Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{*N*,*N*-Bis[3-(phenylysulfanyl)-1-(phenylsulfonyl)-indol-2-ylmethyl]amino}acetaldehyde dimethyl acetal

M. Yogavel,[a] D. Velmurugan,[a]* P. C. Srinivasan[b] and H.-K. Fun[c]

[a]Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, [b]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India, and [c]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia

Correspondence e-mail: d_velu@yahoo.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
Disorder in main residue
R factor = 0.074
wR factor = 0.207
Data-to-parameter ratio = 19.7

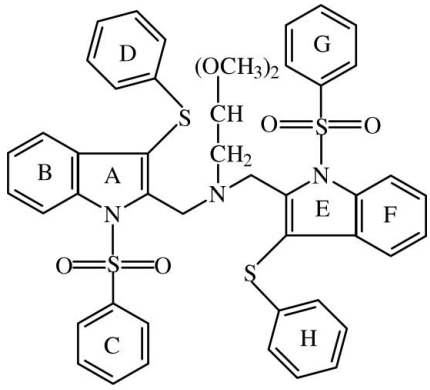
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 11 July 2005
Accepted 6 September 2005
Online 14 September 2005

The structure of the title compound, $C_{46}H_{41}N_3O_6S_4$, is stabilized by C—H···O, C—H···S and C—H···N interactions, and the packing of the molecules is stabilized by several C—H···π interactions, and face-to-face and edge-to-face π–π interactions.

Comment

Indole is present in a large number of natural products, many of which have a wide range of biological activities, such as antibacterial (Okabe & Adachi, 1998), antitumour (Scholl-meyer *et al.*, 1995), antidepressant (Grinev *et al.*, 1984), anti-microbial (El-Sayed *et al.*, 1986; Gadaginamath & Patil, 1999) and anti-inflammatory (Rodriguez *et al.*, 1985). Indoles have been proved to display high aldose reductase inhibitory activity (Rajeswaran *et al.*, 1999). The interaction of phenyl-sulfonyl indole with the calf-thymus DNA has also been studied by spectroscopic methods (Sivaraman *et al.*, 1996). The structure determination of the title compound, (I), was undertaken as part of our studies on indole derivatives.



(I)

The dihedral angle between the indole groups (*AB* and *EF*) and the phenyl rings (*C*, *D*, *G* and *H*) are *AB*/*C* = 75.0 (1)°, *EF*/*G* = 84.0 (1)°, *AB*/*D* = 84.9 (1)° and *EF*/*H* = 66.6 (1)°. The dihedral angle between rings *C*/*D* and *G*/*H* are 69.5 (1) and 77.8 (1)°, respectively. Atom N25 deviates by 0.217 (3) Å from the plane through atoms C26, C29 and S3, and the sum of the angles around N25 is 353.8°. This slight pyramidalization behaviour is also observed in related indole derivatives (Sankaranarayan *et al.*, 2000, 2001; Sankaranarayan, Yogavel, Velmurugan, Sekar, Babu *et al.*, 2003; Sankaranarayan, Yogavel, Velmurugan, Sekar, Srinivasan *et al.*, 2003; Sethu-Sankar *et al.*, 2002; Ganesh *et al.*, 2003; Krishna *et al.*, 2003).

The molecular structure is stabilized by C—H···O, C—H···S and C—H···N interactions. The phenyl rings *C* of the

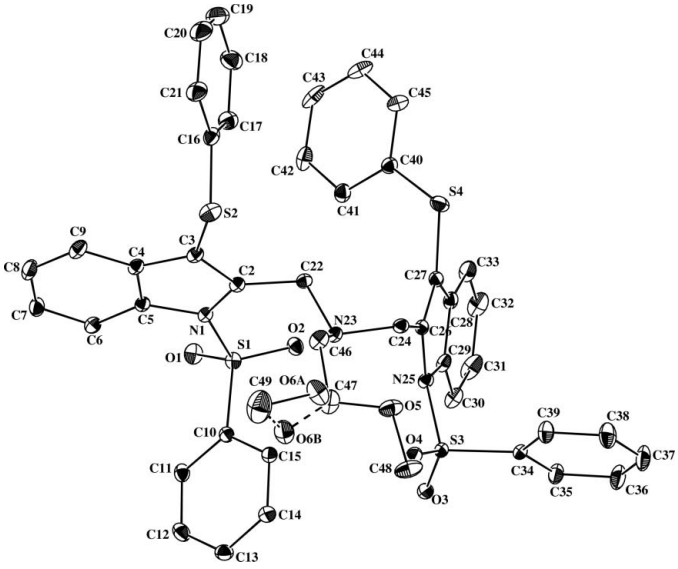


Figure 1
The molecular structure of the title compound, showing 35% probability displacement ellipsoids. H atoms have been omitted. Dashed lines indicate the minor component of the disordered O atom.

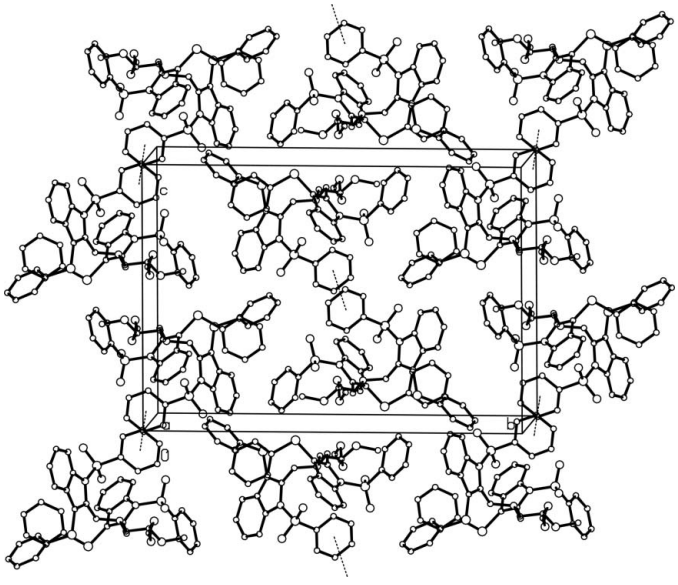


Figure 2
The crystal structure of (I), viewed down the *a* axis. The π–π interactions are indicated as dashed lines. H atoms have been omitted.

molecules at (x, y, z) and ($-x$, $-y$, $-z$) are stacked in a face-to-face manner, with their centroids separated by 3.772 (2) Å. Several intermolecular edge-to-face interactions and several C—H$\cdots\pi$ interactions are also observed (Table 2). Thus, the crystal packing is stabilized by C—H$\cdots\pi$, face-to-face π–π and edge-to-face π–π interactions.

Experimental

To a solution of aminoacetaldehyde dimethyl acetal (4.4 ml, 40 mmol) in chloroform (40 ml) was added a solution of 1-phenylsulfonyl-2-bromomethyl-3-phenylthioindole (10 mmol) in chloroform (15 ml) and the mixture was stirred at room temperature for 4 h. Work-up of the reaction and crystallization of the residue from methanol afforded the title compound (yield 4.1 g, 85%) as the sole product.

Crystal data

$C_{46}H_{41}N_3O_6S_4$	D_x = 1.318 Mg m^{-3}
M_r = 857.03	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 8042 reflections
a = 10.7146 (1) Å	θ = 1.5–28.5°
b = 23.8939 (1) Å	μ = 0.27 mm^{-1}
c = 16.8782 (3) Å	T = 293 (2) K
β = 91.846 (1)°	Block, colourless
V = 4318.81 (9) Å^3	0.40 × 0.36 × 0.28 mm
Z = 4	

Data collection

Siemens SMART CCD area-detector diffractometer	5223 reflections with $I > 2\sigma(I)$
	R_{int} = 0.066
ω scans	θ_{max} = 28.5°
Absorption correction: none	$h = -14 \rightarrow 12$
29148 measured reflections	$k = -31 \rightarrow 30$
10689 independent reflections	$l = -15 \rightarrow 22$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0814P)^2 + 1.9503P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.074	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.207	$\Delta\rho_{max}$ = 0.56 e Å^{-3}
S = 1.01	$\Delta\rho_{min}$ = −0.45 e Å^{-3}
10689 reflections	
543 parameters	
H-atom parameters constrained	

Table 1
Selected interatomic distances (Å).

S1—O2	1.406 (3)	S3—O4	1.426 (3)
S1—O1	1.427 (3)	S3—O3	1.432 (3)
N1—C5	1.415 (4)	N25—C26	1.425 (4)
N1—C2	1.421 (4)	N25—C29	1.435 (4)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C6—H6$\cdots$O1	0.93	2.37	2.923 (5)	118
C11—H11$\cdots$O1	0.93	2.57	2.924 (5)	103
C15—H15$\cdots$N23	0.93	2.48	3.334 (4)	153
C22—H22$A\cdots$O2	0.97	2.36	2.913 (4)	115
C22—H22$B\cdots$S2	0.97	2.85	3.311 (4)	110
C24—H24$A\cdots$O4	0.97	2.33	2.887 (4)	116
C24—H24$A\cdots$O5	0.97	2.39	3.090 (5)	129
C24—H24$B\cdots$S4	0.97	2.84	3.287 (4)	109
C30—H30$\cdots$O3	0.93	2.33	2.920 (5)	121
C35—H35$\cdots$O3	0.93	2.55	2.904 (5)	103
C32—H32$\cdots$CgA^{i}	0.93	2.95	3.728 (5)	143
C32—H32$\cdots$CgB^{i}	0.93	3.09	3.752 (5)	129
C31—H31$\cdots$CgC^{i}	0.93	2.99	3.680 (6)	132
C7—H7$\cdots$CgD^{ii}	0.93	3.09	3.661 (5)	122
C9—H9$\cdots$CgH^{iii}	0.93	3.02	3.682 (5)	130

Symmetry codes: (i) $x+1, y, z$; (ii) $x-\frac{3}{2}, -y-\frac{1}{2}, z-\frac{3}{2}$; (iii) $x-1, y, z$. *CgA*, *CgB*, *CgC*, *CgD* and *CgH* are the centroids of the rings *A*, *B*, *C*, *D* and *H*, respectively.

All the H atoms were positioned geometrically and allowed to ride on their parent atoms [C—H = 0.93–0.98 Å, and U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(C_{methyl})]. Atom O6 was found to be disordered and the site occupancy factors of the major and minor components were refined.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

MY and DV thank the University Grants Commission (UCG) Herbal Science Programme for financial support under the scheme for Universities with Potential for Excellency. The UGC and Department of Science and Technology (DST) are gratefully acknowledged for financial support to the Department of Crystallography and Biophysics under the UGC-SAP and DST-FIST programmes.

References

El-Sayed, K., Barnhart, D. M., Ammon, H. L. & Wassel, G. M. (1986). *Acta Cryst.* C**42**, 1383–1385.
Gadaginamath, G. S. & Patil, S. A. (1999). *Indian J. Chem.* Sect. *B*, **38**, 1070–1074.
Ganesh, V. K., Yogavel, M., D., Velmurugan, D., Shanmuga Sundara Raj, S., Fun, H.-K., Kannadasan, S. & Srinivasan, P. C. (2003). *Acta Cryst.* E**59**, o703–705.
Grinev, A. N., Shevdov, V. L., Krichevskii, E. S., Romanova, O. B., Altukkhova, L. B., Kurilo, G. N., Andreeva, N. I., Golovina, S. M. & Mashkovskii, M. D. (1984). *Khim. Farm, Zh.* **18**, 159–163. (In Russian.)
Krishna, R., Aravindan, P. G., Yogavel, M. D. Velmurugan, D., Shanmuga Sundara Raj, S., Fun, H.-K. & Srinivasan, P. C. (2003). *Acta Cryst.* E**59**, o875–877.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Okabe, N. & Adachi, Y. (1998). *Acta Cryst.* C**54**, 386–387.
Rajeswaran, W. G., Labroo, R. B. & Cohen, L. A. (1999). *J. Org. Chem.* **64**, 1369–1371.
Rodriguez, J. G., Temprano, F., Esteban-Calderon, C., Martinez-Ripoll, M. & Garcia-Blanco, S. (1985). *Tetrahedron*, **41**, 3813–3823.
Sankaranarayan, R., Velmurugan, D., Shanmuga Sundara Raj, S., Fun, H.-K., Babu, G. & Perumal, P. T. (2000). *Acta Cryst.* C**56**, 475–476.
Sankaranarayan, R., Velmurugan, D., Shanmuga Sundara Raj, S., Fun, H.-K., Narasinga Rao, S., Kannadasan, S. & Srinivasan, P. C. (2001). *Acta Cryst.* C**57**, 569–571.
Sankaranarayan, R., Yogavel, M., Velmurugan, D., Sekar, K., Babu, G., Perumal, P. T., Shanmuga Sundara Raj, S. & Fun, H.-K. (2003). *Acta Cryst.* E**59**, o49–o51.
Sankaranarayan, R., Yogavel, M., Velmurugan, D., Sekar, K., Srinivasan, P. C., Shanmuga Sundara Raj, S. & Fun, H.-K. (2003). *Acta Cryst.* E**59**, o99–o101.
Schollmeyer, D., Fischer, G. & Pindur, U. (1995). *Acta Cryst.* C**51**, 2572–2575.
SethuSankar, K., Suresh Babu, N., Velmurugan, D., Shanmuga Sundara Raj, S. & Fun, H.-K. (2002). *Acta Cryst.* E**58**, o134–o136.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray instruments Inc., Madison, Wisconsin, USA.
Sivaraman, J., Subramanian, K., Velmurugan, D., Subramanian, E. & Seetharaman, J. (1996). *J. Mol. Struct.* **385**, 123–128.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Zsolnai, L. (1997). *ZORTEP*. University of Heidelberg, Germany.