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

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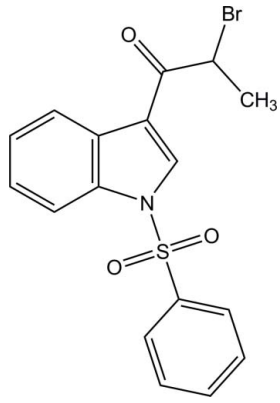
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.050; wR factor = 0.149; data-to-parameter ratio = 18.7.

In the title compound, $C_{17}H_{14}BrNO_3S$, the phenyl ring makes a dihedral angle of 89.78 (16)° with the plane of the indole ring system. The terminal Br atom and the methyl group are disordered over two sets of sites, with site occupancies of 0.860 (2) and 0.140 (2). In the crystal, molecules are linked into a chain along the *b*-axis direction by weak C—H···O hydrogen bonds. The chains are further linked by C—H···π interactions, forming layers parallel to the *bc* plane.

Related literature

For the biological activity of indole derivatives, see: Andreani *et al.* (2001); Singh *et al.* (2000); Pomarnacka & Kozlarska-Kedra (2003); Srivastava & Pandeya (2011). For related structures, see: Umadevi *et al.* (2013); Kanchanadevi *et al.* (2014).



Experimental

Crystal data

$C_{17}H_{14}BrNO_3S$
M_r = 392.26
Monoclinic, $P2_1/c$
a = 8.7539 (3) Å
b = 10.9968 (4) Å
c = 17.5801 (7) Å
β = 99.231 (2)°
V = 1670.43 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.60 mm^{-1}
T = 295 K
0.35 × 0.25 × 0.25 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.416, T_{max} = 0.522
15009 measured reflections
4141 independent reflections
2334 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.149
S = 1.03
4141 reflections
222 parameters
5 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

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

*Cg*2 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1^{i}	0.93	2.57	3.312 (4)	137
C10—H10···O1^{i}	0.93	2.44	3.280 (4)	150
C12—H12···*Cg*2^{ii}	0.93	2.72	3.528 (2)	146

Symmetry codes: (i) $-x+2, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); 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).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: IS5339).

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supplementary materials

Acta Cryst. (2014). E**70**, o295–o296 [doi:10.1107/S1600536814002864]

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

C. Ramathilagam, P. R. Umarani, V. Saravanan, A. K. Mohanakrishnan, B. Gunasekaran and V. Manivannan

1. Comment

Indole derivatives exhibit antibacterial, antifungal (Singh *et al.*, 2000) and antitumour activities (Andreani *et al.*, 2001). These derivatives also exhibit antimicrobial, antibiotic, analgesic, anticancer and anti-HIV (Pomarnacka & Kozlarska-Kedra, 2003; Srivastava & Pandeya, 2011) activities.

The geometric parameters of the title molecule (Fig. 1) agree well with reported similar structures (Umadevi *et al.*, 2013; Kanchanadevi *et al.*, 2014). The phenyl ring makes a dihedral angle of 89.78 (16)° with the indole ring system. The terminal bromine atom and the methyl group are disordered over two positions with site occupancies of 0.860 (2) and 0.140 (2). The sum of bond angles around the atom N1 [356.7 (3) °] indicates sp^2 hybridized state of atom N1 in the molecule. The crystal packing is controlled by weak C—H···O and C—H···π interactions (Table 1).

2. Experimental

A solution of 1-[1-(phenylsulfonyl)-1*H*-indol-3-yl]propan-1-one (1 g, 3.194 mmol) and PTT (phenyltrimethylammonium tribromide) (1.32 g, 3.514 mmol) in dry THF (20 ml) was stirred at room temperature for 3 h. After completion of the reaction (monitored by TLC), it was poured into crushed ice (100 g). The solid obtained was filtered and washed with MeOH (5 ml) to afford 2-bromo-1-[1-(phenylsulfonyl)-1*H*-indol-3-yl]propan-1-one (1.14 g, yield 91%; melting point 130–132 °C).

3. Refinement

The terminal bromine atom and the methyl group are disordered over two positions. The site occupancy factors of disordered atoms were refined to 0.860 (2) and 0.140 (2). In the refinement, *EADP* was used for atoms C17 and C17A. The bond distances of C16—C17 and C16—C17A were restrained to be 1.5200 (1) and 1.5200 (5) Å, respectively, and the distances of C16—Br1 and C16—Br1A were restrained to be 1.9100 (1) and 1.9100 (5) Å, respectively. Also the distance of C17A···Br1A was restrained to be 2.85 (1) Å. H atoms were positioned geometrically and refined using riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic C—H, C—H = 0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) for C—H, C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for CH_3.

Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); 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).

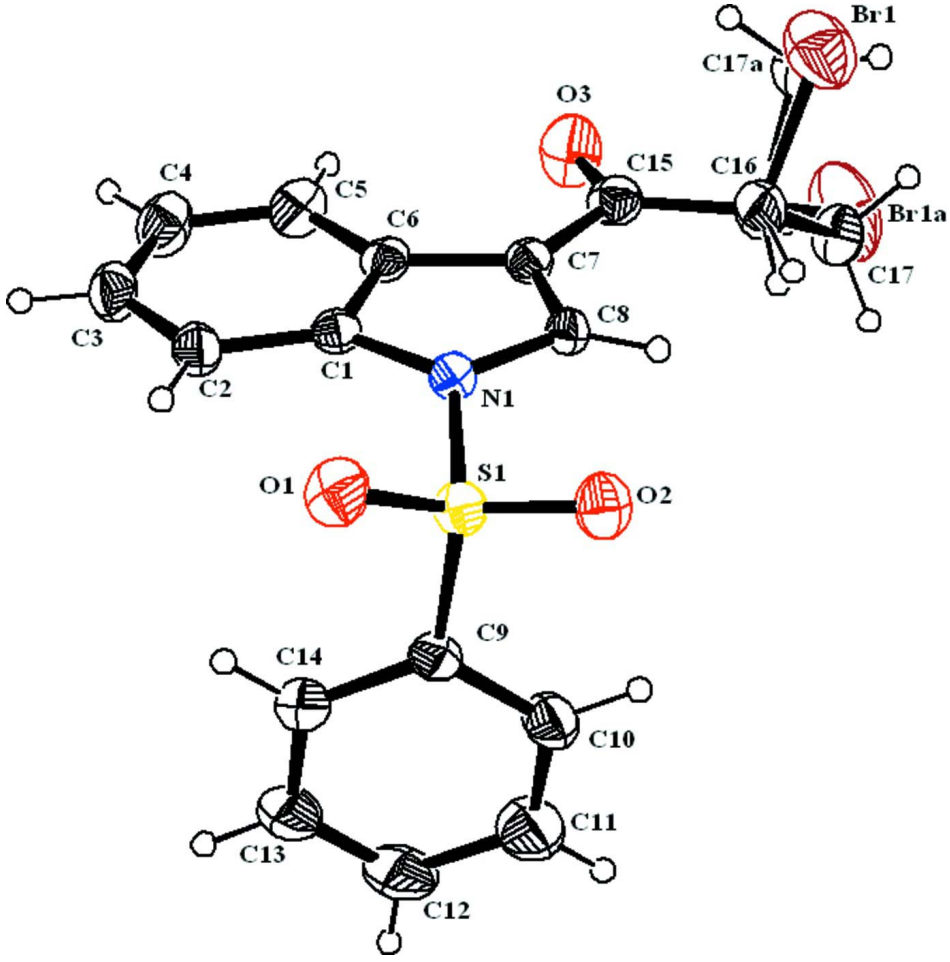

Figure 1

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

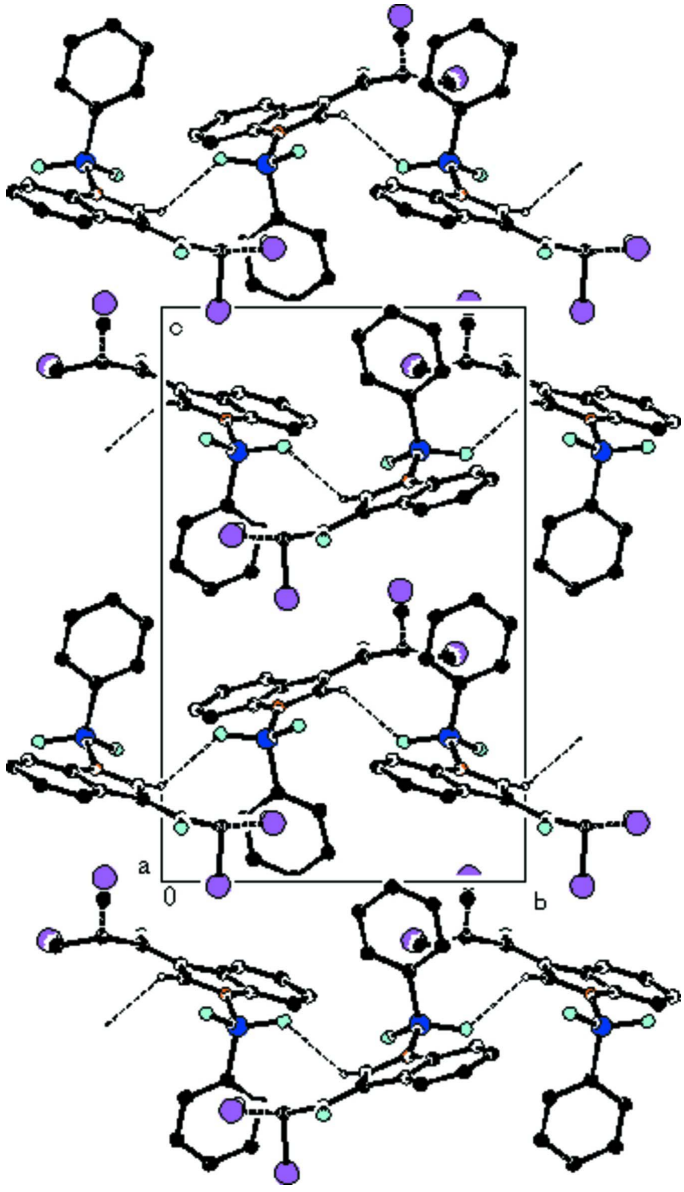

Figure 2

The packing diagram of the title compound, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

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

Crystal data

$C_{17}H_{14}BrNO_3S$
$M_r = 392.26$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.7539$ (3) Å
$b = 10.9968$ (4) Å
$c = 17.5801$ (7) Å
$\beta = 99.231$ (2)°
$V = 1670.43$ (11) Å^3
$Z = 4$

$F(000) = 792$
$D_x = 1.560$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4350 reflections
$\theta = 2.2$–$28.4°$
$\mu = 2.60$ mm^{-1}
$T = 295$ K
Block, yellow
0.35 × 0.25 × 0.25 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.416, T_{max} = 0.522
15009 measured reflections
4141 independent reflections
2334 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 28.5°, θ_{min} = 2.2°
h = −11→8
k = −10→14
l = −21→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.149
S = 1.03
4141 reflections
222 parameters
5 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
$w = 1/[\sigma^2(F_o^2) + (0.0673P)^2 + 0.7073P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0037 (9)

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.7170 (3)	0.2542 (3)	0.30787 (16)	0.0382 (7)	
C2	0.6804 (4)	0.1348 (3)	0.28691 (18)	0.0480 (8)	
H2	0.7480	0.0850	0.2655	0.058*	
C3	0.5365 (4)	0.0944 (3)	0.2998 (2)	0.0558 (9)	
H3	0.5071	0.0148	0.2870	0.067*	
C4	0.4359 (4)	0.1688 (3)	0.3310 (2)	0.0627 (10)	
H4	0.3398	0.1387	0.3380	0.075*	
C5	0.4753 (4)	0.2878 (3)	0.3522 (2)	0.0552 (9)	
H5	0.4072	0.3373	0.3735	0.066*	
C6	0.6184 (3)	0.3308 (3)	0.34090 (16)	0.0392 (7)	
C7	0.6963 (3)	0.4468 (2)	0.35599 (16)	0.0391 (7)	
C8	0.8349 (3)	0.4370 (2)	0.33195 (16)	0.0375 (7)	
H8	0.9074	0.4992	0.3341	0.045*	
C9	0.8963 (3)	0.3192 (3)	0.15480 (17)	0.0427 (7)	
C10	0.9085 (4)	0.4343 (3)	0.12403 (19)	0.0587 (9)	
H10	0.9658	0.4947	0.1527	0.070*	
C11	0.8349 (5)	0.4573 (4)	0.0508 (2)	0.0803 (12)	
H11	0.8417	0.5339	0.0292	0.096*	
C12	0.7501 (5)	0.3665 (4)	0.0088 (2)	0.0820 (13)	
H12	0.6992	0.3830	−0.0407	0.098*	
C13	0.7405 (5)	0.2530 (4)	0.0393 (2)	0.0804 (13)	
H13	0.6845	0.1926	0.0101	0.096*	
C14	0.8121 (4)	0.2279 (3)	0.1120 (2)	0.0614 (9)	
H14	0.8050	0.1508	0.1329	0.074*	

C15	0.6362 (4)	0.5538 (3)	0.39046 (19)	0.0511 (8)	
C16	0.7409 (4)	0.6635 (2)	0.40341 (9)	0.0651 (10)	
H16A	0.8186	0.6547	0.3694	0.078*	0.860 (2)
H16B	0.7916	0.6656	0.3576	0.078*	0.140 (2)
Br1	0.84813 (7)	0.65595 (6)	0.50680 (4)	0.0973 (3)	0.860 (2)
C17	0.6681 (10)	0.7883 (4)	0.3880 (5)	0.0539 (15)	0.860 (2)
H17A	0.7036	0.8411	0.4307	0.081*	0.860 (2)
H17B	0.5575	0.7812	0.3817	0.081*	0.860 (2)
H17C	0.6973	0.8215	0.3419	0.081*	0.860 (2)
Br1A	0.6298 (11)	0.8071 (6)	0.3977 (7)	0.132 (4)	0.140 (2)
C17A	0.875 (2)	0.6591 (18)	0.4701 (12)	0.0539 (15)	0.140 (2)
H17D	0.9557	0.7124	0.4596	0.081*	0.140 (2)
H17E	0.9138	0.5775	0.4763	0.081*	0.140 (2)
H17F	0.8396	0.6846	0.5166	0.081*	0.140 (2)
N1	0.8539 (3)	0.3213 (2)	0.30363 (13)	0.0384 (6)	
O1	1.0168 (3)	0.16368 (19)	0.25653 (14)	0.0591 (6)	
O2	1.1079 (2)	0.3760 (2)	0.27067 (13)	0.0526 (6)	
O3	0.5058 (3)	0.5548 (2)	0.40600 (18)	0.0778 (8)	
S1	0.98775 (9)	0.29060 (7)	0.24862 (4)	0.0422 (2)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0438 (16)	0.0389 (15)	0.0298 (16)	0.0014 (13)	−0.0003 (12)	0.0057 (12)
C2	0.059 (2)	0.0392 (17)	0.0421 (19)	−0.0028 (14)	−0.0019 (15)	0.0011 (13)
C3	0.060 (2)	0.0464 (18)	0.056 (2)	−0.0136 (17)	−0.0088 (16)	0.0034 (16)
C4	0.0454 (19)	0.065 (2)	0.074 (3)	−0.0139 (18)	−0.0001 (17)	0.0101 (19)
C5	0.0441 (18)	0.058 (2)	0.063 (2)	0.0016 (16)	0.0069 (15)	0.0098 (17)
C6	0.0413 (16)	0.0405 (15)	0.0340 (16)	0.0009 (13)	0.0004 (12)	0.0080 (12)
C7	0.0454 (16)	0.0353 (15)	0.0355 (16)	0.0031 (13)	0.0034 (12)	0.0027 (12)
C8	0.0464 (17)	0.0298 (14)	0.0357 (16)	−0.0021 (12)	0.0047 (12)	−0.0002 (11)
C9	0.0470 (17)	0.0435 (17)	0.0393 (17)	0.0018 (13)	0.0115 (13)	−0.0037 (13)
C10	0.083 (2)	0.0438 (19)	0.047 (2)	−0.0007 (17)	0.0053 (18)	−0.0021 (15)
C11	0.118 (4)	0.063 (2)	0.056 (3)	0.003 (2)	0.004 (2)	0.010 (2)
C12	0.097 (3)	0.107 (4)	0.037 (2)	−0.008 (3)	−0.004 (2)	−0.001 (2)
C13	0.099 (3)	0.098 (3)	0.042 (2)	−0.033 (3)	0.008 (2)	−0.012 (2)
C14	0.078 (2)	0.061 (2)	0.047 (2)	−0.0192 (19)	0.0146 (18)	−0.0042 (17)
C15	0.057 (2)	0.051 (2)	0.047 (2)	0.0062 (16)	0.0141 (16)	0.0018 (14)
C16	0.080 (3)	0.051 (2)	0.070 (3)	−0.0090 (18)	0.029 (2)	−0.0180 (17)
Br1	0.0956 (5)	0.0997 (5)	0.0870 (5)	−0.0029 (3)	−0.0142 (3)	−0.0100 (3)
C17	0.067 (4)	0.023 (2)	0.071 (4)	0.016 (2)	0.008 (3)	0.009 (2)
Br1A	0.118 (6)	0.078 (3)	0.192 (7)	0.027 (3)	0.004 (4)	−0.038 (4)
C17A	0.067 (4)	0.023 (2)	0.071 (4)	0.016 (2)	0.008 (3)	0.009 (2)
N1	0.0432 (14)	0.0363 (13)	0.0356 (14)	−0.0015 (10)	0.0062 (10)	−0.0010 (10)
O1	0.0659 (15)	0.0400 (12)	0.0727 (17)	0.0185 (10)	0.0151 (12)	0.0072 (10)
O2	0.0369 (11)	0.0555 (13)	0.0640 (15)	−0.0048 (10)	0.0040 (10)	−0.0037 (11)
O3	0.0651 (17)	0.0646 (16)	0.111 (2)	0.0071 (13)	0.0367 (16)	−0.0143 (15)
S1	0.0431 (4)	0.0378 (4)	0.0458 (5)	0.0067 (3)	0.0078 (3)	0.0012 (3)

Geometric parameters (Å, º)

C1—C2	1.387 (4)	C12—C13	1.366 (6)
C1—C6	1.398 (4)	C12—H12	0.9300
C1—N1	1.420 (4)	C13—C14	1.359 (5)
C2—C3	1.388 (5)	C13—H13	0.9300
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.379 (5)	C15—O3	1.216 (4)
C3—H3	0.9300	C15—C16	1.511 (4)
C4—C5	1.389 (5)	C16—C17	1.5190 (10)
C4—H4	0.9300	C16—C17A	1.520 (5)
C5—C6	1.382 (4)	C16—Br1A	1.849 (4)
C5—H5	0.9300	C16—Br1	1.9092 (10)
C6—C7	1.450 (4)	C16—H16A	0.9800
C7—C8	1.352 (4)	C16—H16B	0.9800
C7—C15	1.460 (4)	C17—H17A	0.9600
C8—N1	1.386 (3)	C17—H17B	0.9600
C8—H8	0.9300	C17—H17C	0.9600
C9—C10	1.388 (4)	C17A—H17D	0.9600
C9—C14	1.392 (5)	C17A—H17E	0.9600
C9—S1	1.743 (3)	C17A—H17F	0.9600
C10—C11	1.368 (5)	N1—S1	1.669 (2)
C10—H10	0.9300	O1—S1	1.422 (2)
C11—C12	1.384 (6)	O2—S1	1.417 (2)
C11—H11	0.9300		
C2—C1—C6	123.3 (3)	C13—C14—C9	119.1 (3)
C2—C1—N1	129.7 (3)	C13—C14—H14	120.5
C6—C1—N1	107.0 (2)	C9—C14—H14	120.5
C1—C2—C3	115.9 (3)	O3—C15—C7	121.0 (3)
C1—C2—H2	122.0	O3—C15—C16	121.8 (3)
C3—C2—H2	122.0	C7—C15—C16	117.1 (3)
C4—C3—C2	121.9 (3)	C15—C16—C17	117.9 (4)
C4—C3—H3	119.0	C15—C16—C17A	117.7 (10)
C2—C3—H3	119.0	C15—C16—Br1A	111.9 (4)
C3—C4—C5	121.3 (3)	C17A—C16—Br1A	113.8 (6)
C3—C4—H4	119.4	C15—C16—Br1	107.61 (19)
C5—C4—H4	119.4	C17—C16—Br1	109.7 (4)
C6—C5—C4	118.4 (3)	C15—C16—H16A	107.0
C6—C5—H5	120.8	C17—C16—H16A	107.0
C4—C5—H5	120.8	Br1—C16—H16A	107.0
C5—C6—C1	119.2 (3)	C15—C16—H16B	103.8
C5—C6—C7	133.2 (3)	C17A—C16—H16B	103.8
C1—C6—C7	107.6 (2)	Br1A—C16—H16B	103.8
C8—C7—C6	107.0 (2)	C16—C17—H17A	109.5
C8—C7—C15	126.5 (3)	C16—C17—H17B	109.5
C6—C7—C15	126.5 (3)	H17A—C17—H17B	109.5
C7—C8—N1	110.6 (2)	C16—C17—H17C	109.5
C7—C8—H8	124.7	H17A—C17—H17C	109.5
N1—C8—H8	124.7	H17B—C17—H17C	109.5

C10—C9—C14	121.0 (3)	C16—C17A—H17D	109.5
C10—C9—S1	118.7 (2)	C16—C17A—H17E	109.5
C14—C9—S1	120.3 (2)	H17D—C17A—H17E	109.5
C11—C10—C9	118.8 (3)	C16—C17A—H17F	109.5
C11—C10—H10	120.6	H17D—C17A—H17F	109.5
C9—C10—H10	120.6	H17E—C17A—H17F	109.5
C10—C11—C12	120.0 (4)	C8—N1—C1	107.9 (2)
C10—C11—H11	120.0	C8—N1—S1	122.02 (19)
C12—C11—H11	120.0	C1—N1—S1	127.03 (19)
C13—C12—C11	120.7 (4)	O2—S1—O1	120.71 (14)
C13—C12—H12	119.6	O2—S1—N1	105.46 (12)
C11—C12—H12	119.6	O1—S1—N1	105.86 (13)
C14—C13—C12	120.4 (4)	O2—S1—C9	110.36 (14)
C14—C13—H13	119.8	O1—S1—C9	108.50 (14)
C12—C13—H13	119.8	N1—S1—C9	104.67 (13)

C6—C1—C2—C3	0.7 (4)	C6—C7—C15—C16	177.8 (2)
N1—C1—C2—C3	178.7 (3)	O3—C15—C16—C17	−37.3 (5)
C1—C2—C3—C4	0.5 (5)	C7—C15—C16—C17	140.8 (4)
C2—C3—C4—C5	−1.1 (5)	O3—C15—C16—C17A	106.8 (12)
C3—C4—C5—C6	0.4 (5)	C7—C15—C16—C17A	−75.1 (12)
C4—C5—C6—C1	0.8 (4)	O3—C15—C16—Br1A	−27.8 (5)
C4—C5—C6—C7	−179.8 (3)	C7—C15—C16—Br1A	150.3 (4)
C2—C1—C6—C5	−1.4 (4)	O3—C15—C16—Br1	87.4 (3)
N1—C1—C6—C5	−179.7 (2)	C7—C15—C16—Br1	−94.5 (3)
C2—C1—C6—C7	179.1 (3)	C7—C8—N1—C1	1.7 (3)
N1—C1—C6—C7	0.7 (3)	C7—C8—N1—S1	163.2 (2)
C5—C6—C7—C8	−179.2 (3)	C2—C1—N1—C8	−179.7 (3)
C1—C6—C7—C8	0.3 (3)	C6—C1—N1—C8	−1.5 (3)
C5—C6—C7—C15	0.7 (5)	C2—C1—N1—S1	20.1 (4)
C1—C6—C7—C15	−179.8 (3)	C6—C1—N1—S1	−161.7 (2)
C6—C7—C8—N1	−1.3 (3)	C8—N1—S1—O2	28.1 (2)
C15—C7—C8—N1	178.9 (3)	C1—N1—S1—O2	−174.2 (2)
C14—C9—C10—C11	0.7 (5)	C8—N1—S1—O1	157.1 (2)
S1—C9—C10—C11	−179.1 (3)	C1—N1—S1—O1	−45.2 (3)
C9—C10—C11—C12	0.0 (6)	C8—N1—S1—C9	−88.4 (2)
C10—C11—C12—C13	−0.8 (7)	C1—N1—S1—C9	69.3 (2)
C11—C12—C13—C14	1.1 (7)	C10—C9—S1—O2	−21.3 (3)
C12—C13—C14—C9	−0.4 (6)	C14—C9—S1—O2	158.9 (3)
C10—C9—C14—C13	−0.4 (5)	C10—C9—S1—O1	−155.7 (3)
S1—C9—C14—C13	179.3 (3)	C14—C9—S1—O1	24.6 (3)
C8—C7—C15—O3	175.7 (3)	C10—C9—S1—N1	91.7 (3)
C6—C7—C15—O3	−4.1 (5)	C14—C9—S1—N1	−88.0 (3)
C8—C7—C15—C16	−2.4 (4)		

Hydrogen-bond geometry (Å, º)

*Cg*2 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O1^{i}	0.93	2.57	3.312 (4)	137

C10—H10···O1^{i}	0.93	2.44	3.280 (4)	150
C12—H12···*Cg*2^{ii}	0.93	2.72	3.528 (2)	146

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