	0.0002 (9)
O2	0.0616 (11)	0.0617 (11)	0.0763 (13)	0.0099 (9)	0.0226 (10)	−0.0013 (10)
O3	0.0890 (15)	0.0806 (14)	0.0485 (10)	−0.0023 (11)	0.0037 (10)	−0.0285 (10)
O4	0.0634 (10)	0.0476 (9)	0.0544 (10)	−0.0169 (8)	−0.0054 (8)	0.0019 (7)
O5	0.1144 (18)	0.0565 (11)	0.0729 (13)	−0.0309 (11)	0.0018 (12)	−0.0271 (10)
N1	0.0493 (10)	0.0366 (8)	0.0368 (9)	−0.0027 (7)	−0.0047 (7)	−0.0028 (7)
C1	0.0475 (11)	0.0364 (10)	0.0378 (10)	−0.0087 (8)	−0.0007 (8)	0.0004 (8)
C2	0.0592 (14)	0.0448 (12)	0.0446 (12)	−0.0003 (10)	−0.0010 (10)	−0.0046 (9)
C3	0.0667 (17)	0.0526 (14)	0.0643 (17)	0.0067 (12)	−0.0043 (13)	0.0026 (12)
C4	0.0731 (18)	0.0632 (15)	0.0666 (17)	−0.0116 (12)	−0.0220 (14)	0.0176 (12)
C5	0.100 (2)	0.0681 (16)	0.0423 (13)	−0.0282 (13)	−0.0172 (13)	0.0013 (11)
C6	0.0832 (18)	0.0457 (12)	0.0405 (12)	−0.0136 (12)	0.0018 (12)	−0.0054 (9)
C7	0.0482 (11)	0.0377 (10)	0.0378 (10)	0.0006 (8)	−0.0085 (9)	−0.0055 (8)
C8	0.0470 (11)	0.0349 (9)	0.0367 (10)	−0.0014 (8)	−0.0108 (8)	−0.0048 (7)
C9	0.0435 (10)	0.0352 (9)	0.0349 (9)	0.0020 (8)	−0.0096 (8)	−0.0046 (7)
C10	0.0501 (12)	0.0476 (12)	0.0379 (10)	−0.0016 (9)	−0.0074 (9)	−0.0051 (9)
C11	0.0588 (14)	0.0557 (13)	0.0393 (11)	0.0059 (11)	−0.0081 (10)	−0.0143 (10)

C12	0.0738 (17)	0.0448 (12)	0.0515 (13)	−0.0005 (11)	−0.0141 (12)	−0.0183 (10)
C13	0.0666 (15)	0.0386 (11)	0.0517 (13)	−0.0078 (10)	−0.0130 (11)	−0.0074 (9)
C14	0.0467 (11)	0.0357 (10)	0.0373 (10)	0.0005 (8)	−0.0099 (8)	−0.0045 (8)
C15	0.0730 (15)	0.0533 (14)	0.0440 (12)	−0.0058 (11)	0.0002 (9)	−0.0152 (10)
C16	0.0666 (18)	0.097 (2)	0.0486 (15)	0.0153 (16)	0.0053 (13)	−0.0143 (15)
C17	0.0561 (13)	0.0395 (11)	0.0464 (12)	−0.0060 (9)	−0.0160 (10)	−0.0033 (9)
C18	0.0631 (16)	0.0593 (16)	0.096 (2)	−0.0238 (13)	−0.0233 (16)	0.0205 (15)
C19	0.065 (2)	0.128 (3)	0.105 (3)	−0.030 (2)	−0.0010 (19)	0.048 (3)

Geometric parameters (Å, °)

Br1—C15	1.914 (3)	C7—C15	1.484 (3)
Br1A—C15	1.9152 (10)	C8—C9	1.439 (3)
S1—O2	1.417 (2)	C8—C17	1.472 (3)
S1—O1	1.419 (2)	C9—C14	1.389 (3)
S1—N1	1.6862 (19)	C9—C10	1.405 (3)
S1—C1	1.751 (2)	C10—C11	1.379 (3)
O3—C11	1.370 (3)	C10—H10	0.9300
O3—C16	1.407 (4)	C11—C12	1.390 (4)
O4—C17	1.320 (3)	C12—C13	1.362 (4)
O4—C18	1.448 (3)	C12—H12	0.9300
O5—C17	1.208 (3)	C13—C14	1.398 (3)
N1—C7	1.405 (3)	C13—H13	0.9300
N1—C14	1.417 (3)	C15—H15A	0.9700
C1—C6	1.372 (3)	C15—H15B	0.9700
C1—C2	1.381 (3)	C15—H15C	0.9700
C2—C3	1.371 (4)	C15—H15D	0.9700
C2—H2	0.9300	C16—H16A	0.9600
C3—C4	1.369 (4)	C16—H16B	0.9600
C3—H3	0.9300	C16—H16C	0.9600
C4—C5	1.365 (5)	C18—C19	1.487 (5)
C4—H4	0.9300	C18—H18A	0.9700
C5—C6	1.388 (4)	C18—H18B	0.9700
C5—H5	0.9300	C19—H19A	0.9600
C6—H6	0.9300	C19—H19B	0.9600
C7—C8	1.364 (3)	C19—H19C	0.9600
O2—S1—O1	120.09 (13)	C11—C12—H12	119.1
O2—S1—N1	106.72 (11)	C12—C13—C14	117.7 (2)
O1—S1—N1	105.29 (11)	C12—C13—H13	121.1
O2—S1—C1	109.30 (12)	C14—C13—H13	121.1
O1—S1—C1	108.93 (11)	C9—C14—C13	121.2 (2)
N1—S1—C1	105.49 (10)	C9—C14—N1	107.98 (17)
C11—O3—C16	117.9 (2)	C13—C14—N1	130.8 (2)
C17—O4—C18	117.3 (2)	C7—C15—Br1	114.7 (2)
C7—N1—C14	107.77 (17)	C7—C15—Br1A	103.7 (4)
C7—N1—S1	127.88 (15)	C7—C15—H15A	108.6
C14—N1—S1	124.15 (15)	Br1—C15—H15A	108.6
C6—C1—C2	121.7 (2)	Br1A—C15—H15A	111.8
C6—C1—S1	119.67 (19)	C7—C15—H15B	108.6

C2—C1—S1	118.53 (18)	Br1—C15—H15B	108.6
C3—C2—C1	118.6 (2)	Br1A—C15—H15B	116.3
C3—C2—H2	120.7	H15A—C15—H15B	107.6
C1—C2—H2	120.7	C7—C15—H15C	111.1
C4—C3—C2	120.6 (3)	Br1—C15—H15C	107.3
C4—C3—H3	119.7	Br1A—C15—H15C	111.0
C2—C3—H3	119.7	H15B—C15—H15C	106.2
C5—C4—C3	120.4 (3)	C7—C15—H15D	111.1
C5—C4—H4	119.8	Br1—C15—H15D	102.7
C3—C4—H4	119.8	Br1A—C15—H15D	110.4
C4—C5—C6	120.3 (3)	H15A—C15—H15D	111.1
C4—C5—H5	119.8	H15C—C15—H15D	109.5
C6—C5—H5	119.8	O3—C16—H16A	109.5
C1—C6—C5	118.4 (3)	O3—C16—H16B	109.5
C1—C6—H6	120.8	H16A—C16—H16B	109.5
C5—C6—H6	120.8	O3—C16—H16C	109.5
C8—C7—N1	108.66 (18)	H16A—C16—H16C	109.5
C8—C7—C15	127.3 (2)	H16B—C16—H16C	109.5
N1—C7—C15	124.1 (2)	O5—C17—O4	123.3 (2)
C7—C8—C9	108.47 (18)	O5—C17—C8	124.7 (2)
C7—C8—C17	124.5 (2)	O4—C17—C8	112.02 (19)
C9—C8—C17	127.0 (2)	O4—C18—C19	107.3 (3)
C14—C9—C10	120.41 (19)	O4—C18—H18A	110.3
C14—C9—C8	107.12 (18)	C19—C18—H18A	110.3
C10—C9—C8	132.5 (2)	O4—C18—H18B	110.3
C11—C10—C9	117.5 (2)	C19—C18—H18B	110.3
C11—C10—H10	121.2	H18A—C18—H18B	108.5
C9—C10—H10	121.2	C18—C19—H19A	109.5
O3—C11—C10	123.9 (2)	C18—C19—H19B	109.5
O3—C11—C12	114.8 (2)	H19A—C19—H19B	109.5
C10—C11—C12	121.3 (2)	C18—C19—H19C	109.5
C13—C12—C11	121.8 (2)	H19A—C19—H19C	109.5
C13—C12—H12	119.1	H19B—C19—H19C	109.5
O2—S1—N1—C7	−30.0 (2)	C17—C8—C9—C10	1.3 (4)
O1—S1—N1—C7	−158.62 (19)	C14—C9—C10—C11	0.3 (3)
C1—S1—N1—C7	86.2 (2)	C8—C9—C10—C11	178.5 (2)
O2—S1—N1—C14	155.94 (18)	C16—O3—C11—C10	−6.6 (4)
O1—S1—N1—C14	27.3 (2)	C16—O3—C11—C12	174.3 (2)
C1—S1—N1—C14	−87.87 (18)	C9—C10—C11—O3	−179.0 (2)
O2—S1—C1—C6	8.6 (2)	C9—C10—C11—C12	0.0 (3)
O1—S1—C1—C6	141.6 (2)	O3—C11—C12—C13	179.0 (2)
N1—S1—C1—C6	−105.8 (2)	C10—C11—C12—C13	−0.1 (4)
O2—S1—C1—C2	−168.24 (19)	C11—C12—C13—C14	−0.1 (4)
O1—S1—C1—C2	−35.3 (2)	C10—C9—C14—C13	−0.5 (3)
N1—S1—C1—C2	77.3 (2)	C8—C9—C14—C13	−179.1 (2)
C6—C1—C2—C3	1.4 (4)	C10—C9—C14—N1	178.12 (19)
S1—C1—C2—C3	178.2 (2)	C8—C9—C14—N1	−0.5 (2)
C1—C2—C3—C4	0.1 (4)	C12—C13—C14—C9	0.4 (3)
C2—C3—C4—C5	−0.9 (5)	C12—C13—C14—N1	−177.8 (2)

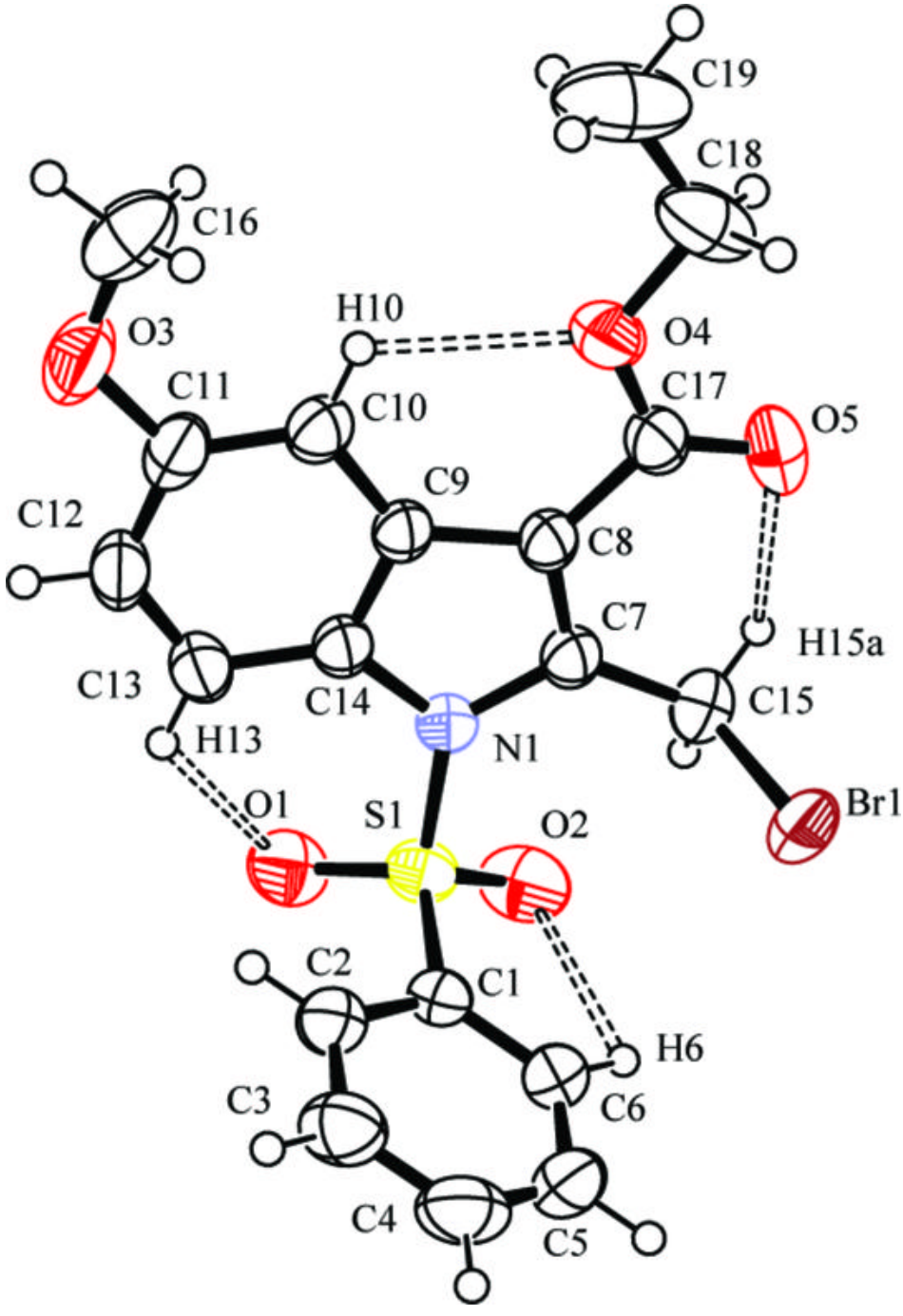
C3—C4—C5—C6	0.2 (5)	C7—N1—C14—C9	0.6 (2)
C2—C1—C6—C5	−2.1 (4)	S1—N1—C14—C9	175.69 (14)
S1—C1—C6—C5	−178.8 (2)	C7—N1—C14—C13	179.0 (2)
C4—C5—C6—C1	1.2 (4)	S1—N1—C14—C13	−5.9 (3)
C14—N1—C7—C8	−0.4 (2)	C8—C7—C15—Br1	90.2 (3)
S1—N1—C7—C8	−175.24 (15)	N1—C7—C15—Br1	−90.1 (2)
C14—N1—C7—C15	179.9 (2)	C8—C7—C15—Br1A	87.5 (3)
S1—N1—C7—C15	5.0 (3)	N1—C7—C15—Br1A	−92.8 (3)
N1—C7—C8—C9	0.0 (2)	C18—O4—C17—O5	2.9 (4)
C15—C7—C8—C9	179.8 (2)	C18—O4—C17—C8	−177.4 (2)
N1—C7—C8—C17	−179.39 (19)	C7—C8—C17—O5	2.7 (4)
C15—C7—C8—C17	0.4 (4)	C9—C8—C17—O5	−176.6 (2)
C7—C8—C9—C14	0.3 (2)	C7—C8—C17—O4	−176.9 (2)
C17—C8—C9—C14	179.7 (2)	C9—C8—C17—O4	3.8 (3)
C7—C8—C9—C10	−178.1 (2)	C17—O4—C18—C19	171.9 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O1^{i}	0.93	2.56	3.472 (3)	165
C2—H2···O5^{ii}	0.93	2.60	3.235 (3)	126
C6—H6···O2	0.93	2.54	2.908 (4)	104
C10—H10···O4	0.93	2.37	2.892 (3)	116
C13—H13···O1	0.93	2.28	2.863 (3)	120
C15—H15A···O5	0.97	2.31	2.911 (4)	119
C15—H15D···O2	0.97	2.16	2.895 (4)	131

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

Fig. 1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C18
C16
H10
O3
O4
C11
C10
C17
O5
C9
C12
C8
C7
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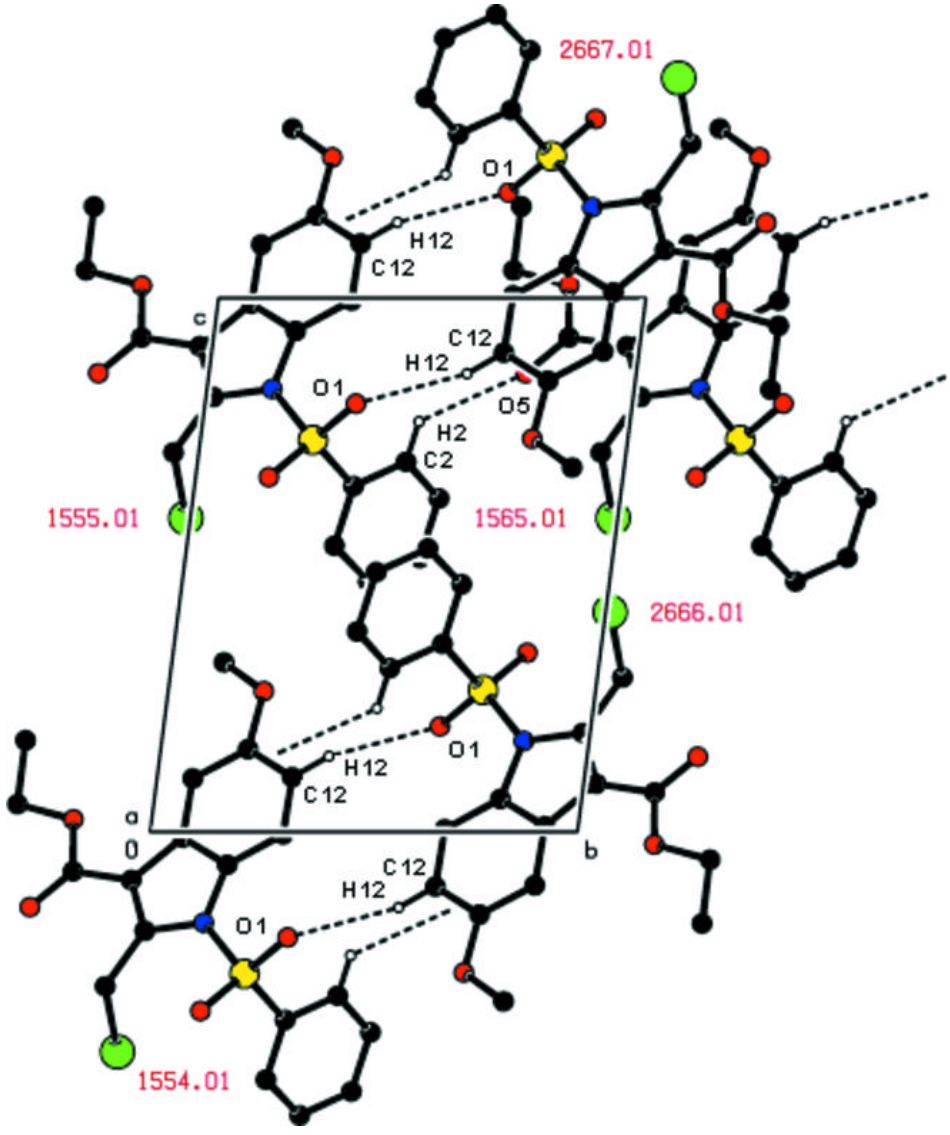
C13
C14
C15
H13
N1
O1
S1
O2
Br1
C2
C1
H6
C3
C6
C4
C5

Fig. 2


2667.01
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C12
c
C12
H12
O1
O5
H2
C2
1555.01
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O1
H12
C12
a
0
b
C12
H12
O1
1554.01