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(4-Bromophenyl)(1-phenylsulfonyl-1*H*-indol-2-yl)methanone

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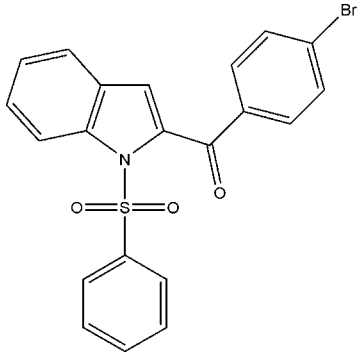
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.044; wR factor = 0.111; data-to-parameter ratio = 19.4.

In the title compound, $C_{21}H_{14}BrNO_3S$, the indole ring system forms dihedral angles of 65.64 (8) and 59.30 (8)°, respectively, with the phenyl and bromophenyl rings. In the crystal, molecules are connected by a C—H···O hydrogen bond, forming a chain along [101]. The chains are further connected by weak intermolecular C—H···π interactions, forming a layer parallel to the *ac* plane.

Related literature

For the biological activity of indole derivatives, see: Joshi & Chand (1982); Pomarnacka & Kozlarska-Kedra (2003); Poter *et al.* (1977). For related structures, see: Chakkaravarthi *et al.* (2007, 2008). 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

$C_{21}H_{14}BrNO_3S$ M_r = 440.30
Monoclinic, $P2_1/n$
a = 8.482 (3) Å
b = 25.780 (4) Å
c = 8.690 (3) Å
β = 93.388 (3)°
V = 1896.9 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.30 mm^{-1}
T = 295 K
0.24 × 0.22 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.609, T_{max} = 0.656
18123 measured reflections
4736 independent reflections
2944 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.111
S = 1.03
4736 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the N1/C7/C8/C9/C14 and C9–C14 rings, respectively

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17···O3^{i}	0.93	2.50	3.383 (3)	158
C4—H4···*Cg*1^{ii}	0.93	2.67	3.635 (4)	127
C4—H4···*Cg*2^{ii}	0.93	2.76	3.681 (4)	169

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

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 DV University of Madras for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2617).

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(4-Bromophenyl)(1-phenylsulfonyl-1*H*-indol-2-yl)methanone

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S1. Comment

Indole derivatives are found abundantly in a variety of natural plants (Poter *et al.*, 1977). Compounds containing the indole moiety exhibit antibacterial and fungicidal activities (Joshi & Chand, 1982). Indole derivatives are also known to exhibit anticancer and anti - HIV (Pomarnacka & Kozlarska-Kedra, 2003) activities.

In continuation of our studies of indole derivatives, we determined the crystal structure of the title compound,(I). The geometric parameters of the molecule of (I) (Fig. 1) agree well with the reported values for similar structures (Chakkaravarthi *et al.*, 2007, 2008). Due to Thorpe–Ignold effect (Bassindale, 1984), bond angles around atom S1 show significant deviation from ideal tetrahedral value, with significant deviations in angles O2—S1—O1 [120.86 (13)°] and N1—S1—C1 [103.79 (11)°].

The phenyl ring forms the dihedral angle of 65.64 (8)° with the indole ring system and the bromophenyl ring makes the dihedral angle of 59.30 (8)° with the indole ring system. The N1—S1—C1 plane is almost orthogonal to both [dihedral angle 72.30 (9)°] indole ring and [dihedral angle 71.68 (12)°] phenyl ring.

The sum of the bond angles around N1 [341.7 (2)°] indicates that N1 atom is sp^3 hybridized (Beddoes *et al.*, 1986). The crystal packing is stabilized by weak intermolecular C—H···O and C—H···π [C4—H4···*Cg*1 (-1 + *x*, *y*, *z*) distance of 3.635 (4)Å and C4—H4···*Cg*2 (-1 + *x*, *y*, *z*) distance of 3.681 (4)Å (*Cg*1 and *Cg*2 are the centroids of the rings defined by the atoms N1/C7/C8/C9/C14 and C9—C14, respectively] interactions.

S2. Experimental

To a solution of *N*-(2-Formylphenyl)benzenesulfonamide (0.5 g, 1.91 mmol) in dry CH_3CN (20 ml), K_2CO_3 (0.8 g, 5.79 mmol), 2-bromo-1-(4-bromophenyl)ethanone (0.63 g, 2.26 mmol) were added. The reaction mixture was stirred at room temperature for 6 h under N_2 atmosphere. The solvent was removed and the residue was quenched with ice-water (50 ml), extracted with chloroform (3 × 10 ml) and dried (Na_2SO_4). Removal of solvent followed by the residue was dissolved in CH_3CN (20 ml), Conc. HCl (3 ml) was added. The reaction mixture was then refluxed for 2 h. It was then poured over ice-water (50 ml), extracted with $CHCl_3$ (3 × 10 ml) and dried (Na_2SO_4). Removal of solvent followed by crystallization from methanol afforded the compound as a colourless crystal.

S3. Refinement

H atoms were positioned geometrically and refined using riding model, with C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C).

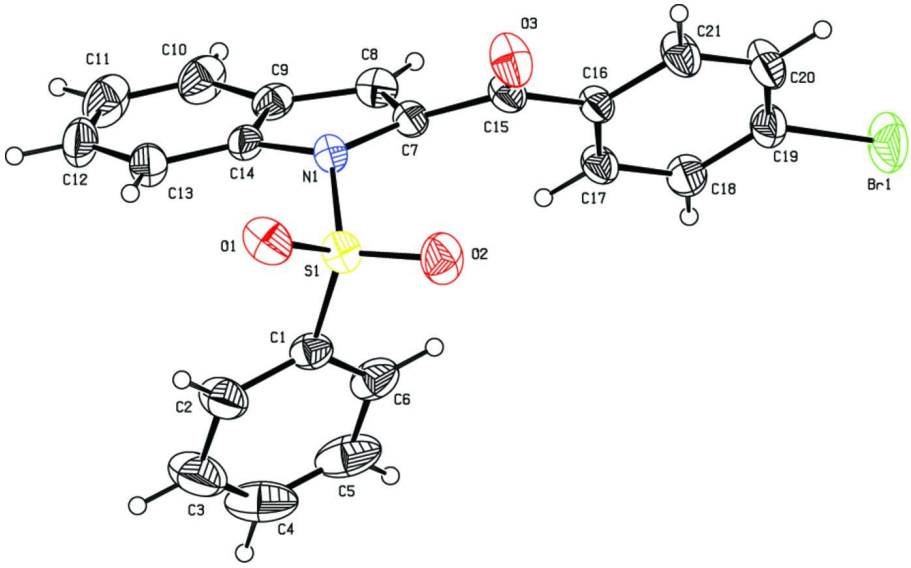

Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids.

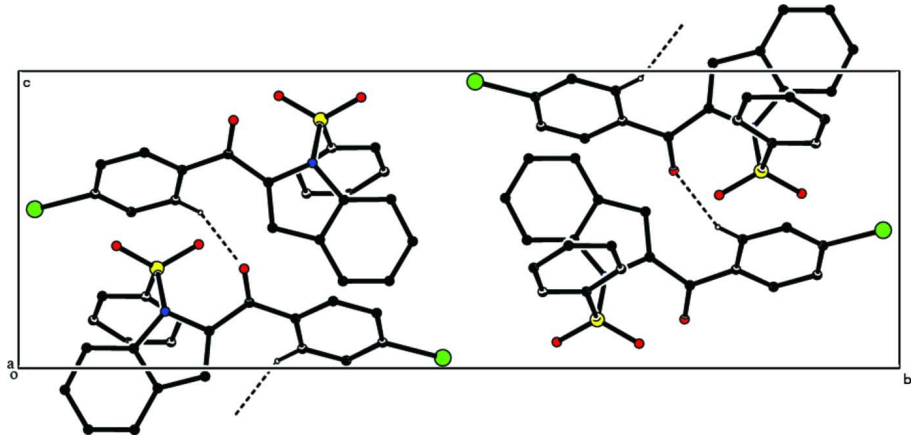

Figure 2

The packing of (I), viewed down the *a* axis. H-bonds are shown as dashed lines; H atoms not involved in hydrogen bonding have been omitted.

(4-Bromophenyl)(1-phenylsulfonyl-1*H*-indol-2-yl)methanone

Crystal data

$C_{21}H_{14}BrNO_3S$
$M_r = 440.30$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.482\ (3)$ Å
$b = 25.780\ (4)$ Å
$c = 8.690\ (3)$ Å
$\beta = 93.388\ (3)°$
$V = 1896.9\ (10)$ Å^3
$Z = 4$

$F(000) = 888$
$D_x = 1.542$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4249 reflections
$\theta = 2.5–24.4°$
$\mu = 2.30$ mm^{-1}
$T = 295$ K
Block, colourless
0.24 × 0.22 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.609, T_{max} = 0.656
18123 measured reflections
4736 independent reflections
2944 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 28.4°, θ_{min} = 1.6°
h = −9→11
k = −29→34
l = −9→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.111
S = 1.03
4736 reflections
244 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
$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2 + 0.6759P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.24312 (5)	0.018422 (12)	0.53534 (5)	0.09126 (18)
S1	0.26404 (8)	0.34303 (3)	0.83609 (7)	0.04855 (18)
O1	0.3198 (2)	0.38893 (8)	0.9118 (2)	0.0648 (5)
O2	0.2576 (3)	0.29550 (8)	0.9169 (2)	0.0737 (6)
O3	0.5440 (2)	0.24395 (7)	0.8349 (2)	0.0671 (6)
N1	0.3837 (2)	0.33357 (7)	0.6910 (2)	0.0421 (5)
C1	0.0793 (3)	0.35548 (11)	0.7418 (3)	0.0494 (6)
C2	0.0204 (4)	0.40492 (12)	0.7428 (4)	0.0703 (9)
H2	0.0751	0.4312	0.7965	0.084*
C3	−0.1230 (4)	0.41519 (17)	0.6619 (5)	0.0963 (12)
H3	−0.1637	0.4487	0.6586	0.116*
C4	−0.2035 (4)	0.3756 (2)	0.5872 (5)	0.1035 (14)
H4	−0.3000	0.3824	0.5347	0.124*
C5	−0.1456 (4)	0.32696 (18)	0.5883 (4)	0.0901 (12)
H5	−0.2021	0.3006	0.5369	0.108*
C6	−0.0021 (4)	0.31602 (12)	0.6658 (3)	0.0650 (8)
H6	0.0386	0.2825	0.6665	0.078*
C7	0.4047 (3)	0.28357 (9)	0.6256 (3)	0.0410 (5)
C8	0.4166 (3)	0.28833 (10)	0.4728 (3)	0.0488 (6)
H8	0.4315	0.2612	0.4045	0.059*
C9	0.4027 (3)	0.34192 (10)	0.4327 (3)	0.0477 (6)
C10	0.4108 (4)	0.36829 (14)	0.2933 (4)	0.0706 (9)
H10	0.4263	0.3505	0.2024	0.085*
C11	0.3955 (4)	0.42089 (15)	0.2939 (4)	0.0827 (11)
H11	0.4003	0.4391	0.2019	0.099*

C12	0.3731 (4)	0.44741 (12)	0.4272 (5)	0.0769 (10)
H12	0.3629	0.4833	0.4230	0.092*
C13	0.3650 (3)	0.42278 (11)	0.5686 (4)	0.0613 (7)
H13	0.3494	0.4410	0.6587	0.074*
C14	0.3816 (3)	0.36928 (9)	0.5669 (3)	0.0438 (6)
C15	0.4561 (3)	0.23788 (10)	0.7209 (3)	0.0471 (6)
C16	0.4037 (3)	0.18560 (9)	0.6675 (3)	0.0430 (6)
C17	0.2741 (3)	0.17786 (10)	0.5660 (3)	0.0486 (6)
H17	0.2187	0.2062	0.5244	0.058*
C18	0.2266 (3)	0.12794 (11)	0.5260 (3)	0.0566 (7)
H18	0.1389	0.1226	0.4584	0.068*
C19	0.3100 (3)	0.08671 (10)	0.5870 (3)	0.0566 (7)
C20	0.4411 (4)	0.09344 (11)	0.6858 (4)	0.0656 (8)
H20	0.4980	0.0650	0.7246	0.079*
C21	0.4865 (3)	0.14285 (10)	0.7260 (3)	0.0586 (7)
H21	0.5744	0.1478	0.7936	0.070*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1039 (3)	0.04279 (18)	0.1244 (4)	−0.01215 (17)	−0.0165 (2)	−0.00695 (18)
S1	0.0576 (4)	0.0482 (4)	0.0396 (3)	0.0031 (3)	0.0004 (3)	−0.0035 (3)
O1	0.0676 (13)	0.0651 (12)	0.0596 (11)	0.0067 (10)	−0.0144 (10)	−0.0246 (10)
O2	0.0985 (17)	0.0670 (13)	0.0573 (12)	0.0100 (11)	0.0197 (11)	0.0186 (10)
O3	0.0788 (14)	0.0531 (11)	0.0650 (12)	0.0036 (10)	−0.0339 (11)	−0.0042 (9)
N1	0.0464 (12)	0.0357 (10)	0.0439 (11)	0.0020 (9)	−0.0010 (9)	0.0010 (8)
C1	0.0446 (15)	0.0566 (15)	0.0475 (14)	−0.0042 (12)	0.0073 (12)	−0.0093 (12)
C2	0.0522 (18)	0.066 (2)	0.092 (2)	0.0062 (15)	−0.0045 (16)	−0.0181 (17)
C3	0.059 (2)	0.103 (3)	0.125 (3)	0.022 (2)	−0.008 (2)	−0.009 (3)
C4	0.045 (2)	0.163 (5)	0.102 (3)	−0.002 (3)	−0.0044 (19)	−0.031 (3)
C5	0.054 (2)	0.129 (4)	0.088 (3)	−0.031 (2)	0.0063 (18)	−0.041 (2)
C6	0.0609 (19)	0.0685 (19)	0.0671 (19)	−0.0180 (15)	0.0171 (16)	−0.0198 (15)
C7	0.0391 (13)	0.0378 (12)	0.0452 (14)	0.0000 (10)	−0.0038 (10)	−0.0029 (10)
C8	0.0482 (15)	0.0539 (15)	0.0439 (15)	−0.0019 (12)	−0.0018 (12)	−0.0090 (12)
C9	0.0382 (14)	0.0604 (16)	0.0438 (14)	−0.0065 (12)	−0.0029 (11)	0.0067 (12)
C10	0.071 (2)	0.086 (2)	0.0539 (18)	−0.0102 (17)	−0.0008 (15)	0.0200 (16)
C11	0.079 (2)	0.095 (3)	0.073 (2)	−0.014 (2)	−0.0080 (18)	0.041 (2)
C12	0.067 (2)	0.0518 (17)	0.110 (3)	−0.0056 (15)	−0.0073 (19)	0.0329 (19)
C13	0.0565 (18)	0.0475 (15)	0.079 (2)	−0.0009 (13)	−0.0005 (15)	0.0073 (14)
C14	0.0349 (13)	0.0428 (13)	0.0533 (15)	−0.0032 (10)	−0.0025 (11)	0.0084 (11)
C15	0.0449 (14)	0.0445 (13)	0.0508 (15)	0.0057 (11)	−0.0058 (12)	−0.0023 (11)
C16	0.0421 (14)	0.0387 (12)	0.0475 (14)	0.0047 (10)	−0.0035 (11)	0.0000 (10)
C17	0.0422 (14)	0.0431 (13)	0.0590 (16)	0.0047 (11)	−0.0100 (12)	−0.0004 (11)
C18	0.0470 (16)	0.0503 (16)	0.0707 (18)	−0.0045 (12)	−0.0114 (14)	−0.0017 (13)
C19	0.0585 (17)	0.0387 (13)	0.0719 (19)	−0.0029 (12)	−0.0005 (14)	−0.0020 (12)
C20	0.071 (2)	0.0425 (15)	0.080 (2)	0.0129 (14)	−0.0178 (16)	0.0013 (14)
C21	0.0556 (17)	0.0489 (15)	0.0685 (18)	0.0082 (13)	−0.0212 (14)	0.0000 (13)

Geometric parameters (Å, º)

Br1—C19	1.895 (3)	C8—H8	0.9300
S1—O2	1.415 (2)	C9—C14	1.384 (4)
S1—O1	1.4211 (19)	C9—C10	1.394 (4)
S1—N1	1.682 (2)	C10—C11	1.362 (5)
S1—C1	1.754 (3)	C10—H10	0.9300
O3—C15	1.215 (3)	C11—C12	1.368 (5)
N1—C14	1.417 (3)	C11—H11	0.9300
N1—C7	1.424 (3)	C12—C13	1.388 (4)
C1—C2	1.369 (4)	C12—H12	0.9300
C1—C6	1.376 (4)	C13—C14	1.386 (3)
C2—C3	1.394 (5)	C13—H13	0.9300
C2—H2	0.9300	C15—C16	1.485 (3)
C3—C4	1.370 (5)	C16—C17	1.382 (3)
C3—H3	0.9300	C16—C21	1.387 (3)
C4—C5	1.346 (6)	C17—C18	1.387 (4)
C4—H4	0.9300	C17—H17	0.9300
C5—C6	1.385 (5)	C18—C19	1.367 (4)
C5—H5	0.9300	C18—H18	0.9300
C6—H6	0.9300	C19—C20	1.375 (4)
C7—C8	1.343 (3)	C20—C21	1.370 (4)
C7—C15	1.490 (3)	C20—H20	0.9300
C8—C9	1.428 (4)	C21—H21	0.9300
O2—S1—O1	120.86 (13)	C11—C10—C9	118.2 (3)
O2—S1—N1	106.80 (11)	C11—C10—H10	120.9
O1—S1—N1	105.58 (12)	C9—C10—H10	120.9
O2—S1—C1	109.31 (14)	C10—C11—C12	121.2 (3)
O1—S1—C1	109.10 (12)	C10—C11—H11	119.4
N1—S1—C1	103.79 (11)	C12—C11—H11	119.4
C14—N1—C7	106.31 (19)	C11—C12—C13	122.5 (3)
C14—N1—S1	119.67 (16)	C11—C12—H12	118.7
C7—N1—S1	121.71 (16)	C13—C12—H12	118.7
C2—C1—C6	121.2 (3)	C14—C13—C12	115.8 (3)
C2—C1—S1	118.9 (2)	C14—C13—H13	122.1
C6—C1—S1	119.9 (2)	C12—C13—H13	122.1
C1—C2—C3	118.8 (3)	C9—C14—C13	122.3 (2)
C1—C2—H2	120.6	C9—C14—N1	108.3 (2)
C3—C2—H2	120.6	C13—C14—N1	129.4 (2)
C4—C3—C2	119.6 (4)	O3—C15—C16	122.0 (2)
C4—C3—H3	120.2	O3—C15—C7	119.8 (2)
C2—C3—H3	120.2	C16—C15—C7	118.1 (2)
C5—C4—C3	121.3 (4)	C17—C16—C21	119.0 (2)
C5—C4—H4	119.4	C17—C16—C15	122.8 (2)
C3—C4—H4	119.4	C21—C16—C15	118.1 (2)
C4—C5—C6	120.2 (3)	C16—C17—C18	120.2 (2)
C4—C5—H5	119.9	C16—C17—H17	119.9

C6—C5—H5	119.9	C18—C17—H17	119.9
C1—C6—C5	119.0 (3)	C19—C18—C17	119.2 (2)
C1—C6—H6	120.5	C19—C18—H18	120.4
C5—C6—H6	120.5	C17—C18—H18	120.4
C8—C7—N1	109.3 (2)	C18—C19—C20	121.7 (3)
C8—C7—C15	125.8 (2)	C18—C19—Br1	119.3 (2)
N1—C7—C15	122.2 (2)	C20—C19—Br1	119.0 (2)
C7—C8—C9	108.6 (2)	C21—C20—C19	118.8 (3)
C7—C8—H8	125.7	C21—C20—H20	120.6
C9—C8—H8	125.7	C19—C20—H20	120.6
C14—C9—C10	120.0 (3)	C20—C21—C16	121.1 (2)
C14—C9—C8	107.5 (2)	C20—C21—H21	119.4
C10—C9—C8	132.5 (3)	C16—C21—H21	119.4

O2—S1—N1—C14	163.63 (18)	C10—C11—C12—C13	0.1 (5)
O1—S1—N1—C14	−66.5 (2)	C11—C12—C13—C14	0.2 (5)
C1—S1—N1—C14	48.2 (2)	C10—C9—C14—C13	1.2 (4)
O2—S1—N1—C7	26.6 (2)	C8—C9—C14—C13	179.6 (2)
O1—S1—N1—C7	156.43 (18)	C10—C9—C14—N1	−177.8 (2)
C1—S1—N1—C7	−88.8 (2)	C8—C9—C14—N1	0.6 (3)
O2—S1—C1—C2	138.5 (2)	C12—C13—C14—C9	−0.9 (4)
O1—S1—C1—C2	4.3 (3)	C12—C13—C14—N1	177.9 (3)
N1—S1—C1—C2	−107.9 (2)	C7—N1—C14—C9	−0.8 (3)
O2—S1—C1—C6	−42.9 (3)	S1—N1—C14—C9	−143.64 (18)
O1—S1—C1—C6	−177.1 (2)	C7—N1—C14—C13	−179.7 (2)
N1—S1—C1—C6	70.7 (2)	S1—N1—C14—C13	37.5 (3)
C6—C1—C2—C3	−1.5 (5)	C8—C7—C15—O3	127.2 (3)
S1—C1—C2—C3	177.1 (3)	N1—C7—C15—O3	−32.1 (4)
C1—C2—C3—C4	1.8 (6)	C8—C7—C15—C16	−49.7 (4)
C2—C3—C4—C5	−1.1 (7)	N1—C7—C15—C16	151.0 (2)
C3—C4—C5—C6	0.0 (6)	O3—C15—C16—C17	162.2 (3)
C2—C1—C6—C5	0.5 (4)	C7—C15—C16—C17	−20.9 (4)
S1—C1—C6—C5	−178.1 (2)	O3—C15—C16—C21	−16.0 (4)
C4—C5—C6—C1	0.3 (5)	C7—C15—C16—C21	160.8 (2)
C14—N1—C7—C8	0.7 (3)	C21—C16—C17—C18	1.2 (4)
S1—N1—C7—C8	142.63 (19)	C15—C16—C17—C18	−177.0 (2)
C14—N1—C7—C15	163.0 (2)	C16—C17—C18—C19	−0.5 (4)
S1—N1—C7—C15	−55.1 (3)	C17—C18—C19—C20	−0.8 (5)
N1—C7—C8—C9	−0.4 (3)	C17—C18—C19—Br1	178.9 (2)
C15—C7—C8—C9	−161.9 (2)	C18—C19—C20—C21	1.4 (5)
C7—C8—C9—C14	−0.1 (3)	Br1—C19—C20—C21	−178.3 (2)
C7—C8—C9—C10	178.0 (3)	C19—C20—C21—C16	−0.7 (5)
C14—C9—C10—C11	−0.8 (4)	C17—C16—C21—C20	−0.6 (4)
C8—C9—C10—C11	−178.7 (3)	C15—C16—C21—C20	177.7 (3)
C9—C10—C11—C12	0.2 (5)		

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*2 are the centroids of the N1/C7/C8/C9/C14 and C9—C14 rings, respectively

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17···O3^{i}	0.93	2.50	3.383 (3)	158
C4—H4···*Cg*1^{ii}	0.93	2.67	3.635 (4)	127
C4—H4···*Cg*2^{ii}	0.93	2.76	3.681 (4)	169

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