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

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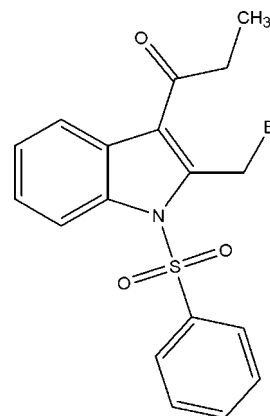
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.052; wR factor = 0.133; data-to-parameter ratio = 33.5.

In the title compound, $\text{C}_{18}\text{H}_{16}\text{BrNO}_3\text{S}$, the dihedral angle between the phenyl ring and the indole ring system is $89.91(11)^\circ$. The molecular structure features weak $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{Br}$ hydrogen bonds. In the crystal, molecules are linked by weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, forming chains along the a -axis direction. The chains are further linked by $\text{C}-\text{H}\cdots\pi$ 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

$\text{C}_{18}\text{H}_{16}\text{BrNO}_3\text{S}$
 $M_r = 406.29$
 Monoclinic, $P2_1/c$
 $a = 10.2772(7)$ Å
 $b = 8.6610(6)$ Å
 $c = 18.8980(14)$ Å
 $\beta = 90.676(2)^\circ$
 $V = 1682.0(2)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 2.58$ mm⁻¹
 $T = 295$ K
 $0.38 \times 0.34 \times 0.30$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.036$

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, °).

$\text{Cg}2$ and $\text{Cg}3$ are the centroids of the $\text{C}1-\text{C}6$ and $\text{C}9-\text{C}14$ rings, respectively.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}6-\text{H}6\cdots\text{Br}1$	0.93	2.89	3.815 (2)	171
$\text{C}13-\text{H}13\cdots\text{O}2$	0.93	2.39	2.978 (3)	121
$\text{C}15-\text{H}15\text{B}\cdots\text{O}1$	0.97	2.15	2.833 (3)	126
$\text{C}2-\text{H}2\cdots\text{O}3^i$	0.93	2.59	3.191 (3)	123
$\text{C}15-\text{H}15\text{A}\cdots\text{Cg}3^{\text{ii}}$	0.97	2.74	3.486 (3)	134
$\text{C}18-\text{H}18\text{B}\cdots\text{Cg}2^{\text{iii}}$	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).

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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

S1. 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 [$\text{O1—S1—O2} = 120.16 (13)^\circ$ and $\text{N1—S1—C1} = 105.11 (10)^\circ$] 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 $2.00 (12)^\circ$. The phenyl ring (C1–C6) makes the dihedral angle of $89.91 (11)^\circ$ with the indole ring system. The molecular structure is stabilized by weak intramolecular C—H \cdots O and C—H \cdots Br hydrogen bonds (Table 1). The crystal structure exhibit weak intermolecular C—H \cdots O and C—H \cdots π (Table 1 & Fig. 2) interactions.

S2. 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.

S3. Refinement

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

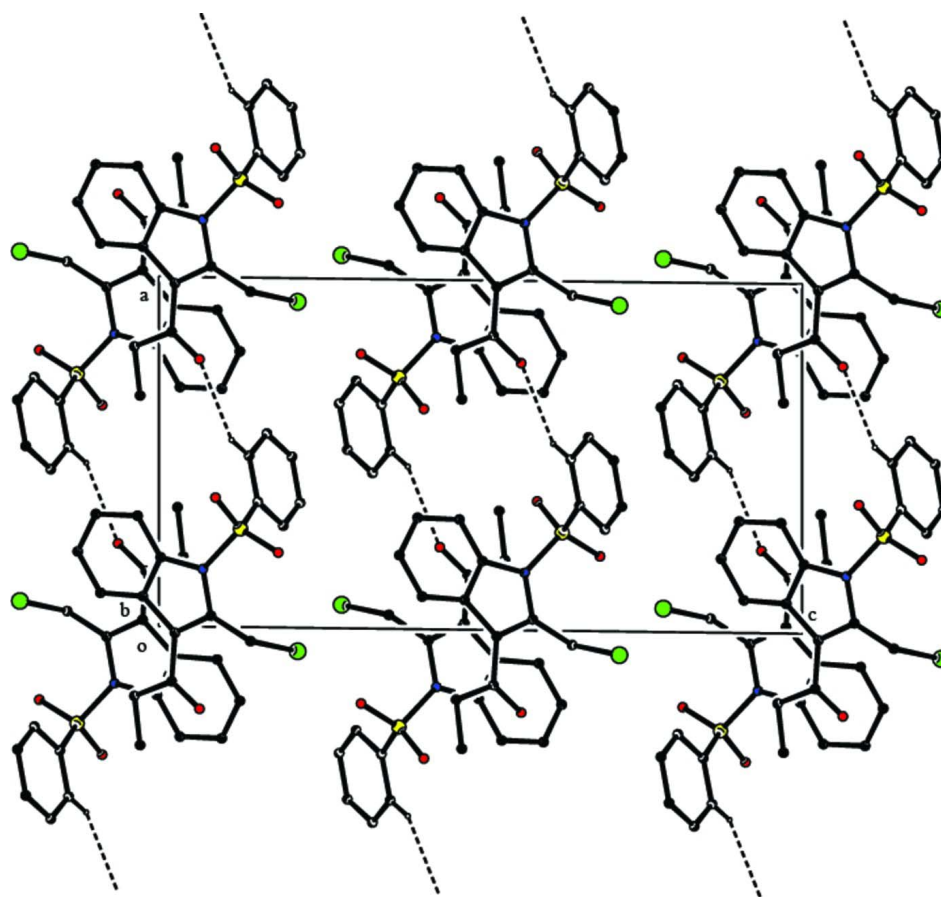


Figure 2

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: $-P\ 2_1/c$

$a = 10.2772\ (7)\ \text{\AA}$

$b = 8.6610\ (6)\ \text{\AA}$

$c = 18.8980\ (14)\ \text{\AA}$

$\beta = 90.676\ (2)^\circ$

$V = 1682.0\ (2)\ \text{\AA}^3$

$Z = 4$

$F(000) = 824$

$D_x = 1.604\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5675 reflections

$\theta = 2.6\text{--}28.2^\circ$

$\mu = 2.58\ \text{mm}^{-1}$

$T = 295\ \text{K}$

Block, colourless

$0.38 \times 0.34 \times 0.30\ \text{mm}$

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 $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$
 $\theta_{\text{max}} = 35.0^\circ$, $\theta_{\text{min}} = 2.2^\circ$
 $h = -16 \rightarrow 15$

$k = -13 \rightarrow 13$
 $l = -30 \rightarrow 30$

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 $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 1.11 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.90 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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, °)

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 (\AA , $^\circ$)

Cg2 and Cg3 are the centroids of the C1–C6 and C9–C14 rings, respectively.

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C6—H6 \cdots Br1	0.93	2.89	3.815 (2)	171
C13—H13 \cdots O2	0.93	2.39	2.978 (3)	121
C15—H15B \cdots O1	0.97	2.15	2.833 (3)	126
C2—H2 \cdots O3 ⁱ	0.93	2.59	3.191 (3)	123

C15—H15A...Cg3 ⁱⁱ	0.97	2.74	3.486 (3)	134
C18—H18B...Cg2 ⁱⁱⁱ	0.96	2.66	3.616 (3)	174

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