organic papers

Ethyl 2-{[N-(2-iodophenyl)phenylsulfonamido]-methyl}-1-phenylsulfonyl-1H-indole-3-carboxylate

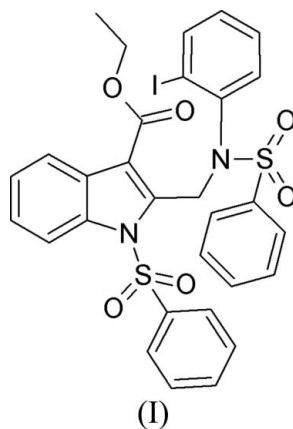**G. Senthil Kumar,ª K. Chinnakali,ª‡ N. Ramesh,ᵇ A. K. Mohanakrishnanᵇ and Hoong-Kun Funᶜ***

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In the title compound, $C_{31}H_{26}IN_2O_6S_2$, molecules are linked into a sheet parallel to the *bc* plane by C—H⋯O hydrogen bonds and C—H⋯π interactions. The sheets are interlinked *via* C—H⋯O hydrogen bonds.

Comment

N-(Phenylsulfonyl)indoles exhibit a high affinity towards the 5-HT6 receptor (Zhou *et al.*, 2005). Certain 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). We report here the structure of the title compound, (I).

(I)

The geometry of the phenylsulfonylindole system agrees with those reported for similar structures (Beddoes *et al.*, 1986; Senthil Kumar, Chinnakali, Balamurugan *et al.*, 2006*a,b*; Senthil Kumar, Chinnakali, Ramesh *et al.*, 2006*a,b,c*). Bond lengths and angles involving the S atom of the two phenyl-sufonyl groups present in the molecule agree with each other; the O—S—O, N—S—C and N—S—O angles deviate significantly from the ideal tetrahedral value (Table 1).

The indole ring system (N1/C1–C8) is planar to within 0.013 (1) Å. Atoms O3, C15, O4 and C16 of the ethyl-carboxylate substituent are coplanar, with an r.m.s. deviation of 0.009 Å. The C9–C14 and O3/C15/O4/C16 planes form dihedral angles of 78.99 (5) and 12.86 (9)°, respectively, with the indole ring system. The dihedral angle between the planes of the C19–C24 and C25–C30 benzene rings is 31.79 (6)°. The torsion angles describing the conformation of the group attached at C1 are given in Table 1.

The intramolecular C—H⋯O interactions (Table 2) involving the sulfonyl O1 and O2 atoms, and the carboxylate O3 and O4 atoms, generate rings of graph-set motif *S*(6)
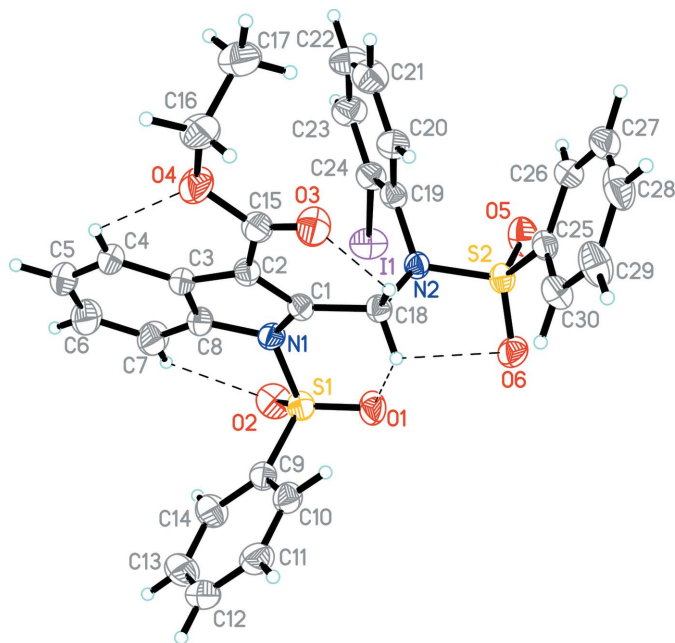
Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 80% probability level. Hydrogen bonds are shown as dashed lines.
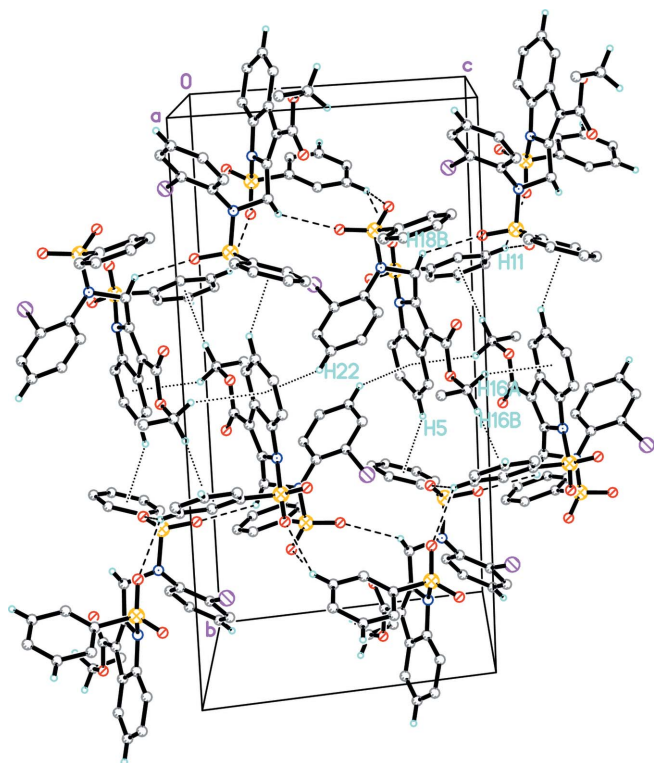

Figure 2
A view of a hydrogen-bonded sheet in (I). Dashed and dotted lines indicate C—H⋯O and C—H⋯π interactions, respectively. For the sake of clarity, H atoms not involved in hydrogen bonding have been omitted.

(Bernstein *et al.*, 1995) (Fig. 1). Glide-related molecules are linked through C11—H11⋯O1^i, C11—H11⋯O6^i and C18—H18B⋯O5^i hydrogen bonds, forming a chain along the c axis.

Adjacent chains are interconnected *via* C—H⋯π interactions involving the C25–C30 phenyl ring (centroid *Cg*1), the C3–C8 benzene ring (centroid *Cg*2) and the C9–C14 phenyl ring (centroid *Cg*3), leading to the formation of a sheet parallel to the *bc* plane (Fig. 2). Molecules in adjacent sheets are linked through C13—H13⋯O3^{ii} hydrogen bonds along the *a* axis. The symmetry codes are given in Table 2.

Experimental

Ethyl-1-phenylsulfonyl-2-methylindole-3-carboxylate (1.18 mmol) was added to a stirred suspension of 2-iodobenzenesulfonamide (1.11 mmol), potassium carbonate (2.4 mmol) and dimethyl-acetamide (10 ml). After 3 h, the reaction mixture was poured into ice–water; the precipitated solid was filtered off and dried with $CaCl_2$. It was recrystallized from ethyl acetate.

Crystal data

$C_{30}H_{25}IN_2O_6S_2$	$Z = 4$
$M_r = 700.56$	$D_x = 1.640$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 10.9098$ (2) Å	$\mu = 1.32$ mm^{-1}
$b = 22.7150$ (4) Å	$T = 100.0$ (1) K
$c = 11.8579$ (2) Å	Block, colourless
$\beta = 105.011$ (1)°	$0.58 \times 0.53 \times 0.29$ mm
$V = 2838.30$ (9) Å^3	

Data collection

Bruker SMART APEX2 CCD diffractometer	41126 measured reflections
ω scans	12373 independent reflections
Absorption correction: multi-scan	10729 reflections with $I > 2\sigma(I)$
(*SADABS*; Bruker, 2005)	$R_{int} = 0.021$
$T_{min} = 0.544$, $T_{max} = 0.699$	$\theta_{max} = 35.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0359P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.033$	$+ 3.3196P]$
$wR(F^2) = 0.088$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.002$
12373 reflections	$\Delta\rho_{max} = 2.87$ e Å^{-3}
371 parameters	$\Delta\rho_{min} = -1.11$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

I1—C24	2.0903 (16)	S2—N2	1.6587 (13)
S1—O1	1.4255 (13)	S2—C25	1.7648 (15)
S1—O2	1.4296 (13)	N1—C1	1.4118 (19)
S1—N1	1.6915 (13)	N1—C8	1.4198 (19)
S1—C9	1.7576 (16)	N2—C19	1.4420 (19)
S2—O6	1.4291 (13)	N2—C18	1.4907 (18)
S2—O5	1.4352 (12)		
O1—S1—O2	120.41 (8)	O5—S2—N2	105.65 (7)
O1—S1—N1	106.90 (7)	O6—S2—C25	107.03 (7)
O2—S1—N1	106.42 (7)	O5—S2—C25	108.07 (8)
O1—S1—C9	108.93 (8)	N2—S2—C25	107.82 (7)
O2—S1—C9	109.13 (8)	C19—N2—C18	117.32 (12)
N1—S1—C9	103.77 (7)	C19—N2—S2	116.28 (10)
O6—S2—O5	120.70 (8)	C18—N2—S2	115.16 (9)
O6—S2—N2	107.00 (7)		
C25—S2—N2—C18	−67.89 (12)	S2—N2—C18—C1	−164.98 (10)
C19—N2—C18—C1	52.53 (17)	N1—C1—C18—N2	66.85 (17)

Table 2
Hydrogen-bond geometry (Å, °).

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
C4—H4$\cdots$O4	0.95	2.41	2.932 (2)	114
C7—H7$\cdots$O2	0.95	2.35	2.958 (2)	121
C11—H11$\cdots$O1^i	0.95	2.49	3.150 (2)	127
C11—H11$\cdots$O6^i	0.95	2.38	3.159 (2)	139
C13—H13$\cdots$O3^{ii}	0.95	2.33	3.248 (2)	162
C18—H18$A\cdots$O3	0.99	2.25	2.981 (2)	130
C18—H18$B\cdots$O1	0.99	2.31	2.852 (2)	113
C18—H18$B\cdots$O6	0.99	2.48	2.9184 (18)	106
C18—H18$B\cdots$O5^i	0.99	2.55	3.1223 (18)	116
C5—H5$\cdots$Cg1^{iii}	0.95	2.63	3.4645 (17)	148
C16—H16$A\cdots$Cg2^{iv}	0.99	2.92	3.638 (2)	131
C16—H16$B\cdots$Cg3^{iv}	0.99	2.83	3.655 (2)	141
C22—H22$\cdots$Cg2^v	0.95	2.81	3.635 (2)	146

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x-1, y, z$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+1, -y+1, -z+2$; (v) $-x+1, -y+1, -z+1$.

The H atoms were positioned geometrically (C—H = 0.95–0.99 Å) and treated as riding on their parent atoms, with U_{iso}(H) = xU_{eq}(carrier atom), where x = 1.5 for methyl and 1.2 for other H atoms. The highest residual electron density peak is located 0.67 Å from atom C21 and the deepest hole is located 0.60 Å from atom I1.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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