Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structure of (2-methyl-1-phenylsulfonyl-1*H*-indol-3-yl)(phenyl)methanone

M. Umadevi,[a,b] V. Saravanan,[c] R. Yamuna,[d]* A. K. Mohanakrishnan[c] and G. Chakkaravarthi[e]*

[a]Research and Development Centre, Bharathiyar University, Coimbatore 641 046, India, [b]Department of Chemistry, Pallavan College of Engineering, Kanchipuram 631 502, India, [c]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India, [d]Department of Sciences, Chemistry and Materials Research Lab, Amrita Vishwa Vidyapeetham University, Ettimadai, Coimbatore 641 112, India, and [e]Department of Physics, CPCL Polytechnic College, Chennai 600 068, India. *Correspondence e-mail: ryamuna1@gmail.com, chakkaravarthi_2005@yahoo.com

Received 13 December 2014
Accepted 24 December 2014

Edited by H. Ishida, Okayama University, Japan

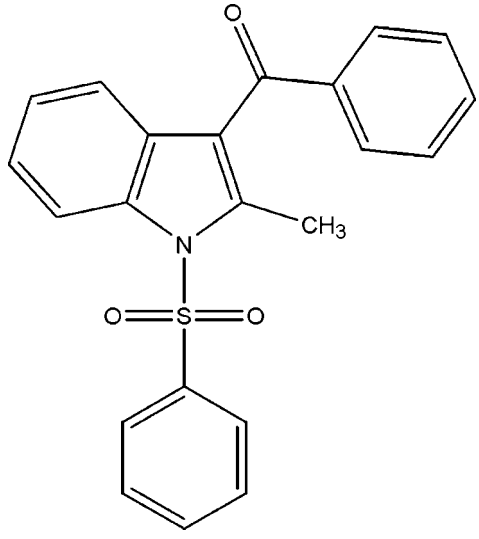
Keywords: Indole derivative; crystal structure; C—H···O hydrogen bonds

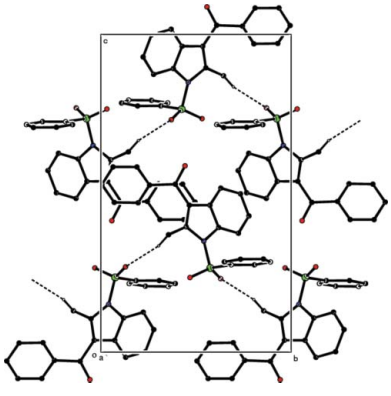
CCDC reference: 1040926
Supporting information: this article has supporting information at journals.iucr.org/e

In the title compound, $C_{22}H_{17}NO_3S$, the sulfonyl-bound phenyl ring is almost orthogonal to the indole ring system, making a dihedral angle of 84.89 (7)°. The carbonyl-bound phenyl ring forms a dihedral angle of 57.32 (5)° with the indole ring system. The two phenyl rings are inclined at 52.68 (7)°. The S atom has a distorted tetrahedral configuration. In the crystal, weak C—H···O interactions link the molecules, forming a helical chain along the *b*-axis direction.

1. Chemical context

In a continuation of our studies on indole derivatives, which possess various biological activities such as antihepatitis B virus (Chai *et al.*, 2006) and antibacterial (Nieto *et al.*, 2005) *etc*, we herein report the synthesis and the crystal structure of the title compound, (I).





2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The sulfonyl-bound phenyl ring (C1–C6) is almost orthogonal to the indole ring system (N1/C7–C14), making a dihedral angle of 84.89 (7)°. The carbonyl-bound phenyl ring (C17–C22) forms a dihedral angle of 57.32 (5)° with the indole ring system. The two phenyl rings are inclined at an angle of 52.68 (7)°. Atom S1 has a distorted tetrahedral configuration

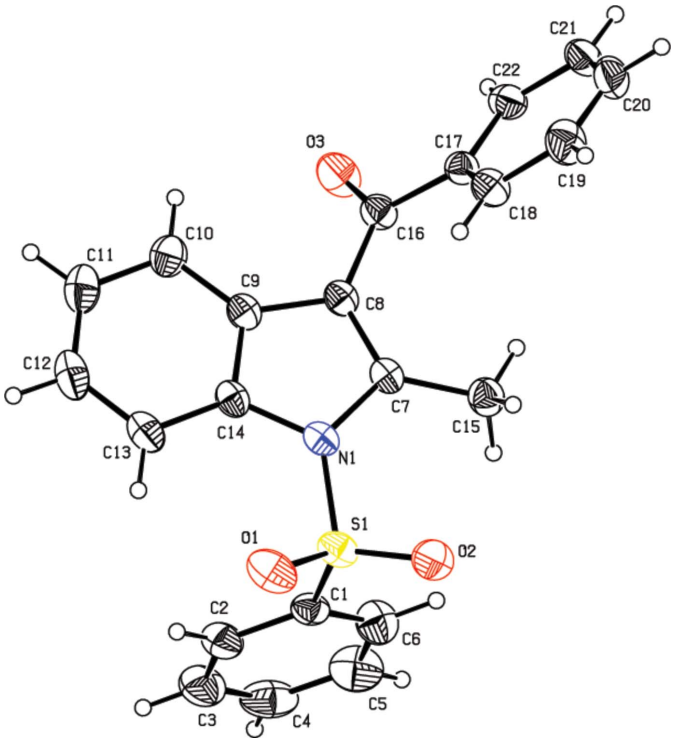


Figure 1
The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

with angles O1—S1—O2 [119.97 (10)°] and N1—S1—C1 [104.99 (8)°] differing from the ideal tetrahedral value. As a result of the electron-withdrawing character of the phenylsulfonyl group, the bond lengths N1—C7 [1.420 (2) Å] and N1—C14 [1.419 (2) Å] are longer than the mean value of 1.355 (14) Å (Allen *et al.*, 1987). The geometric parameters of (I) agree well with those in similar reported structures (Chakkaravarthi *et al.*, 2008, 2009).

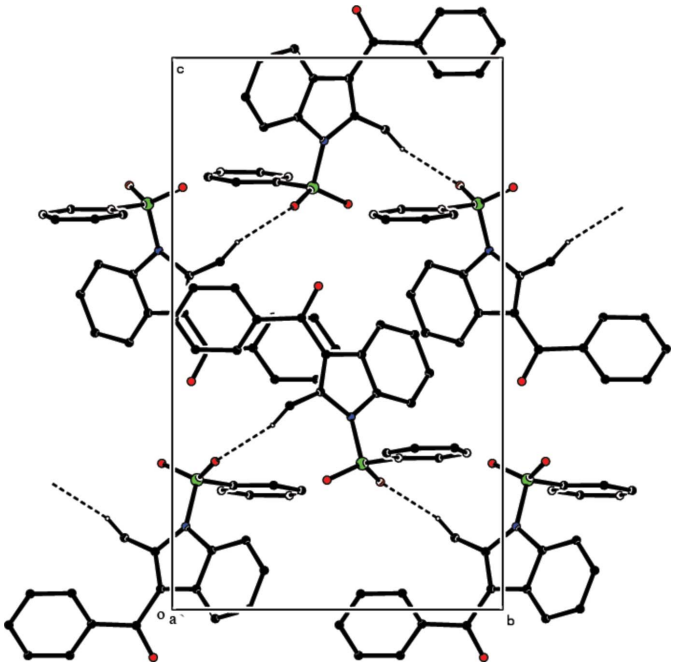


Figure 2
The packing diagram of the title compound, viewed down the *a* axis. Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15C···O1^{i}	0.96	2.59	3.525 (3)	165

Symmetry code: (i) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$.

3. Supramolecular features

In the crystal, weak C—H···O interactions link the molecules, forming a helical chain along the *b*-axis direction (Table 1 and Fig. 2). No significant π–π or C—H···π interactions are observed.

4. Database survey

A search of the Cambridge Structural Database (Version 5.35, last update May 2014; Groom & Allen, 2014). indicated 123 compounds having a phenylsulfonyl-1*H*-indole moiety. Of these compounds, several similar structures have been

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{17}NO_3S$
M_r	375.43
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	295
a, b, c (Å)	8.9989 (7), 11.0036 (9), 18.4209 (16)
V (Å^3)	1824.0 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.20
Crystal size (mm)	0.28 × 0.24 × 0.20
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 1996)
T_{min}, T_{max}	0.946, 0.961
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26244, 5020, 3493
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.708
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.091, 1.02
No. of reflections	5020
No. of parameters	246
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.25
Absolute structure	Flack (1983), 2109 Friedel pairs
Absolute structure parameter	−0.01 (7)

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

reported earlier, *i.e.* ethyl 2-acetoxymethyl-1-phenylsulfonyl-1*H*-indole-3-carboxylate (Gunasekaran *et al.*, 2009), 3-iodo-2-methyl-1-phenylsulfonyl-1*H*-indole (Ramathilagam *et al.*, 2011) and 1-(2-bromomethyl-1-phenylsulfonyl-1*H*-indol-3-yl)propan-1-one (Umadevi *et al.*, 2013). In these structures, the sulfonyl-bound phenyl ring is almost orthogonal to the indole ring system, the dihedral angles of 83.35 (5), 82.84 (9) and 89.91 (11)°, respectively, being are comparable with that in the title compound.

5. Synthesis and crystallization

To a solution of benzoyl chloride (1.55 g, 11.07 mmol) in dry DCM (25 ml), $SnCl_4$ (2.88 g, 10.10 mmol) at 273 K was added dropwise. To this, phenylsulfonyl-1*H*-indole (2 g, 7.38 mmol) in dry DCM (10 ml) was added dropwise (5 min) and stirred for 30 min at the same temperature. After completion of the reaction (monitored by TLC), it was poured over ice–water (50 ml) and extracted with saturated aqueous $NaHCO_3$ (2 × 30 ml) and brine (2 × 30 ml), dried (Na_2SO_4) and concentrated under reduced pressure. Then, the crude product was crystallized from methanol to afford single crystals of the title compound suitable for X-ray diffraction.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms for $C_{aromatic}$ and C_{methyl} were positioned geometrically and refined using a riding model, with C—H = 0.93 and 0.97 Å, respectively with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for other H atoms.

Acknowledgements

The authors wish to acknowledge the SAIF, IIT, Madras, for the data collection.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin. Trans. 2*, pp. S1–19.
Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chai, H., Zhao, C., Zhao, C. & Gong, P. (2006). *Bioorg. Med. Chem.* **14**, 911–917.
Chakkaravarthi, G., Marx, A., Dhayalan, V., Mohanakrishnan, A. K. & Manivannan, V. (2009). *Acta Cryst.* E**65**, o464–o465.
Chakkaravarthi, G., Sureshbabu, R., Mohanakrishnan, A. K. & Manivannan, V. (2008). *Acta Cryst.* E**64**, o751.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Groom, C. R. & Allen, F. H. (2014). *Angew. Chem. Int. Ed.* **53**, 662–671.
Gunasekaran, B., Sureshbabu, R., Mohanakrishnan, A. K., Chakkaravarthi, G. & Manivannan, V. (2009). *Acta Cryst.* E**65**, o2069.
Nieto, M. J., Alovero, F. L., Manzo, R. H. & Mazzieri, M. R. (2005). *Eur. J. Med. Chem.* **40**, 361–369.
Ramathilagam, C., Saravanan, V., Mohanakrishnan, A. K., Chakkaravarthi, G., Umarani, P. R. & Manivannan, V. (2011). *Acta Cryst.* E**67**, o632.
Sheldrick, G. M. (1996). *SADABS*, University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Umadevi, M., Saravanan, V., Yamuna, R., Mohanakrishnan, A. K. & Chakkaravarthi, G. (2013). *Acta Cryst.* E**69**, o1802–o1803.

supporting information

Acta Cryst. (2015). E**71**, 133-135 [doi:10.1107/S2056989014028059]

Crystal structure of (2-methyl-1-phenylsulfonyl-1*H*-indol-3-yl)(phenyl)-methanone

M. Umadevi, V. Saravanan, R. Yamuna, A. K. Mohanakrishnan and G. Chakkaravarthi

Computing details

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

(2-Methyl-1-phenylsulfonyl-1*H*-indol-3-yl)(phenyl)methanone

Crystal data

$C_{22}H_{17}NO_3S$
M_r = 375.43
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
a = 8.9989 (7) Å
b = 11.0036 (9) Å
c = 18.4209 (16) Å
V = 1824.0 (3) Å^3
Z = 4
$F(000)$ = 784
D_x = 1.367 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 812 reflections
θ = 2.2–30.2°
μ = 0.20 mm^{-1}
T = 295 K
Block, colourless
0.28 × 0.24 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.946, T_{max} = 0.961
26244 measured reflections
5020 independent reflections
3493 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 30.2°, θ_{min} = 2.2°
h = −12→12
k = −14→14
l = −25→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.091
S = 1.02
5020 reflections
246 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0353P)^2 + 0.2764P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0039 (8)

Absolute structure: Flack (1983), 2109 Friedel pairs
Absolute structure parameter: −0.01 (7)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2369 (2)	0.81475 (17)	0.72517 (9)	0.0469 (4)
C2	0.2009 (3)	0.69315 (19)	0.72539 (12)	0.0623 (6)
H2	0.1029	0.6684	0.7318	0.075*
C3	0.3119 (4)	0.6089 (2)	0.71605 (14)	0.0779 (8)
H3	0.2891	0.5265	0.7160	0.093*
C4	0.4552 (4)	0.6457 (3)	0.70682 (13)	0.0797 (8)
H4	0.5295	0.5881	0.6999	0.096*
C5	0.4904 (3)	0.7661 (3)	0.70759 (15)	0.0815 (8)
H5	0.5889	0.7903	0.7025	0.098*
C6	0.3812 (3)	0.8512 (2)	0.71586 (13)	0.0658 (6)
H6	0.4047	0.9335	0.7152	0.079*
C7	0.1037 (2)	1.05176 (15)	0.60528 (9)	0.0405 (4)
C8	0.0471 (2)	1.03514 (16)	0.53755 (10)	0.0417 (4)
C9	−0.0431 (2)	0.92698 (17)	0.53745 (10)	0.0421 (4)
C10	−0.1247 (2)	0.86956 (18)	0.48385 (12)	0.0566 (5)
H10	−0.1258	0.8998	0.4367	0.068*
C11	−0.2046 (3)	0.7663 (2)	0.50152 (15)	0.0667 (6)
H11	−0.2593	0.7266	0.4659	0.080*
C12	−0.2040 (3)	0.72186 (19)	0.57128 (15)	0.0651 (6)
H12	−0.2588	0.6524	0.5819	0.078*
C13	−0.1248 (2)	0.77715 (17)	0.62583 (13)	0.0549 (5)
H13	−0.1251	0.7466	0.6729	0.066*
C14	−0.0439 (2)	0.88084 (16)	0.60774 (11)	0.0429 (4)
C15	0.2119 (2)	1.14443 (19)	0.63034 (11)	0.0521 (5)
H15A	0.2445	1.1921	0.5897	0.078*
H15B	0.2959	1.1047	0.6520	0.078*
H15C	0.1654	1.1964	0.6655	0.078*
C16	0.0714 (2)	1.10898 (16)	0.47141 (10)	0.0462 (4)
C17	0.0621 (2)	1.24405 (16)	0.47428 (10)	0.0425 (4)
C18	−0.0098 (2)	1.30428 (18)	0.52995 (12)	0.0513 (5)
H18	−0.0503	1.2605	0.5683	0.062*
C19	−0.0215 (3)	1.4297 (2)	0.52874 (14)	0.0667 (6)

H19	−0.0699	1.4700	0.5663	0.080*
C20	0.0380 (3)	1.4945 (2)	0.47233 (15)	0.0684 (7)
H20	0.0296	1.5787	0.4716	0.082*
C21	0.1096 (3)	1.4360 (2)	0.41704 (13)	0.0633 (6)
H21	0.1511	1.4805	0.3792	0.076*
C22	0.1204 (2)	1.31043 (19)	0.41723 (11)	0.0512 (5)
H22	0.1671	1.2707	0.3789	0.061*
N1	0.04557 (17)	0.95902 (13)	0.65071 (8)	0.0436 (4)
O1	−0.02677 (18)	0.87038 (14)	0.76860 (8)	0.0700 (4)
O2	0.16072 (19)	1.03169 (12)	0.76515 (8)	0.0632 (4)
O3	0.0922 (2)	1.05764 (13)	0.41366 (7)	0.0699 (4)
S1	0.09803 (6)	0.92484 (4)	0.73525 (3)	0.04934 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0585 (12)	0.0484 (10)	0.0339 (9)	0.0054 (9)	0.0015 (9)	0.0024 (9)
C2	0.0712 (14)	0.0513 (12)	0.0644 (14)	0.0075 (11)	−0.0075 (12)	0.0094 (11)
C3	0.103 (2)	0.0516 (14)	0.0789 (17)	0.0201 (14)	−0.0139 (16)	−0.0001 (12)
C4	0.098 (2)	0.0856 (19)	0.0556 (14)	0.0464 (17)	−0.0027 (14)	−0.0015 (13)
C5	0.0655 (17)	0.095 (2)	0.0836 (19)	0.0196 (15)	0.0100 (14)	0.0062 (16)
C6	0.0626 (14)	0.0606 (13)	0.0743 (15)	0.0054 (12)	0.0048 (12)	−0.0017 (11)
C7	0.0405 (9)	0.0364 (9)	0.0448 (9)	0.0027 (8)	0.0077 (8)	0.0009 (7)
C8	0.0453 (10)	0.0362 (9)	0.0436 (10)	0.0040 (8)	0.0065 (8)	−0.0015 (8)
C9	0.0441 (9)	0.0346 (9)	0.0476 (10)	0.0067 (8)	0.0068 (8)	−0.0029 (8)
C10	0.0608 (13)	0.0529 (11)	0.0560 (12)	−0.0004 (11)	0.0006 (11)	−0.0103 (10)
C11	0.0660 (15)	0.0526 (13)	0.0813 (16)	−0.0068 (11)	0.0007 (13)	−0.0177 (12)
C12	0.0555 (14)	0.0402 (11)	0.0995 (19)	−0.0051 (10)	0.0087 (13)	−0.0040 (12)
C13	0.0497 (12)	0.0417 (10)	0.0732 (13)	0.0019 (10)	0.0084 (11)	0.0106 (10)
C14	0.0395 (9)	0.0350 (9)	0.0541 (11)	0.0043 (8)	0.0071 (8)	0.0014 (8)
C15	0.0556 (12)	0.0503 (11)	0.0505 (11)	−0.0049 (10)	0.0045 (10)	0.0007 (9)
C16	0.0526 (12)	0.0440 (10)	0.0422 (10)	0.0019 (9)	0.0055 (9)	0.0012 (8)
C17	0.0403 (10)	0.0430 (10)	0.0443 (10)	−0.0004 (8)	−0.0011 (8)	0.0036 (8)
C18	0.0530 (12)	0.0469 (11)	0.0539 (12)	0.0055 (9)	0.0062 (10)	0.0011 (10)
C19	0.0682 (14)	0.0498 (12)	0.0821 (16)	0.0095 (12)	−0.0013 (13)	−0.0096 (13)
C20	0.0693 (15)	0.0408 (11)	0.095 (2)	−0.0042 (11)	−0.0175 (15)	0.0054 (13)
C21	0.0614 (13)	0.0547 (12)	0.0736 (14)	−0.0124 (12)	−0.0097 (12)	0.0233 (12)
C22	0.0468 (11)	0.0554 (12)	0.0512 (11)	−0.0008 (10)	−0.0007 (9)	0.0098 (9)
N1	0.0454 (9)	0.0403 (8)	0.0452 (8)	0.0020 (7)	0.0056 (7)	0.0064 (7)
O1	0.0734 (10)	0.0768 (10)	0.0599 (9)	0.0050 (8)	0.0309 (8)	0.0169 (8)
O2	0.0924 (11)	0.0505 (8)	0.0466 (8)	0.0073 (7)	0.0019 (8)	−0.0101 (7)
O3	0.1119 (13)	0.0526 (8)	0.0453 (8)	0.0015 (10)	0.0186 (9)	−0.0054 (7)
S1	0.0614 (3)	0.0477 (3)	0.0389 (2)	0.0074 (2)	0.0117 (2)	0.0022 (2)

Geometric parameters (Å, º)

C1—C6	1.369 (3)	C12—H12	0.9300
C1—C2	1.377 (3)	C13—C14	1.394 (3)

C1—S1	1.750 (2)	C13—H13	0.9300
C2—C3	1.373 (3)	C14—N1	1.419 (2)
C2—H2	0.9300	C15—H15A	0.9600
C3—C4	1.362 (4)	C15—H15B	0.9600
C3—H3	0.9300	C15—H15C	0.9600
C4—C5	1.363 (4)	C16—O3	1.219 (2)
C4—H4	0.9300	C16—C17	1.490 (3)
C5—C6	1.366 (3)	C17—C18	1.382 (3)
C5—H5	0.9300	C17—C22	1.383 (3)
C6—H6	0.9300	C18—C19	1.384 (3)
C7—C8	1.360 (2)	C18—H18	0.9300
C7—N1	1.420 (2)	C19—C20	1.369 (3)
C7—C15	1.483 (3)	C19—H19	0.9300
C8—C9	1.441 (3)	C20—C21	1.366 (3)
C8—C16	1.481 (2)	C20—H20	0.9300
C9—C10	1.383 (3)	C21—C22	1.385 (3)
C9—C14	1.391 (3)	C21—H21	0.9300
C10—C11	1.384 (3)	C22—H22	0.9300
C10—H10	0.9300	N1—S1	1.6701 (16)
C11—C12	1.375 (4)	O1—S1	1.4134 (15)
C11—H11	0.9300	O2—S1	1.4156 (15)
C12—C13	1.374 (3)		

C6—C1—C2	120.5 (2)	C9—C14—C13	121.60 (19)
C6—C1—S1	119.18 (17)	C9—C14—N1	107.17 (16)
C2—C1—S1	120.28 (17)	C13—C14—N1	131.22 (19)
C3—C2—C1	119.0 (2)	C7—C15—H15A	109.5
C3—C2—H2	120.5	C7—C15—H15B	109.5
C1—C2—H2	120.5	H15A—C15—H15B	109.5
C4—C3—C2	120.3 (2)	C7—C15—H15C	109.5
C4—C3—H3	119.9	H15A—C15—H15C	109.5
C2—C3—H3	119.9	H15B—C15—H15C	109.5
C3—C4—C5	120.5 (3)	O3—C16—C8	119.11 (16)
C3—C4—H4	119.7	O3—C16—C17	120.13 (17)
C5—C4—H4	119.7	C8—C16—C17	120.66 (16)
C4—C5—C6	120.0 (3)	C18—C17—C22	119.23 (18)
C4—C5—H5	120.0	C18—C17—C16	122.10 (17)
C6—C5—H5	120.0	C22—C17—C16	118.58 (17)
C5—C6—C1	119.7 (2)	C17—C18—C19	120.1 (2)
C5—C6—H6	120.1	C17—C18—H18	119.9
C1—C6—H6	120.1	C19—C18—H18	119.9
C8—C7—N1	107.82 (15)	C20—C19—C18	120.1 (2)
C8—C7—C15	128.60 (16)	C20—C19—H19	120.0
N1—C7—C15	123.54 (16)	C18—C19—H19	120.0
C7—C8—C9	108.87 (16)	C21—C20—C19	120.3 (2)
C7—C8—C16	128.73 (17)	C21—C20—H20	119.8
C9—C8—C16	122.38 (17)	C19—C20—H20	119.8
C10—C9—C14	119.69 (18)	C20—C21—C22	120.1 (2)

C10—C9—C8	132.63 (18)	C20—C21—H21	120.0
C14—C9—C8	107.64 (17)	C22—C21—H21	120.0
C9—C10—C11	118.9 (2)	C17—C22—C21	120.1 (2)
C9—C10—H10	120.6	C17—C22—H22	119.9
C11—C10—H10	120.6	C21—C22—H22	119.9
C12—C11—C10	120.6 (2)	C14—N1—C7	108.41 (14)
C12—C11—H11	119.7	C14—N1—S1	122.94 (12)
C10—C11—H11	119.7	C7—N1—S1	127.40 (13)
C13—C12—C11	121.9 (2)	O1—S1—O2	119.97 (10)
C13—C12—H12	119.1	O1—S1—N1	106.03 (10)
C11—C12—H12	119.1	O2—S1—N1	106.76 (8)
C12—C13—C14	117.3 (2)	O1—S1—C1	108.67 (10)
C12—C13—H13	121.4	O2—S1—C1	109.36 (10)
C14—C13—H13	121.4	N1—S1—C1	104.99 (8)

C6—C1—C2—C3	−0.1 (3)	C8—C16—C17—C18	−19.3 (3)
S1—C1—C2—C3	178.83 (18)	O3—C16—C17—C22	−19.3 (3)
C1—C2—C3—C4	0.1 (4)	C8—C16—C17—C22	164.22 (18)
C2—C3—C4—C5	0.8 (4)	C22—C17—C18—C19	−0.6 (3)
C3—C4—C5—C6	−1.6 (4)	C16—C17—C18—C19	−177.1 (2)
C4—C5—C6—C1	1.6 (4)	C17—C18—C19—C20	0.0 (3)
C2—C1—C6—C5	−0.8 (3)	C18—C19—C20—C21	−0.2 (4)
S1—C1—C6—C5	−179.70 (19)	C19—C20—C21—C22	1.0 (4)
N1—C7—C8—C9	−2.92 (19)	C18—C17—C22—C21	1.4 (3)
C15—C7—C8—C9	174.62 (18)	C16—C17—C22—C21	178.01 (19)
N1—C7—C8—C16	178.71 (17)	C20—C21—C22—C17	−1.6 (3)
C15—C7—C8—C16	−3.8 (3)	C9—C14—N1—C7	−1.39 (19)
C7—C8—C9—C10	−179.9 (2)	C13—C14—N1—C7	179.84 (19)
C16—C8—C9—C10	−1.4 (3)	C9—C14—N1—S1	−169.49 (12)
C7—C8—C9—C14	2.1 (2)	C13—C14—N1—S1	11.7 (3)
C16—C8—C9—C14	−179.42 (16)	C8—C7—N1—C14	2.70 (19)
C14—C9—C10—C11	−0.5 (3)	C15—C7—N1—C14	−174.99 (17)
C8—C9—C10—C11	−178.31 (19)	C8—C7—N1—S1	170.12 (13)
C9—C10—C11—C12	0.5 (3)	C15—C7—N1—S1	−7.6 (2)
C10—C11—C12—C13	−0.1 (4)	C14—N1—S1—O1	−40.28 (16)
C11—C12—C13—C14	−0.1 (3)	C7—N1—S1—O1	153.97 (15)
C10—C9—C14—C13	0.2 (3)	C14—N1—S1—O2	−169.29 (14)
C8—C9—C14—C13	178.55 (17)	C7—N1—S1—O2	24.96 (17)
C10—C9—C14—N1	−178.67 (16)	C14—N1—S1—C1	74.67 (16)
C8—C9—C14—N1	−0.37 (19)	C7—N1—S1—C1	−91.08 (16)
C12—C13—C14—C9	0.1 (3)	C6—C1—S1—O1	−159.68 (17)
C12—C13—C14—N1	178.71 (19)	C2—C1—S1—O1	21.40 (19)
C7—C8—C16—O3	137.3 (2)	C6—C1—S1—O2	−27.02 (19)
C9—C8—C16—O3	−40.9 (3)	C2—C1—S1—O2	154.07 (17)
C7—C8—C16—C17	−46.2 (3)	C6—C1—S1—N1	87.22 (18)
C9—C8—C16—C17	135.63 (18)	C2—C1—S1—N1	−91.69 (17)
O3—C16—C17—C18	157.2 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15*C*···O1^{i}	0.96	2.59	3.525 (3)	165

Symmetry code: (i) −*x*, *y*+1/2, −*z*+3/2.