Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-[(3-Phenylsulfanyl-1-phenylsulfonyl-1*H*-indol-2-yl)methyl]acetamide

S. Thenmozhi,[a] A. SubbiahPandi,[a]* V. Dhayalan[b] and A. K. MohanaKrishnan[b]

[a]Department of Physics, Presidency College (Autonomous), Chennai 600 005, India, and [b]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India
Correspondence e-mail: a_spandian@yahoo.com

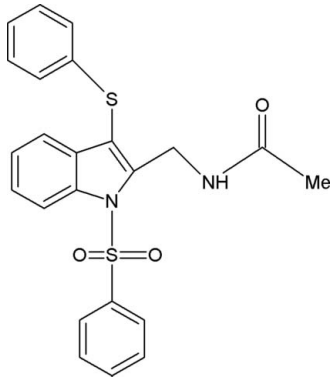
Received 30 March 2009; accepted 2 April 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.121; data-to-parameter ratio = 26.3.

In the title compound, $C_{23}H_{20}N_2O_3S_2$, the phenylsulfonyl ring and phenylthio ring make dihedral angles of 66.5 (7) and 81.2 (6)°, respectively, with the indole unit. In the crystal, molecules are linked into centrosymmetric dimers *via* pairs of N—H···O hydrogen bonds with graph-set motif $R_2^2(14)$. The crystal structure is further stabilized by weak intermolecular C—H···O and very weak C—H···π interactions.

Related literature

For the biological activity of indole derivatives, see: Singh *et al.* (2000); Andreani *et al.* (2001); Quetin-Leclercq (1994); Mukhopadhyay *et al.* (1981); Taylor *et al.* (1999); Williams *et al.* (1993); Sivaraman *et al.* (1996). For a related structure, see: Ravishankar *et al.* (2005).



Experimental

Crystal data

$C_{23}H_{20}N_2O_3S_2$
M_r = 436.53
Triclinic, $P\overline{1}$
a = 8.8129 (2) Å
b = 10.8880 (3) Å
c = 11.3711 (3) Å
α = 86.698 (1)°
β = 76.494 (1)°
γ = 83.317 (1)°
V = 1053.21 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 293 K
0.21 × 0.19 × 0.17 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.943, T_{max} = 0.953
28160 measured reflections
7167 independent reflections
5294 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.121
S = 0.98
7167 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2^{i}	0.86	2.48	3.3179 (15)	165
C21—H21···O1^{ii}	0.93	2.44	3.2666 (18)	149
C5—H5···$Cg3^{iii}$	0.93	2.94	3.7634 (18)	149
C9—H9A···$Cg4^{iv}$	0.97	2.95	3.5792 (16)	124
C11—H11A···$Cg2^{v}$	0.96	2.91	3.5974 (21)	129
C16—H16···$Cg4^{vi}$	0.93	2.95	3.7453 (21)	145

Symmetry codes: (i) $-x+2, -y+1, -z+2$; (ii) $x, y, z-1$; (iii) $x-1, y, z$; (iv) $-x+2, -y+1, -z+1$; (v) $-x+1, -y+1, -z+2$; (vi) $-x+2, -y, -z+1$. *Cg*2, *Cg*3 and *Cg*4 are the centroids of the C1–C6, C12–C17 and C18–C23 rings, respectively.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

ST and ASP thank Dr J. Jothi Kumar, Principal of Presidency College (Autonomous), Chennai, for providing computer and internet facilities. Dr Babu Vargheese, SAIF, IIT, Madras, India, is thanked for his help with the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2922).

References

Andreani, A., Granaiola, M., Leoni, A., Locatelli, A., Morigi, R., Rambaldi, M., Giorgi, G., Salvini, L. & Garaliene, V. (2001). *Anticancer Drug Des.* **16**, 167–174.
Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Mukhopadhyay, S., Handy, G. A., Funayama, S. & Cordell, G. A. (1981). *J. Nat. Prod.* **44**, 696–700.
Quetin-Leclercq, J. (1994). *J. Pharm. Belg.* **49**, 181–192.
Ravishankar, T., Chinnakali, K., Arumugam, N., Srinivasan, P. C., Usman, A. & Fun, H.-K. (2005). *Acta Cryst.* E**61**, o2455–o2457.
Sheldrick, G. M. (1996). *SADABS*. University of Gottingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Singh, U. P., Sarma, B. K., Mishra, P. K. & Ray, A. B. (2000). *Folia Microbiol.* **45**, 173–176.
Sivaraman, J., Subramanian, K., Velmurugan, D., Subramanian, E. & Seetharaman, J. (1996). *J. Mol. Struct.* **385**, 123–128.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Taylor, D. L., Ahmed, P. S., Chambers, P., Tyms, A. S., Bedard, J., Duchaine, J., Falardeau, G., Lavallee, J. F., Brown, W., Rando, R. F. & Bowlin, T. (1999). *Antiviral Chem. Chemother.* **10**, 79–86.
Williams, T. M., Ciccarone, T. M., MacTough, S. C., Rooney, C. S., Balani, S. K., Condra, J. H., Emini, E. A., Goldman, M. E., Greenlee, W. J. & Kauffman, L. R. (1993). *J. Med. Chem.* **36**, 1291–1294.

supplementary materials

Acta Cryst. (2009). E**65**, o1020-o1021 [**doi:10.1107/S1600536809012525**]

N-[(3-Phenylsulfanyl-1-phenylsulfonyl-1*H*-indol-2-yl)methyl]acetamide

S. Thenmozhi, A. SubbiahPandi, V. Dhayalan and A. K. MohanaKrishnan

Comment

Indole derivatives have been found to exhibit antibacterial, antifungal (Singh *et al.*, 2000) and antitumour activities (Andreani *et al.*, 2001). Some of the indole alkaloids extracted from plants possess interesting cytotoxic, antitumour or antiparasitic properties (Quetin-Leclercq, 1994; Mukhopadhyay *et al.*, 1981). Pyrido[1,2-*a*] indole derivatives have been identified as potent inhibitors of human immunodeficiency virus type 1 (Taylor *et al.*, 1999), and 5-chloro-3-(phenylsulfonyl) indole-2-carboxamide is reported to be a highly potent non-nucleoside inhibitor of HIV-1 reverse transcriptase (Williams *et al.*, 1993). The interaction of phenylsulfonylindole with calf thymus DNA has also been studied by spectroscopic methods (Sivaraman *et al.*, 1996). Against this background, and in order to obtain detailed information on molecular conformations in the solid state, X-ray studies of the title compound (Fig. 1) have been carried out.

The mean plane of the indole ring system makes dihedral angles of 66.5 (7) and 81.2 (6)° with respect to the phenyl rings. The S–O, S–C, and S–N distances are 1.419 (11), 1.750 (13) and 1.679 (11) Å, respectively, these are comparable as observed in similar structures (Ravishankar *et al.*, 2005). As a result of the electron-withdrawing character of the phenylsulfonyl group, the N–Csp^2 bond lengths, *viz*. N1–C1 [1.422 (9) Å] and N1–C8 [1.433 (6) Å], are longer than the mean value of 1.355 (14)Å for N atoms with planar configurations.

Via N2–H2···O2 hydrogen bonds the molecules form cyclic centrosymmetric dimers [$R_2^2(14)$] shown in Fig.2. The structure is further stabilized by intermolecular C–H···π and C–H···O interactions as shown in Table. 1.

Experimental

To a solution of 1-phenylsulfonyl-2-(bromomethyl)-3-(phenylthio)-1*H*-indole (0.5 g, 1.09 mmol) in dry acetonitrile (20 ml), $ZnBr_2$ (0.49 g, 2.18 mmol), was added. The reaction mixture was then refluxed for 5 hr under N_2 atmosphere. It was then poured over ice-water (30 ml) containing 1 ml of conc.HCl, extracted with $CHCl_3$ (30 ml) and dried (Na_2 SO_4). Removal of solvent followed by crystallization from methanol afforded amide product. The amide was recrystallization from $CDCl_3$. Single crystals of the title compound suitable for X-ray diffraction were obtained by slow evaporation of a solution in methanol.

Refinement

All H atoms were fixed geometrically and allowed to ride on their parent C atoms, with C–H distances fixed in the range 0.93–0.97 Å with U_{iso}(H) = 1.5U_{eq}(C) for methyl H 1.2U_{eq}(C) for other H atoms.

Figures

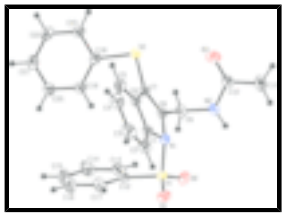


Fig. 1. View of the title molecule with the atom labeling scheme. The displacement ellipsoids are drawn at the 30% probability level while the H atoms are shown as small spheres of arbitrary radii.

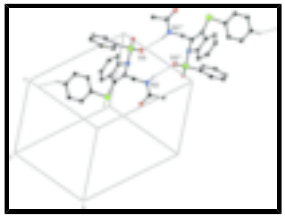


Fig. 2. The crystal structure showing the centrosymmetric hydrogen bond motif $R_2^2(14)$. For the sake of clarity, the H atoms not involved in the motif have been omitted. The atoms marked with an asterisk (*) are at the symmetry position (-*x*, 1 - *y*, 2 - *z*). The dashed lines indicate the hydrogen bonds.

N-[(3-Phenylsulfanyl-1-phenylsulfonyl-1*H*-indol-2- yl)methyl]acetamide

Crystal data

$C_{23}H_{20}N_2O_3S_2$	$Z = 2$
$M_r = 436.53$	$F_{000} = 456$
Triclinic, $P\overline{1}$	$D_x = 1.377$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.8129$ (2) Å	Cell parameters from 7167 reflections
$b = 10.8880$ (3) Å	$\theta = 2.4$–31.9°
$c = 11.3711$ (3) Å	$\mu = 0.28$ mm^{-1}
$\alpha = 86.698$ (1)°	$T = 293$ K
$\beta = 76.494$ (1)°	Block, colourless
$\gamma = 83.317$ (1)°	0.21 × 0.19 × 0.17 mm
$V = 1053.21$ (5) Å^3	

Data collection

Bruker Kappa APEXII CCD diffractometer	7167 independent reflections
Radiation source: fine-focus sealed tube	5294 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
$T = 293$ K	$\theta_{max} = 31.9^\circ$
ω scans	$\theta_{min} = 2.4^\circ$
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	$h = -13 \rightarrow 13$
$T_{min} = 0.943$, $T_{max} = 0.953$	$k = -16 \rightarrow 16$
28160 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.121$	$w = 1/[\sigma^2(F_o^2) + (0.0595P)^2 + 0.2774P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{max} = 0.005$
7167 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
272 parameters	$\Delta\rho_{min} = -0.39$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.80217 (15)	0.18662 (12)	0.83970 (11)	0.0347 (3)
C2	0.79544 (18)	0.07935 (15)	0.91125 (14)	0.0470 (3)
H2	0.8532	0.0644	0.9703	0.056*
C3	0.6993 (2)	−0.00414 (16)	0.89092 (17)	0.0567 (4)
H3	0.6929	−0.0775	0.9370	0.068*
C4	0.6116 (2)	0.01768 (16)	0.80390 (17)	0.0561 (4)
H4	0.5467	−0.0404	0.7937	0.067*
C5	0.61930 (18)	0.12411 (15)	0.73246 (14)	0.0465 (3)
H5	0.5611	0.1385	0.6736	0.056*
C6	0.71616 (15)	0.20927 (12)	0.75069 (11)	0.0348 (3)
C7	0.74318 (15)	0.33121 (12)	0.69884 (11)	0.0338 (3)
C8	0.83792 (15)	0.38163 (12)	0.75660 (11)	0.0329 (2)
C9	0.87341 (16)	0.51288 (13)	0.75136 (13)	0.0393 (3)
H9A	0.9854	0.5152	0.7415	0.047*
H9B	0.8427	0.5560	0.6822	0.047*
C10	0.64041 (17)	0.62259 (15)	0.87510 (15)	0.0463 (3)
C11	0.5609 (2)	0.66919 (19)	0.99829 (18)	0.0619 (5)
H11A	0.4948	0.7443	0.9901	0.093*

H11B	0.6387	0.6850	1.0405	0.093*
H11C	0.4982	0.6081	1.0430	0.093*
C12	1.17375 (14)	0.22315 (13)	0.72453 (12)	0.0355 (3)
C13	1.23409 (17)	0.30613 (15)	0.63391 (14)	0.0458 (3)
H13	1.2222	0.3904	0.6477	0.055*
C14	1.31247 (19)	0.26126 (19)	0.52229 (16)	0.0560 (4)
H14	1.3537	0.3157	0.4601	0.067*
C15	1.3295 (2)	0.1370 (2)	0.50313 (16)	0.0602 (5)
H15	1.3821	0.1075	0.4277	0.072*
C16	1.2700 (2)	0.05551 (18)	0.59387 (19)	0.0656 (5)
H16	1.2830	−0.0288	0.5798	0.079*
C17	1.19143 (19)	0.09758 (15)	0.70519 (16)	0.0517 (4)
H17	1.1506	0.0425	0.7669	0.062*
C18	0.76928 (15)	0.32193 (12)	0.45609 (11)	0.0336 (3)
C19	0.90885 (16)	0.24822 (14)	0.45385 (12)	0.0417 (3)
H19	0.9484	0.2367	0.5232	0.050*
C20	0.98919 (19)	0.19193 (16)	0.34812 (14)	0.0503 (4)
H20	1.0825	0.1418	0.3468	0.060*
C21	0.9327 (2)	0.20926 (16)	0.24488 (14)	0.0512 (4)
H21	0.9882	0.1719	0.1738	0.061*
C22	0.7938 (2)	0.28199 (17)	0.24709 (13)	0.0524 (4)
H22	0.7551	0.2934	0.1774	0.063*
C23	0.71127 (17)	0.33808 (15)	0.35210 (13)	0.0440 (3)
H23	0.6169	0.3867	0.3533	0.053*
N1	0.87779 (12)	0.29375 (10)	0.84621 (9)	0.0346 (2)
N2	0.78974 (13)	0.57402 (11)	0.86117 (11)	0.0403 (3)
H2A	0.8371	0.5792	0.9185	0.048*
O1	1.06998 (14)	0.18125 (12)	0.95384 (10)	0.0559 (3)
O2	1.09978 (14)	0.39630 (11)	0.88318 (11)	0.0552 (3)
O3	0.57273 (17)	0.62503 (18)	0.79379 (14)	0.0910 (5)
S1	1.06294 (4)	0.27656 (3)	0.86411 (3)	0.03906 (10)
S2	0.65950 (4)	0.40353 (3)	0.58434 (3)	0.04266 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0339 (6)	0.0363 (7)	0.0294 (6)	0.0033 (5)	−0.0017 (5)	−0.0011 (5)
C2	0.0472 (8)	0.0473 (8)	0.0409 (8)	0.0023 (6)	−0.0049 (6)	0.0087 (6)
C3	0.0589 (10)	0.0442 (9)	0.0590 (10)	−0.0056 (7)	−0.0003 (8)	0.0117 (7)
C4	0.0557 (9)	0.0456 (9)	0.0646 (11)	−0.0137 (7)	−0.0041 (8)	−0.0036 (8)
C5	0.0465 (8)	0.0474 (8)	0.0459 (8)	−0.0054 (6)	−0.0093 (6)	−0.0084 (6)
C6	0.0363 (6)	0.0365 (7)	0.0288 (6)	0.0022 (5)	−0.0039 (5)	−0.0048 (5)
C7	0.0373 (6)	0.0350 (6)	0.0270 (5)	0.0056 (5)	−0.0072 (5)	−0.0034 (5)
C8	0.0341 (6)	0.0346 (6)	0.0268 (5)	0.0043 (5)	−0.0043 (4)	−0.0025 (5)
C9	0.0388 (6)	0.0359 (7)	0.0403 (7)	−0.0002 (5)	−0.0049 (5)	−0.0030 (5)
C10	0.0393 (7)	0.0476 (8)	0.0508 (8)	0.0029 (6)	−0.0097 (6)	−0.0097 (7)
C11	0.0522 (9)	0.0638 (11)	0.0635 (11)	0.0005 (8)	0.0013 (8)	−0.0246 (9)
C12	0.0307 (6)	0.0404 (7)	0.0362 (6)	−0.0001 (5)	−0.0105 (5)	−0.0041 (5)

C13	0.0396 (7)	0.0441 (8)	0.0503 (8)	−0.0011 (6)	−0.0060 (6)	0.0022 (6)
C14	0.0432 (8)	0.0730 (12)	0.0446 (8)	−0.0027 (7)	0.0002 (6)	0.0076 (8)
C15	0.0448 (8)	0.0834 (14)	0.0490 (9)	−0.0026 (8)	−0.0006 (7)	−0.0234 (9)
C16	0.0572 (10)	0.0559 (11)	0.0783 (13)	−0.0077 (8)	0.0028 (9)	−0.0295 (10)
C17	0.0490 (8)	0.0422 (8)	0.0576 (9)	−0.0052 (6)	0.0015 (7)	−0.0055 (7)
C18	0.0365 (6)	0.0355 (6)	0.0295 (6)	−0.0043 (5)	−0.0093 (5)	0.0010 (5)
C19	0.0411 (7)	0.0508 (8)	0.0330 (6)	0.0029 (6)	−0.0113 (5)	−0.0029 (6)
C20	0.0460 (8)	0.0584 (10)	0.0411 (8)	0.0068 (7)	−0.0043 (6)	−0.0064 (7)
C21	0.0606 (9)	0.0569 (10)	0.0322 (7)	−0.0065 (7)	−0.0015 (6)	−0.0070 (6)
C22	0.0645 (10)	0.0649 (10)	0.0310 (7)	−0.0076 (8)	−0.0170 (7)	−0.0010 (7)
C23	0.0449 (7)	0.0534 (9)	0.0355 (7)	−0.0003 (6)	−0.0163 (6)	0.0022 (6)
N1	0.0343 (5)	0.0400 (6)	0.0282 (5)	0.0025 (4)	−0.0076 (4)	−0.0017 (4)
N2	0.0391 (6)	0.0397 (6)	0.0439 (6)	0.0019 (5)	−0.0137 (5)	−0.0120 (5)
O1	0.0594 (7)	0.0743 (8)	0.0344 (5)	0.0054 (6)	−0.0204 (5)	0.0089 (5)
O2	0.0576 (6)	0.0579 (7)	0.0580 (7)	−0.0021 (5)	−0.0261 (5)	−0.0220 (5)
O3	0.0563 (8)	0.1470 (15)	0.0704 (9)	0.0362 (9)	−0.0318 (7)	−0.0335 (9)
S1	0.04034 (17)	0.0485 (2)	0.03049 (16)	0.00304 (14)	−0.01514 (13)	−0.00580 (13)
S2	0.04688 (19)	0.0454 (2)	0.03417 (17)	0.01400 (14)	−0.01465 (14)	−0.00459 (14)

Geometric parameters (Å, °)

C1—C2	1.3834 (19)	C12—S1	1.7496 (13)
C1—C6	1.3949 (18)	C13—C14	1.382 (2)
C1—N1	1.4226 (18)	C13—H13	0.9300
C2—C3	1.376 (2)	C14—C15	1.368 (3)
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.385 (3)	C15—C16	1.370 (3)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.375 (2)	C16—C17	1.369 (2)
C4—H4	0.9300	C16—H16	0.9300
C5—C6	1.386 (2)	C17—H17	0.9300
C5—H5	0.9300	C18—C19	1.3840 (18)
C6—C7	1.4439 (19)	C18—C23	1.3885 (17)
C7—C8	1.3543 (18)	C18—S2	1.7727 (13)
C7—S2	1.7477 (12)	C19—C20	1.382 (2)
C8—N1	1.4332 (16)	C19—H19	0.9300
C8—C9	1.4930 (19)	C20—C21	1.374 (2)
C9—N2	1.4482 (17)	C20—H20	0.9300
C9—H9A	0.9700	C21—C22	1.375 (2)
C9—H9B	0.9700	C21—H21	0.9300
C10—O3	1.2093 (19)	C22—C23	1.379 (2)
C10—N2	1.3368 (18)	C22—H22	0.9300
C10—C11	1.500 (2)	C23—H23	0.9300
C11—H11A	0.9600	N1—S1	1.6789 (11)
C11—H11B	0.9600	N2—H2A	0.8600
C11—H11C	0.9600	O1—S1	1.4193 (11)
C12—C13	1.382 (2)	O2—S1	1.4198 (12)
C12—C17	1.382 (2)		
C2—C1—C6	121.75 (14)	C14—C13—H13	120.7

C2—C1—N1	130.00 (13)	C15—C14—C13	120.14 (16)
C6—C1—N1	108.02 (11)	C15—C14—H14	119.9
C3—C2—C1	116.88 (15)	C13—C14—H14	119.9
C3—C2—H2	121.6	C14—C15—C16	120.71 (16)
C1—C2—H2	121.6	C14—C15—H15	119.6
C2—C3—C4	122.07 (15)	C16—C15—H15	119.6
C2—C3—H3	119.0	C17—C16—C15	120.32 (17)
C4—C3—H3	119.0	C17—C16—H16	119.8
C5—C4—C3	120.89 (16)	C15—C16—H16	119.8
C5—C4—H4	119.6	C16—C17—C12	119.01 (16)
C3—C4—H4	119.6	C16—C17—H17	120.5
C4—C5—C6	118.11 (15)	C12—C17—H17	120.5
C4—C5—H5	120.9	C19—C18—C23	119.60 (13)
C6—C5—H5	120.9	C19—C18—S2	123.85 (10)
C5—C6—C1	120.29 (13)	C23—C18—S2	116.52 (10)
C5—C6—C7	132.35 (13)	C20—C19—C18	119.66 (13)
C1—C6—C7	107.20 (12)	C20—C19—H19	120.2
C8—C7—C6	109.04 (11)	C18—C19—H19	120.2
C8—C7—S2	125.89 (11)	C21—C20—C19	120.68 (15)
C6—C7—S2	125.02 (10)	C21—C20—H20	119.7
C7—C8—N1	108.48 (11)	C19—C20—H20	119.7
C7—C8—C9	128.32 (12)	C20—C21—C22	119.72 (14)
N1—C8—C9	122.13 (11)	C20—C21—H21	120.1
N2—C9—C8	110.29 (11)	C22—C21—H21	120.1
N2—C9—H9A	109.6	C21—C22—C23	120.40 (14)
C8—C9—H9A	109.6	C21—C22—H22	119.8
N2—C9—H9B	109.6	C23—C22—H22	119.8
C8—C9—H9B	109.6	C22—C23—C18	119.92 (13)
H9A—C9—H9B	108.1	C22—C23—H23	120.0
O3—C10—N2	121.55 (15)	C18—C23—H23	120.0
O3—C10—C11	122.30 (15)	C1—N1—C8	107.23 (10)
N2—C10—C11	116.11 (14)	C1—N1—S1	119.17 (9)
C10—C11—H11A	109.5	C8—N1—S1	118.64 (9)
C10—C11—H11B	109.5	C10—N2—C9	121.31 (12)
H11A—C11—H11B	109.5	C10—N2—H2A	119.3
C10—C11—H11C	109.5	C9—N2—H2A	119.3
H11A—C11—H11C	109.5	O1—S1—O2	119.66 (7)
H11B—C11—H11C	109.5	O1—S1—N1	106.41 (7)
C13—C12—C17	121.18 (14)	O2—S1—N1	106.61 (6)
C13—C12—S1	120.19 (11)	O1—S1—C12	108.97 (7)
C17—C12—S1	118.52 (12)	O2—S1—C12	110.17 (7)
C12—C13—C14	118.64 (15)	N1—S1—C12	103.77 (6)
C12—C13—H13	120.7	C7—S2—C18	101.32 (6)
C6—C1—C2—C3	−0.2 (2)	C19—C20—C21—C22	−0.9 (3)
N1—C1—C2—C3	173.51 (14)	C20—C21—C22—C23	0.3 (3)
C1—C2—C3—C4	−0.6 (2)	C21—C22—C23—C18	0.5 (2)
C2—C3—C4—C5	1.0 (3)	C19—C18—C23—C22	−0.8 (2)
C3—C4—C5—C6	−0.5 (2)	S2—C18—C23—C22	177.16 (12)
C4—C5—C6—C1	−0.3 (2)	C2—C1—N1—C8	−175.59 (13)

C4—C5—C6—C7	−175.17 (14)	C6—C1—N1—C8	−1.19 (13)
C2—C1—C6—C5	0.7 (2)	C2—C1—N1—S1	46.01 (18)
N1—C1—C6—C5	−174.30 (12)	C6—C1—N1—S1	−139.59 (9)
C2—C1—C6—C7	176.72 (12)	C7—C8—N1—C1	0.11 (13)
N1—C1—C6—C7	1.76 (14)	C9—C8—N1—C1	169.22 (11)
C5—C6—C7—C8	173.66 (14)	C7—C8—N1—S1	138.76 (10)
C1—C6—C7—C8	−1.72 (14)	C9—C8—N1—S1	−52.12 (14)
C5—C6—C7—S2	−3.8 (2)	O3—C10—N2—C9	−5.2 (3)
C1—C6—C7—S2	−179.22 (9)	C11—C10—N2—C9	172.65 (14)
C6—C7—C8—N1	0.98 (14)	C8—C9—N2—C10	−83.42 (16)
S2—C7—C8—N1	178.45 (9)	C1—N1—S1—O1	−43.85 (11)
C6—C7—C8—C9	−167.25 (12)	C8—N1—S1—O1	−177.59 (10)
S2—C7—C8—C9	10.2 (2)	C1—N1—S1—O2	−172.62 (10)
C7—C8—C9—N2	104.47 (15)	C8—N1—S1—O2	53.64 (11)
N1—C8—C9—N2	−62.33 (15)	C1—N1—S1—C12	71.05 (10)
C17—C12—C13—C14	0.4 (2)	C8—N1—S1—C12	−62.69 (11)
S1—C12—C13—C14	−175.91 (12)	C13—C12—S1—O1	−156.18 (11)
C12—C13—C14—C15	−0.2 (2)	C17—C12—S1—O1	27.46 (13)
C13—C14—C15—C16	−0.2 (3)	C13—C12—S1—O2	−23.05 (13)
C14—C15—C16—C17	0.4 (3)	C17—C12—S1—O2	160.59 (12)
C15—C16—C17—C12	−0.2 (3)	C13—C12—S1—N1	90.75 (12)
C13—C12—C17—C16	−0.2 (2)	C17—C12—S1—N1	−85.61 (12)
S1—C12—C17—C16	176.18 (14)	C8—C7—S2—C18	108.39 (12)
C23—C18—C19—C20	0.2 (2)	C6—C7—S2—C18	−74.53 (12)
S2—C18—C19—C20	−177.54 (12)	C19—C18—S2—C7	−15.37 (14)
C18—C19—C20—C21	0.6 (2)	C23—C18—S2—C7	166.79 (11)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O2^{i}	0.86	2.48	3.3179 (15)	165
C21—H21···O1^{ii}	0.93	2.44	3.2666 (18)	149
C5—H5···Cg3^{iii}	0.93	2.94	3.7634 (18)	149
C9—H9A···Cg4^{iv}	0.97	2.95	3.5792 (16)	124
C11—H11A···Cg2^{v}	0.96	2.91	3.5974 (21)	129
C16—H16···Cg4^{vi}	0.93	2.95	3.7453 (21)	145

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

Fig. 1

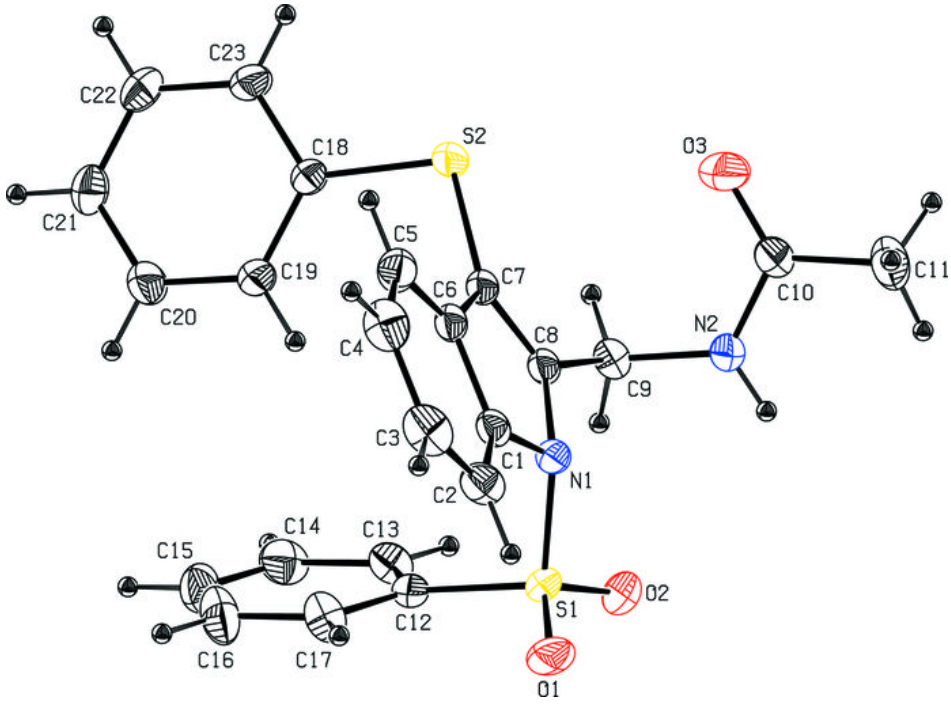

C23
C22
C18
S2
O3
C21
C5
C19
C6
C7
C11
C10
C20
C4
C8
N2
C9
C3
C1
N1
C2
C14
C13
C15
O2
S1
C12
C16
C17
O1

Fig. 2