3-(1-Phenylsulfonyl-2-methylindol-3-yl carbonyl)propanoic acid

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In the title compound, $C_{19}H_{17}NO_5S$, the indole system is not strictly planar and the dihedral angle between the fused rings is 2.1 (1)°. The indole and phenyl rings are orthogonal to each other and the dihedral angle between them is 87.2 (1)°. The molecules are joined into head-to-head dimers by hydrogen bonds involving the butyric acid groups. The centrosymmetrically related C—H···O hydrogen bond pattern joins the head-to-head dimers into chains running parallel to the c axis. Neighbouring chains are held together by weak C—H···π and π–π interactions.

Comment

Indole is an important heterocyclic compound whose ring system is present in a large number of natural products. Many of these natural products, as well as the synthetic derivatives, show a variety of useful biological properties, such as antibacterial (Okabe & Adachi, 1998), antitumour (Schollmeyer *et al.*, 1995), antidepressant (Grinev *et al.*, 1984), antimicrobial (El-Sayed *et al.*, 1986; Gadaginamath & Patil, 1999) and anti-inflammatory (Rodriguez *et al.*, 1985) activities. 4-(3-Indolyl)butyric acid (IBA) is known to possess growth-regulating activity (Steward & Kirkorian, 1971). IBA shows a root-promoting effect in all lemon and lime varieties (Sircar, 1971) and is also effective in bud inhibition in many plants. The interaction of phenylsulfonylindole with the calf-thymus DNA has also been studied by spectroscopic methods (Sivaraman *et al.*, 1996). Indoles have been proved to display high aldose reductase inhibitory activity (Rajeswaran *et al.*, 1999). The structure determination of the title compound, (I), was undertaken as part of our studies on indole derivatives.
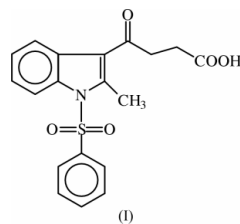
The indole system is not strictly planar and the dihedral angle formed by the pyrrole and benzene planes is 2.1 (1)°. The dihedral angle between the indole system and the phenyl ring is 87.2 (1)°. The 4-oxobutyric acid group is characterized by two planes, *viz.* the 3-oxopropyl group and the acid group. The plane of the indole system makes angles of 36.3 (1) and 68.2 (1)° with the 3-oxopropyl group and the acid group, respectively. Atoms S1, C16 and C17 deviate from the weighted least-squares plane through the indole system by
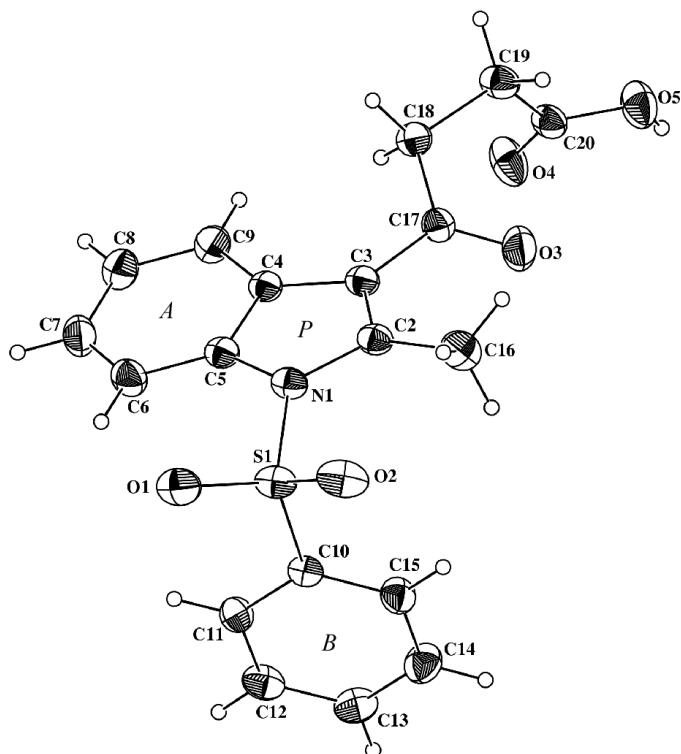
Figure 1
The molecular structure of the title compound, showing 35% probability displacement ellipsoids and the atom-numbering scheme.

Figure 2
The crystal structure of (I), viewed down the *a* axis.

−0.392 (1), 0.072 (3) and −0.108 (2) Å, respectively. Atom N1 deviates by 0.155 (2) Å from the plane passing through atoms C2, C5 and S1. This slight pyramidalization behaviour is also observed in related indole derivatives (Sankaranarayanan *et al.*, 2000, 2001). The bond angles around S1 show distorted tetrahedral geometry. The widening of the O1—S1—O2 angle [120.1 (1)°] from the tetrahedral value is presumably the result of repulsive interactions between the short S=O bonds. Similar observations have been noted in the related structure (Sankaranarayanan *et al.*, 2001). The S—C bond distance [1.757 (2) Å] agrees well with the literature value of 1.758 (13) Å (Allen *et al.*, 1987) and the S—N [1.698 (2) Å] bond distance is slightly longer than the literature value of 1.642 (24) Å (Allen *et al.*, 1987). The lengthening of the C—N distances in the pyrrole ring is due to the electron-withdrawing character of the phenylsulfonyl group. The 3-oxopropyl chain bond lengths and angles are in the expected ranges but its conformation is of interest. The torsion angles C2—C3—C17—O3, C4—C3—C17—C18, C3—C17—C18—C19, C17—C18—C19—C20, and C18—C19—C20—O4 are 24.3 (3), 24.7 (3), 171.8 (2), 79.6 (2) and 32.9 (3)°, respectively.

C—H⋯O interactions have been recognized as important secondary interactions and, in many cases, play a dominant role in the molecular conformation (Steiner, 1997). Four such intramolecular interactions can be identified in the present structure. The conformation of the aliphatic chain is governed by two C—H⋯O intramolecular interactions. Evidence for steric strain is seen at the point where the phenylsulfonyl group joins the indole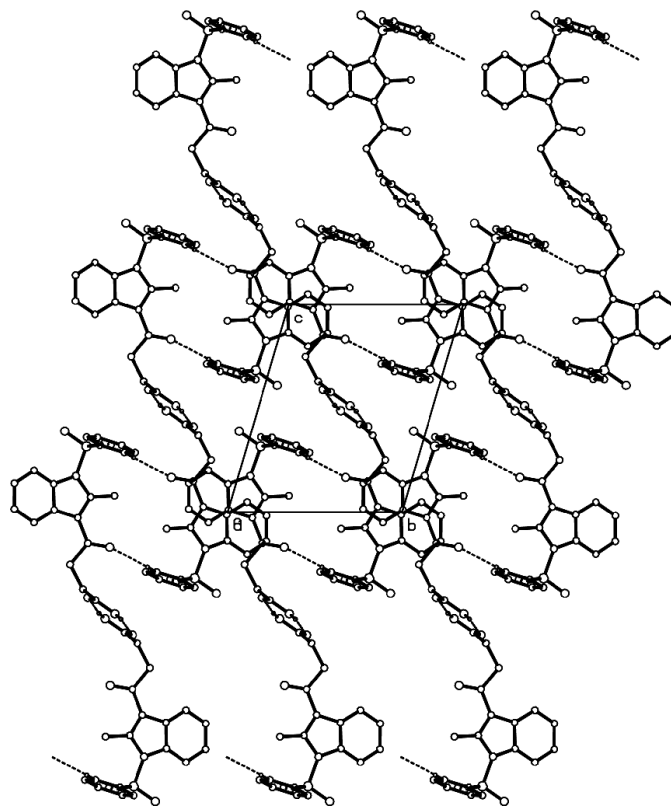. The sulfonyl group, comprising atoms O1, O2 and S1, is prevented from lying in the plane of the indole ring by the close approach of O1 and the H atom bound to C6, while O2 is close to the methyl substituent at C2. Thus, the orientation of the indole substituent is influenced by weak C6—H6⋯O1 and C16—H16B⋯O2 interactions, defined by the torsion angles C6—C5—N1—S1, C5—N1—S1—C10, C16—C2—N1—S1 and C2—N1—S1—C10.

The molecules are joined into head-to-head dimers with graph-set $R_2^2(8)$ (Bernstein *et al.*, 1995) by hydrogen bonds involving the carboxylic acid groups. The O5⋯O4 distance is 2.715 (2) Å. Centrosymmetric hydrogen bonds between atom C15 of the phenyl ring and carbonyl atom O3 of the 4-oxobutyric acid form another dimer with graph-set $R_2^2(18)$. This hydrogen-bond pattern joins the head-to-head dimers into chains running parallel to the *c* axis. Close edge-to-face interactions are observed between *A* and *B*[iii] and the equivalent pair *B* and *A*[iii], with an interplanar angle of 87.8 (1)° and a centroid–centroid distance of 5.088 (1) Å [symmetry code: (iii) 2 − *x*, −*y*, −*z*]. Face-to-face ring interactions between (pyrrole) ring *P* and *P*[v] and between ring *A* and *A*[iii] are observed; these stack in the crystal along *a*, with centroid–centroid distances of 4.129 (2) and 3.986 (2) Å, respectively [symmetry code: (v) 1 − *x*, −*y*, −*z*].

Experimental

The title compound was prepared by the Friedel–Crafts acylation of 1-phenylsulfonyl-2-methylindole with succinic anhydride in the presence of anhydrous aluminium chloride in dry methylene chloride.

Crystal data

$C_{19}H_{17}NO_5S$	$Z = 2$
$M_r = 371.40$	$D_x = 1.423$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 8.1825$ (2) Å	Cell parameters from 3857
$b = 9.9758$ (1) Å	reflections
$c = 12.3121$ (1) Å	$\theta = 1.8$–28.3°
$\alpha = 69.281$ (1)°	$\mu = 0.22$ mm^{-1}
$\beta = 72.067$ (1)°	$T = 293$ (2) K
$\gamma = 70.878$ (1)°	Block, colourless
$V = 866.92$ (2) Å^3	$0.46 \times 0.42 \times 0.24$ mm

Data collection

Siemens SMART CCD area-detector diffractometer	3144 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.025$
Absorption correction: none	$\theta_{max} = 28.3°$
6104 measured reflections	$h = -10 \rightarrow 8$
4175 independent reflections	$k = -13 \rightarrow 12$
	$l = -16 \rightarrow 13$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.052$	$w = 1/[\sigma^2(F_o^2) + (0.091P)^2]$
$wR(F^2) = 0.149$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
4175 reflections	$\Delta\rho_{max} = 0.54$ e Å^{-3}
236 parameters	$\Delta\rho_{min} = -0.48$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O2	1.422 (2)	O4—C20	1.215 (3)
S1—O1	1.424 (2)	O5—C20	1.309 (3)
S1—N1	1.698 (2)	N1—C2	1.414 (2)
S1—C10	1.757 (2)	N1—C5	1.422 (2)
O3—C17	1.212 (2)		
O2—S1—O1	120.1 (1)	N1—S1—C10	103.7 (1)
O2—S1—N1	106.9 (1)	C2—N1—C5	108.5 (1)
O1—S1—N1	105.6 (1)	C2—N1—S1	125.8 (1)
O2—S1—C10	109.3 (1)	C5—N1—S1	122.6 (1)
O1—S1—C10	109.9 (1)		
C10—S1—N1—C2	−78.7 (2)	S1—N1—C2—C16	−23.9 (3)
C10—S1—N1—C5	78.8 (2)	S1—N1—C5—C6	16.4 (3)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C6—H6···O1	0.93	2.30	2.901 (3)	122
C16—H16B···O2	0.96	2.37	2.871 (3)	112
C16—H16C···O3	0.96	2.40	2.954 (3)	117
C18—H18B···O4	0.97	2.49	2.851 (3)	102
O5—H5···O4^i	0.82	1.90	2.715 (2)	173
C15—H15···O3^{ii}	0.93	2.40	3.180 (3)	142
C8—H8···Cg^{iii}	0.93	3.39	3.997 (2)	125
C9—H9···Cg^{iii}	0.93	3.19	3.893 (3)	134
C19—H19A···Cg^{iv}	0.97	3.04	3.910 (3)	150

Symmetry codes: (i) $2 - x, 1 - y, -1 - z$; (ii) $1 - x, 1 - y, -z$; (iii) $2 - x, -y, -z$; (iv) $x, y, z - 1$. Cg denotes the centroid of phenyl ring C10–C15.

All H atoms were included in calculated positions and allowed to ride on their corresponding parent atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai, 1997) and *PLATON* (Spek, 1990); software used to prepare material for publication: *SHELXL*97 and *PARST* (Nardelli, 1995).

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