Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(2-Bromomethyl-1-phenylsulfonyl-1*H*-indol-3-yl)propan-1-one

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

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

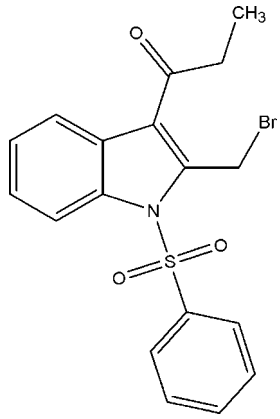
Received 13 November 2013; accepted 16 November 2013

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.052; wR factor = 0.133; data-to-parameter ratio = 33.5.

In the title compound, $C_{18}H_{16}BrNO_3S$, the dihedral angle between the phenyl ring and the indole ring system is 89.91 (11)°. The molecular structure features weak C—H···O and C—H···Br hydrogen bonds. In the crystal, molecules are linked by weak C—H···O hydrogen bonds, forming chains along the *a*-axis direction. The chains are further linked by C—H···π interactions, forming a layer parallel to the *ab* plane.

Related literature

For the biological activity of indole derivatives, see: Chai *et al.* (2006); Nieto *et al.* (2005). For related structures, see: Chakkaravarthi *et al.* (2008, 2010). For details of the configuration at the S atom, see: Bassindale (1984). For details of N-atom hybridization, see: Beddoes *et al.* (1986).



Experimental

Crystal data

$C_{18}H_{16}BrNO_3S$
M_r = 406.29
Monoclinic, $P2_1/c$
a = 10.2772 (7) Å
b = 8.6610 (6) Å
c = 18.8980 (14) Å
β = 90.676 (2)°
V = 1682.0 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.58 mm^{-1}
T = 295 K
0.38 × 0.34 × 0.30 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.397, T_{max} = 0.461
25944 measured reflections
7303 independent reflections
3726 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.133
S = 1.00
7303 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-3}

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

*Cg*2 and *Cg*3 are the centroids of the C1–C6 and C9–C14 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···Br1	0.93	2.89	3.815 (2)	171
C13—H13···O2	0.93	2.39	2.978 (3)	121
C15—H15*B*···O1	0.97	2.15	2.833 (3)	126
C2—H2···O3^{i}	0.93	2.59	3.191 (3)	123
C15—H15*A*···*Cg*3^{ii}	0.97	2.74	3.486 (3)	134
C18—H18*B*···*Cg*2^{iii}	0.96	2.66	3.616 (3)	174

Symmetry codes: (i) $x+1, y, z$; (ii) $-x, -y+1, -z+2$; (iii) $-x, -y, -z+2$.

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: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5323).

References

Bassindale, A. (1984). In *The Third Dimension in Organic Chemistry*. New York: John Wiley and Sons.

Beddoes, R. L., Dalton, L., Joule, T. A., Mills, O. S., Street, J. D. & Watt, C. I. F. (1986). *J. Chem. Soc. Perkin Trans. 2*, pp. 787–797.

Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Chai, H., Zhao, C. & Gong, P. (2006). *Bioorg. Med. Chem.* **14**, 911–917.

Chakkaravarthi, G., Dhayalan, V., Mohanakrishnan, A. K. & Manivannan, V. (2008). *Acta Cryst.* E**64**, o749.

Chakkaravarthi, G., Panchatcharam, R., Dhayalan, V., Mohanakrishnan, A. K. & Manivannan, V. (2010). *Acta Cryst.* E**66**, o2957.

Nieto, M. J., Alovero, F. L., Manzo, R. H. & Mazzieri, M. R. (2005). *Eur. J. Med. Chem.* **40**, 361–369.

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.

supplementary materials

Acta Cryst. (2013). E**69**, o1802–o1803 [doi:10.1107/S1600536813031413]

1-(2-Bromomethyl-1-phenylsulfonyl-1*H*-indol-3-yl)propan-1-one

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

1. Comment

Indole derivatives exhibit antihepatitis B virus (Chai *et al.*, 2006) and antibacterial (Nieto *et al.*, 2005) activities. We herein report the crystal structure of the title compound (I) (Fig. 1). The bond distances of (I) are comparable with the reported similar structures (Chakkaravarthi *et al.*, 2008, 2010). The bond angles around atom S1 show significant deviation from ideal tetrahedral value [O1—S1—O2 = 120.16 (13)° and N1—S1—C1 = 105.11 (10)°] due to Thorpe-Ignold effect (Bassindale, 1984). The sum of the bond angles around N1 (358.05°) indicates the sp^2 hybridization of N1 atom (Beddoes *et al.*, 1986).

The indole ring system is planar, with the dihedral angle between the two rings (N1/C7/C8/C9/C14) and (C9–C14) is 2.00 (12)°. The phenyl ring (C1–C6) makes the dihedral angle of 89.91 (11)° with the indole ring system. The molecular structure is stabilized by weak intramolecular C—H···O and C—H···Br hydrogen bonds (Table 1). The crystal structure exhibit weak intermolecular C—H···O and C—H···π (Table 1 & Fig. 2) interactions.

2. Experimental

A mixture of 1-[2-methyl-1-(phenylsulfonyl)-1*H*-indol-3-yl]propan-1-one (15 g, 45.87 mmol) and *N*-bromosuccinimide (9.8 g, 55 mmol) in dry CCl_4 (250 ml) containing a catalytic amount of 2,2′-azobis(isobutyronitrile) (50 mg) was refluxed for 3 h. Then, the reaction mixture was cooled to room temperature, filtered off the floated succinimide through Na_2SO_4 pad and washed with CCl_4 (20 ml). Removal of the solvent followed by trituration of the crude product with MeOH (50 ml) gave the title compound, suitable for X-ray diffraction quality.

3. Refinement

H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}).

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).

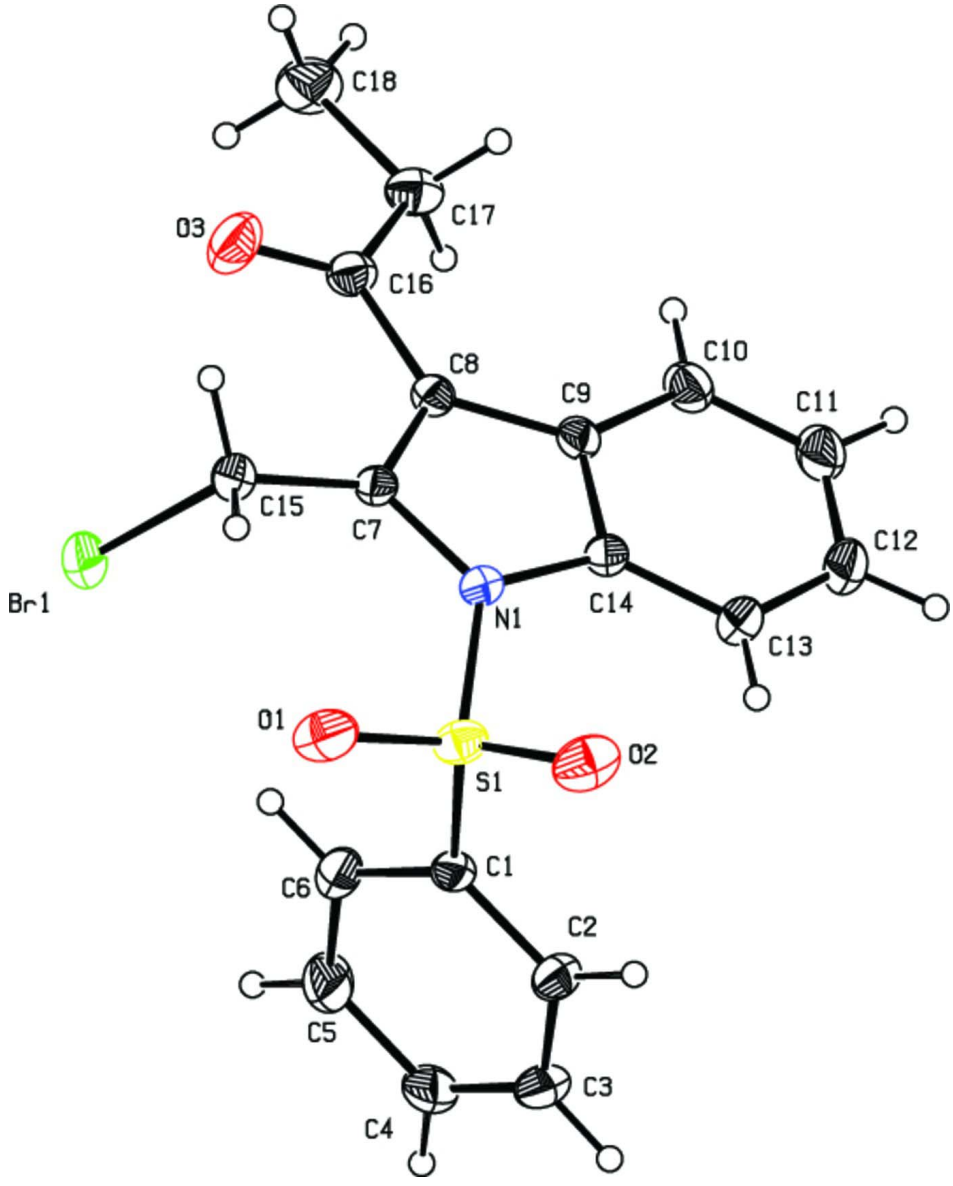


Figure 1

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

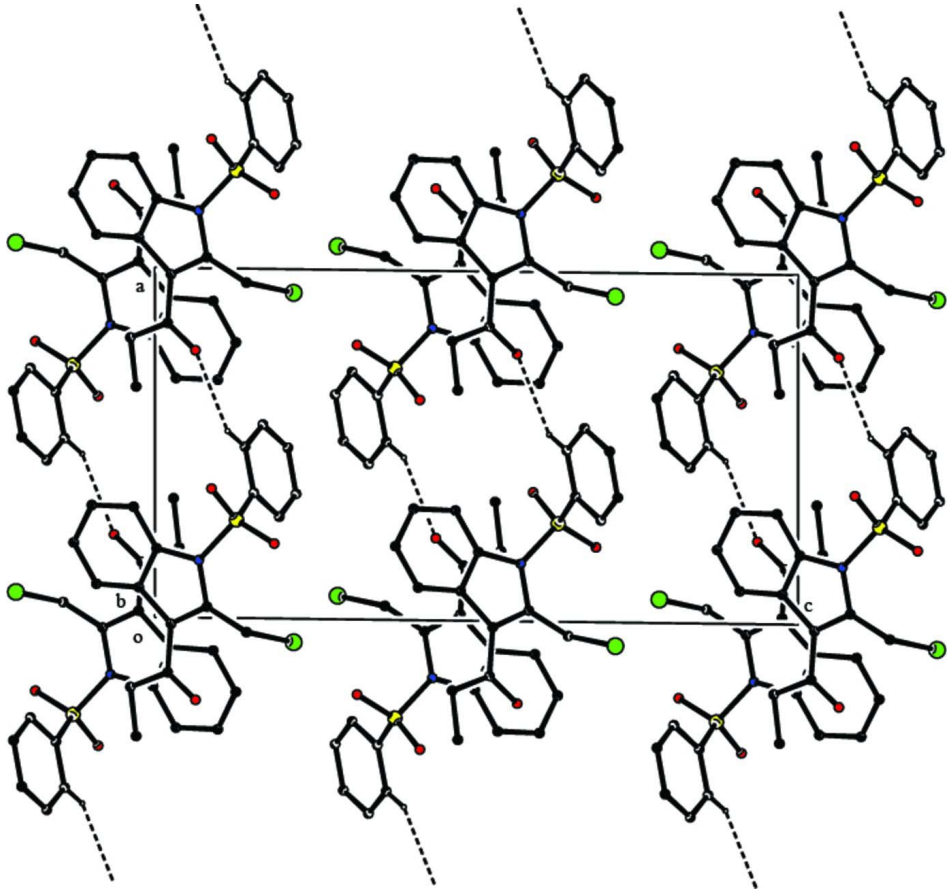


Figure 2

A packing diagram of the title compound viewed down the *b* axis. Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involving hydrogen bonding have been omitted.

1-(2-Bromomethyl-1-phenylsulfonyl-1*H*-indol-3-yl)propan-1-one

Crystal data

$C_{18}H_{16}BrNO_3S$
$M_r = 406.29$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.2772$ (7) Å
$b = 8.6610$ (6) Å
$c = 18.8980$ (14) Å
$\beta = 90.676$ (2)°
$V = 1682.0$ (2) Å^3
$Z = 4$
$F(000) = 824$
$D_x = 1.604$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5675 reflections
$\theta = 2.6$–$28.2°$
$\mu = 2.58$ mm^{-1}
$T = 295$ K
Block, colourless
0.38 × 0.34 × 0.30 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.397$, $T_{max} = 0.461$
25944 measured reflections
7303 independent reflections
3726 reflections with $I > 2\sigma(I)$

R_{int} = 0.036
θ_{max} = 35.0°, θ_{min} = 2.2°
h = −16→15
k = −13→13
l = −30→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.133
S = 1.00
7303 reflections
218 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
$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 0.8633P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3590 (2)	0.2855 (3)	1.15387 (11)	0.0316 (4)
C2	0.4906 (2)	0.2669 (3)	1.14030 (14)	0.0388 (5)
H2	0.5349	0.3387	1.1130	0.047*
C3	0.5545 (2)	0.1404 (3)	1.16792 (14)	0.0478 (6)
H3	0.6429	0.1276	1.1599	0.057*
C4	0.4891 (3)	0.0341 (4)	1.20682 (14)	0.0527 (7)
H4	0.5334	−0.0508	1.2251	0.063*
C5	0.3573 (3)	0.0506 (4)	1.21952 (16)	0.0594 (8)
H5	0.3134	−0.0236	1.2456	0.071*
C6	0.2917 (2)	0.1775 (3)	1.19338 (14)	0.0468 (6)
H6	0.2035	0.1906	1.2021	0.056*
C7	0.03158 (18)	0.3688 (2)	1.08099 (11)	0.0276 (4)
C8	−0.0180 (2)	0.2867 (2)	1.02518 (11)	0.0290 (4)
C9	0.0851 (2)	0.2600 (2)	0.97521 (11)	0.0304 (4)
C10	0.0935 (2)	0.1861 (3)	0.90938 (12)	0.0407 (5)
H10	0.0217	0.1359	0.8898	0.049*
C11	0.2110 (3)	0.1894 (3)	0.87400 (14)	0.0492 (7)
H11	0.2173	0.1407	0.8303	0.059*
C12	0.3188 (3)	0.2635 (3)	0.90221 (14)	0.0491 (7)
H12	0.3957	0.2646	0.8768	0.059*
C13	0.3152 (2)	0.3356 (3)	0.96705 (13)	0.0411 (6)
H13	0.3880	0.3847	0.9861	0.049*
C14	0.19702 (19)	0.3317 (3)	1.00296 (11)	0.0306 (4)
C15	−0.0399 (2)	0.4324 (3)	1.14247 (12)	0.0358 (5)
H15A	−0.1235	0.4717	1.1264	0.043*
H15B	0.0090	0.5179	1.1625	0.043*

C16	−0.1576 (2)	0.2394 (3)	1.02006 (13)	0.0355 (5)
C17	−0.2006 (2)	0.1315 (3)	0.96217 (14)	0.0419 (6)
H17A	−0.1440	0.0418	0.9621	0.050*
H17B	−0.1922	0.1829	0.9169	0.050*
C18	−0.3408 (3)	0.0787 (4)	0.97091 (16)	0.0561 (7)
H18A	−0.3494	0.0268	1.0155	0.084*
H18B	−0.3639	0.0093	0.9332	0.084*
H18C	−0.3975	0.1668	0.9696	0.084*
N1	0.16494 (16)	0.3982 (2)	1.06867 (9)	0.0299 (4)
O1	0.21453 (16)	0.5195 (2)	1.18571 (10)	0.0523 (5)
O2	0.36972 (17)	0.5470 (2)	1.08811 (11)	0.0523 (5)
O3	−0.23528 (17)	0.2863 (3)	1.06323 (11)	0.0571 (5)
S1	0.28085 (5)	0.45547 (7)	1.12687 (3)	0.03548 (14)
Br1	−0.06733 (3)	0.27582 (4)	1.215850 (15)	0.06069 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0272 (9)	0.0409 (12)	0.0268 (10)	0.0035 (9)	−0.0028 (8)	−0.0044 (9)
C2	0.0273 (10)	0.0475 (14)	0.0417 (13)	−0.0015 (9)	0.0007 (9)	−0.0020 (11)
C3	0.0305 (11)	0.0644 (18)	0.0484 (15)	0.0119 (11)	−0.0046 (10)	−0.0013 (13)
C4	0.0490 (14)	0.0675 (19)	0.0415 (14)	0.0214 (14)	−0.0025 (12)	0.0139 (13)
C5	0.0545 (16)	0.072 (2)	0.0515 (16)	0.0105 (15)	0.0129 (13)	0.0290 (15)
C6	0.0332 (11)	0.0619 (17)	0.0456 (15)	0.0068 (11)	0.0090 (10)	0.0126 (13)
C7	0.0253 (8)	0.0293 (11)	0.0281 (10)	0.0034 (8)	0.0001 (8)	0.0040 (8)
C8	0.0285 (9)	0.0303 (11)	0.0281 (10)	0.0006 (8)	−0.0007 (8)	0.0036 (8)
C9	0.0324 (10)	0.0318 (11)	0.0270 (10)	0.0045 (8)	0.0001 (8)	0.0047 (8)
C10	0.0456 (13)	0.0457 (14)	0.0307 (12)	0.0055 (11)	−0.0012 (10)	−0.0033 (10)
C11	0.0534 (15)	0.0605 (17)	0.0339 (13)	0.0191 (13)	0.0064 (11)	−0.0038 (12)
C12	0.0409 (12)	0.0657 (18)	0.0411 (14)	0.0144 (12)	0.0138 (11)	0.0046 (13)
C13	0.0302 (10)	0.0525 (15)	0.0409 (13)	0.0053 (10)	0.0052 (10)	0.0047 (11)
C14	0.0283 (9)	0.0341 (11)	0.0294 (10)	0.0056 (8)	0.0008 (8)	0.0040 (9)
C15	0.0331 (10)	0.0424 (13)	0.0321 (11)	0.0050 (9)	0.0036 (9)	−0.0016 (10)
C16	0.0308 (10)	0.0373 (13)	0.0383 (12)	−0.0023 (9)	−0.0034 (9)	0.0044 (10)
C17	0.0404 (12)	0.0399 (14)	0.0452 (14)	−0.0030 (10)	−0.0091 (11)	0.0015 (11)
C18	0.0482 (15)	0.0594 (18)	0.0606 (18)	−0.0179 (13)	−0.0115 (13)	−0.0020 (15)
N1	0.0244 (7)	0.0356 (10)	0.0296 (9)	0.0016 (7)	−0.0013 (7)	−0.0002 (8)
O1	0.0429 (9)	0.0590 (12)	0.0548 (11)	0.0097 (8)	−0.0095 (8)	−0.0286 (9)
O2	0.0412 (9)	0.0383 (10)	0.0774 (14)	−0.0094 (8)	−0.0049 (9)	0.0062 (10)
O3	0.0341 (9)	0.0783 (14)	0.0593 (13)	−0.0117 (9)	0.0086 (8)	−0.0156 (11)
S1	0.0297 (2)	0.0333 (3)	0.0434 (3)	0.0002 (2)	−0.0058 (2)	−0.0068 (2)
Br1	0.04826 (16)	0.0928 (3)	0.04125 (16)	0.01267 (15)	0.01231 (12)	0.02479 (15)

Geometric parameters (Å, º)

C1—C6	1.386 (3)	C11—C12	1.382 (4)
C1—C2	1.389 (3)	C11—H11	0.9300
C1—S1	1.750 (2)	C12—C13	1.376 (4)
C2—C3	1.376 (4)	C12—H12	0.9300
C2—H2	0.9300	C13—C14	1.399 (3)

C3—C4	1.361 (4)	C13—H13	0.9300
C3—H3	0.9300	C14—N1	1.411 (3)
C4—C5	1.385 (4)	C15—Br1	1.963 (2)
C4—H4	0.9300	C15—H15A	0.9700
C5—C6	1.378 (4)	C15—H15B	0.9700
C5—H5	0.9300	C16—O3	1.218 (3)
C6—H6	0.9300	C16—C17	1.502 (3)
C7—C8	1.366 (3)	C17—C18	1.522 (3)
C7—N1	1.416 (2)	C17—H17A	0.9700
C7—C15	1.488 (3)	C17—H17B	0.9700
C8—C9	1.446 (3)	C18—H18A	0.9600
C8—C16	1.494 (3)	C18—H18B	0.9600
C9—C10	1.403 (3)	C18—H18C	0.9600
C9—C14	1.403 (3)	N1—S1	1.6864 (18)
C10—C11	1.387 (4)	O1—S1	1.4236 (18)
C10—H10	0.9300	O2—S1	1.4193 (19)

C6—C1—C2	121.0 (2)	C12—C13—C14	117.0 (2)
C6—C1—S1	119.62 (17)	C12—C13—H13	121.5
C2—C1—S1	119.21 (19)	C14—C13—H13	121.5
C3—C2—C1	118.9 (2)	C13—C14—C9	122.8 (2)
C3—C2—H2	120.6	C13—C14—N1	129.1 (2)
C1—C2—H2	120.6	C9—C14—N1	108.08 (17)
C4—C3—C2	120.5 (2)	C7—C15—Br1	111.86 (16)
C4—C3—H3	119.8	C7—C15—H15A	109.2
C2—C3—H3	119.8	Br1—C15—H15A	109.2
C3—C4—C5	120.9 (2)	C7—C15—H15B	109.2
C3—C4—H4	119.5	Br1—C15—H15B	109.2
C5—C4—H4	119.5	H15A—C15—H15B	107.9
C6—C5—C4	119.7 (3)	O3—C16—C8	120.1 (2)
C6—C5—H5	120.2	O3—C16—C17	120.4 (2)
C4—C5—H5	120.2	C8—C16—C17	119.5 (2)
C5—C6—C1	119.1 (2)	C16—C17—C18	112.2 (2)
C5—C6—H6	120.5	C16—C17—H17A	109.2
C1—C6—H6	120.5	C18—C17—H17A	109.2
C8—C7—N1	108.64 (18)	C16—C17—H17B	109.2
C8—C7—C15	127.79 (19)	C18—C17—H17B	109.2
N1—C7—C15	123.36 (19)	H17A—C17—H17B	107.9
C7—C8—C9	108.54 (18)	C17—C18—H18A	109.5
C7—C8—C16	122.81 (19)	C17—C18—H18B	109.5
C9—C8—C16	128.6 (2)	H18A—C18—H18B	109.5
C10—C9—C14	118.3 (2)	C17—C18—H18C	109.5
C10—C9—C8	134.9 (2)	H18A—C18—H18C	109.5
C14—C9—C8	106.79 (19)	H18B—C18—H18C	109.5
C11—C10—C9	118.8 (2)	C14—N1—C7	107.94 (17)
C11—C10—H10	120.6	C14—N1—S1	121.55 (14)
C9—C10—H10	120.6	C7—N1—S1	128.56 (14)
C12—C11—C10	121.5 (2)	O2—S1—O1	120.16 (13)
C12—C11—H11	119.3	O2—S1—N1	106.36 (11)

C10—C11—H11	119.3	O1—S1—N1	106.44 (9)
C13—C12—C11	121.6 (2)	O2—S1—C1	108.93 (11)
C13—C12—H12	119.2	O1—S1—C1	108.79 (11)
C11—C12—H12	119.2	N1—S1—C1	105.11 (10)
C6—C1—C2—C3	−1.2 (4)	N1—C7—C15—Br1	−103.6 (2)
S1—C1—C2—C3	173.4 (2)	C7—C8—C16—O3	7.0 (4)
C1—C2—C3—C4	1.2 (4)	C9—C8—C16—O3	−171.7 (2)
C2—C3—C4—C5	−0.1 (5)	C7—C8—C16—C17	−171.8 (2)
C3—C4—C5—C6	−1.0 (5)	C9—C8—C16—C17	9.5 (3)
C4—C5—C6—C1	0.9 (5)	O3—C16—C17—C18	−6.7 (4)
C2—C1—C6—C5	0.2 (4)	C8—C16—C17—C18	172.2 (2)
S1—C1—C6—C5	−174.4 (2)	C13—C14—N1—C7	177.2 (2)
N1—C7—C8—C9	0.5 (2)	C9—C14—N1—C7	−0.8 (2)
C15—C7—C8—C9	175.3 (2)	C13—C14—N1—S1	−17.4 (3)
N1—C7—C8—C16	−178.40 (19)	C9—C14—N1—S1	164.61 (15)
C15—C7—C8—C16	−3.7 (3)	C8—C7—N1—C14	0.2 (2)
C7—C8—C9—C10	−179.2 (2)	C15—C7—N1—C14	−174.9 (2)
C16—C8—C9—C10	−0.4 (4)	C8—C7—N1—S1	−163.90 (16)
C7—C8—C9—C14	−1.0 (2)	C15—C7—N1—S1	21.1 (3)
C16—C8—C9—C14	177.8 (2)	C14—N1—S1—O2	49.4 (2)
C14—C9—C10—C11	−1.1 (3)	C7—N1—S1—O2	−148.47 (19)
C8—C9—C10—C11	176.9 (2)	C14—N1—S1—O1	178.65 (18)
C9—C10—C11—C12	0.0 (4)	C7—N1—S1—O1	−19.2 (2)
C10—C11—C12—C13	0.8 (4)	C14—N1—S1—C1	−66.04 (19)
C11—C12—C13—C14	−0.5 (4)	C7—N1—S1—C1	96.1 (2)
C12—C13—C14—C9	−0.7 (4)	C6—C1—S1—O2	179.4 (2)
C12—C13—C14—N1	−178.4 (2)	C2—C1—S1—O2	4.7 (2)
C10—C9—C14—C13	1.5 (3)	C6—C1—S1—O1	46.8 (2)
C8—C9—C14—C13	−177.0 (2)	C2—C1—S1—O1	−127.98 (19)
C10—C9—C14—N1	179.7 (2)	C6—C1—S1—N1	−66.9 (2)
C8—C9—C14—N1	1.1 (2)	C2—C1—S1—N1	118.35 (19)
C8—C7—C15—Br1	82.3 (2)		

Hydrogen-bond geometry (Å, º)

*Cg*2 and *Cg*3 are the centroids of the C1–C6 and C9–C14 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···Br1	0.93	2.89	3.815 (2)	171
C13—H13···O2	0.93	2.39	2.978 (3)	121
C15—H15*B*···O1	0.97	2.15	2.833 (3)	126
C2—H2···O3^{i}	0.93	2.59	3.191 (3)	123
C15—H15*A*···*Cg*3^{ii}	0.97	2.74	3.486 (3)	134
C18—H18*B*···*Cg*2^{iii}	0.96	2.66	3.616 (3)	174

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