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(Phenyl)(1-phenylsulfonyl-1*H*-indol-3-yl)-methanone

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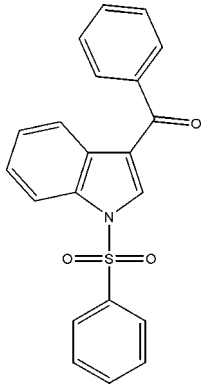
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.109; data-to-parameter ratio = 18.2.

In the title compound, $C_{21}H_{15}NO_3S$, the sulfonyl-bound phenyl ring forms a dihedral angle of 86.28 (5)° with the indole ring system. The molecular structure is stabilized by intramolecular C—H···O hydrogen bonds. The crystal packing is stabilized by weak intermolecular C—H···O and C—H···π interactions.

Related literature

For the structures of closely related compounds, see: Chakkaravarthi *et al.* (2007, 2008).



Experimental

Crystal data

$C_{21}H_{15}NO_3S$ M_r = 361.40
Triclinic, $P\overline{1}$
a = 7.567 (1) Å
b = 10.571 (2) Å
c = 12.083 (3) Å
α = 66.302 (2)°
β = 80.740 (1)°
γ = 78.403 (1)°
V = 863.5 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.21 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} = 0.952, T_{max} = 0.960
15638 measured reflections
4276 independent reflections
3187 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
Standard reflections: 0

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.109
S = 1.01
4276 reflections
235 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

*Cg*1 is the centroid of the C16–C21 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O1	0.93	2.42	2.999 (2)	120
C6—H6···O2^{i}	0.93	2.58	3.493 (2)	167
C7—H7···O2^{i}	0.93	2.54	3.429 (2)	160
C4—H4···*Cg*1^{ii}	0.93	2.98	3.774 (3)	144

Symmetry codes: (i) $-x+2, -y, -z$; (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: BT5379).

References

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

Acta Cryst. (2010). E**66**, o2895 [https://doi.org/10.1107/S1600536810042261]

(Phenyl)(1-phenylsulfonyl-1*H*-indol-3-yl)methanone

G. Chakkaravarthi, R. Panchatcharam, V. Dhayalan, A. K. Mohanakrishnan and V. Manivannan

S1. Comment

The geometric parameters of the molecule of (I) (Fig. 1) agree well with the reported values of similar structures (Chakkaravarthi *et al.*, 2007; Chakkaravarthi *et al.*, 2008). The phenyl rings C1—C6 and C16—C21 form the dihedral angles of 86.28 (5)° and 51.91 (5)°, respectively with the indole ring system. The mean planes of the two phenyl rings are inclined at an angle of 42.16 (6)°.

The sum of the bond angles around N1 [358.53°] indicates that N1 atom is sp^2 hybridized. The molecular structure is stabilized by intra molecular C—H···O hydrogen bonds and 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 3.774 (3)Å (*Cg*1 is the centroid of the ring defined by the atoms C16—C21)] interactions.

S2. Experimental

To a solution of 1-phenylsulfonyl-(1*H*-indol-3-yl)(phenyl)methanol (1 g, 2.75 mmol) in dry 1,2-Dichloroethane (30 ml), manganese dioxide (6 g. 68.96 mmol) was added then stirred at room temperature for 4 h and then refluxed for 3 h. Then the resulting solution was passed through celite pad and washed with DCM (2 *x* 30 ml). 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 U_{iso}(H) = 1.2Ueq(C) for aromatic C—H. The components of the anisotropic displacement parameters in direction of the bond of C3and C4; C18 and C19 were restrained to be equal within an effective standard deviation of 0.001 using the DELU command in *SHELXL* (Sheldrick, 2008).

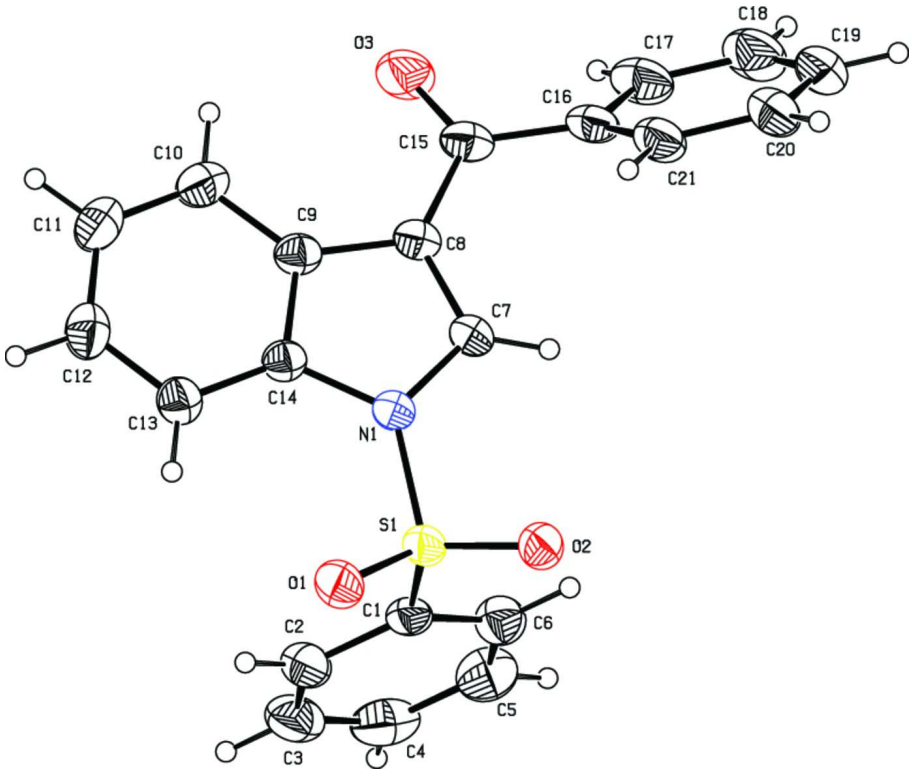

Figure 1

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

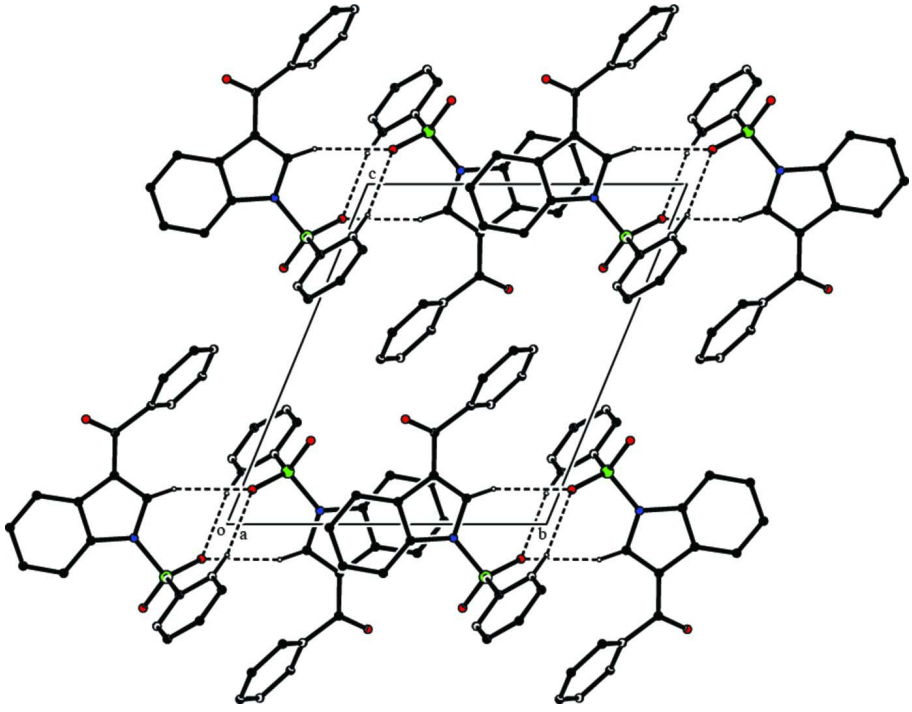

Figure 2

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.

(Phenyl)(1-phenylsulfonyl-1*H*-indol-3-yl)methanone

Crystal data

$C_{21}H_{15}NO_3S$
$M_r = 361.40$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.567$ (1) Å
$b = 10.571$ (2) Å
$c = 12.083$ (3) Å
$\alpha = 66.302$ (2)°
$\beta = 80.740$ (1)°
$\gamma = 78.403$ (1)°
$V = 863.5$ (3) Å^3
$Z = 2$
$F(000) = 376$
$D_x = 1.390$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6196 reflections
$\theta = 2.2$–$27.1°$
$\mu = 0.21$ 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)
$T_{min} = 0.952$, $T_{max} = 0.960$
15638 measured reflections
4276 independent reflections
3187 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 28.3°$, $\theta_{min} = 1.9°$
$h = -10 \rightarrow 10$
$k = -14 \rightarrow 13$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.109$
$S = 1.01$
4276 reflections
235 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 0.1447P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.7233 (2)	0.05722 (16)	0.20701 (13)	0.0494 (4)
C2	0.6154 (3)	0.0869 (2)	0.29978 (15)	0.0648 (5)
H2	0.6523	0.1388	0.3360	0.078*
C3	0.4508 (3)	0.0376 (2)	0.33759 (18)	0.0791 (5)
H3	0.3759	0.0567	0.3997	0.095*
C4	0.3975 (3)	−0.0394 (2)	0.2838 (2)	0.0806 (6)
H4	0.2866	−0.0718	0.3097	0.097*
C5	0.5061 (3)	−0.0687 (2)	0.1928 (2)	0.0757 (5)
H5	0.4690	−0.1215	0.1575	0.091*
C6	0.6701 (2)	−0.02074 (19)	0.15289 (17)	0.0615 (4)
H6	0.7440	−0.0403	0.0906	0.074*
C14	0.80636 (19)	0.40437 (16)	0.04797 (13)	0.0448 (3)

C13	0.7914 (2)	0.44779 (18)	0.14366 (15)	0.0547 (4)
H13	0.8305	0.3873	0.2188	0.066*
C12	0.7164 (2)	0.5838 (2)	0.12251 (18)	0.0641 (5)
H12	0.7018	0.6157	0.1853	0.077*
C11	0.6617 (3)	0.6751 (2)	0.00966 (19)	0.0681 (5)
H11	0.6130	0.7671	−0.0019	0.082*
C10	0.6778 (2)	0.63262 (18)	−0.08489 (17)	0.0609 (4)
H10	0.6412	0.6948	−0.1603	0.073*
C9	0.75050 (19)	0.49375 (16)	−0.06607 (14)	0.0472 (3)
C8	0.7882 (2)	0.41551 (16)	−0.14359 (13)	0.0474 (3)
C7	0.86292 (19)	0.28383 (16)	−0.07641 (12)	0.0469 (3)
H7	0.8982	0.2113	−0.1040	0.056*
C15	0.7413 (2)	0.46868 (18)	−0.26928 (14)	0.0546 (4)
C16	0.8200 (2)	0.39033 (18)	−0.34881 (13)	0.0553 (4)
C21	0.9990 (3)	0.32957 (19)	−0.35204 (14)	0.0634 (5)
H21	1.0737	0.3291	−0.2978	0.076*
C20	1.0679 (3)	0.2692 (2)	−0.43577 (17)	0.0807 (6)
H20	1.1893	0.2301	−0.4391	0.097*
C19	0.9549 (4)	0.2676 (2)	−0.51451 (18)	0.0891 (6)
H19	1.0000	0.2259	−0.5700	0.107*
C18	0.7771 (4)	0.3274 (3)	−0.51087 (19)	0.0900 (6)
H18	0.7017	0.3266	−0.5642	0.108*
C17	0.7103 (3)	0.3879 (2)	−0.42929 (16)	0.0742 (5)
H17	0.5894	0.4283	−0.4275	0.089*
N1	0.87874 (17)	0.27365 (13)	0.04012 (10)	0.0461 (3)
O1	0.98538 (16)	0.15404 (13)	0.24616 (10)	0.0602 (3)
O2	1.04747 (14)	0.03484 (12)	0.10209 (10)	0.0543 (3)
O3	0.63449 (19)	0.57703 (15)	−0.30880 (11)	0.0789 (4)
S1	0.92933 (5)	0.12195 (4)	0.15505 (3)	0.04628 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0554 (8)	0.0428 (8)	0.0381 (7)	0.0021 (7)	−0.0076 (6)	−0.0064 (6)
C2	0.0723 (11)	0.0626 (11)	0.0470 (9)	−0.0010 (9)	0.0007 (8)	−0.0146 (8)
C3	0.0696 (12)	0.0795 (14)	0.0578 (11)	0.0037 (10)	0.0110 (9)	−0.0082 (9)
C4	0.0579 (10)	0.0687 (13)	0.0827 (14)	−0.0089 (9)	−0.0036 (10)	0.0032 (9)
C5	0.0669 (11)	0.0698 (13)	0.0848 (14)	−0.0156 (10)	−0.0104 (10)	−0.0201 (11)
C6	0.0619 (10)	0.0604 (11)	0.0593 (10)	−0.0069 (8)	−0.0060 (8)	−0.0209 (8)
C14	0.0447 (7)	0.0433 (8)	0.0444 (7)	−0.0093 (6)	−0.0023 (6)	−0.0140 (6)
C13	0.0606 (9)	0.0553 (10)	0.0513 (9)	−0.0105 (8)	−0.0034 (7)	−0.0234 (8)
C12	0.0666 (10)	0.0632 (12)	0.0739 (12)	−0.0113 (9)	−0.0011 (9)	−0.0391 (10)
C11	0.0712 (11)	0.0486 (10)	0.0844 (13)	−0.0044 (8)	−0.0049 (10)	−0.0280 (10)
C10	0.0611 (10)	0.0473 (9)	0.0632 (10)	−0.0049 (8)	−0.0074 (8)	−0.0107 (8)
C9	0.0440 (7)	0.0465 (8)	0.0456 (8)	−0.0096 (6)	−0.0016 (6)	−0.0115 (6)
C8	0.0483 (8)	0.0496 (9)	0.0386 (7)	−0.0083 (6)	−0.0041 (6)	−0.0105 (6)
C7	0.0535 (8)	0.0499 (9)	0.0359 (7)	−0.0072 (7)	−0.0052 (6)	−0.0149 (6)
C15	0.0546 (8)	0.0571 (10)	0.0403 (8)	−0.0080 (7)	−0.0082 (7)	−0.0053 (7)

C16	0.0677 (10)	0.0550 (10)	0.0337 (7)	−0.0120 (8)	−0.0094 (7)	−0.0041 (7)
C21	0.0728 (11)	0.0691 (12)	0.0399 (8)	−0.0044 (9)	−0.0087 (8)	−0.0138 (8)
C20	0.1019 (15)	0.0786 (14)	0.0471 (10)	0.0032 (12)	0.0000 (10)	−0.0194 (9)
C19	0.1479 (17)	0.0736 (14)	0.0441 (9)	−0.0172 (13)	−0.0036 (12)	−0.0223 (10)
C18	0.1306 (15)	0.0951 (17)	0.0512 (10)	−0.0334 (13)	−0.0220 (12)	−0.0222 (11)
C17	0.0873 (13)	0.0821 (14)	0.0465 (9)	−0.0182 (11)	−0.0203 (9)	−0.0097 (9)
N1	0.0566 (7)	0.0434 (7)	0.0357 (6)	−0.0037 (6)	−0.0071 (5)	−0.0132 (5)
O1	0.0728 (7)	0.0643 (7)	0.0457 (6)	−0.0020 (6)	−0.0197 (5)	−0.0220 (5)
O2	0.0551 (6)	0.0540 (7)	0.0498 (6)	0.0039 (5)	−0.0072 (5)	−0.0205 (5)
O3	0.0817 (9)	0.0791 (9)	0.0539 (7)	0.0174 (7)	−0.0184 (6)	−0.0119 (7)
S1	0.0526 (2)	0.0470 (2)	0.03579 (19)	0.00011 (16)	−0.00991 (15)	−0.01356 (15)

Geometric parameters (Å, º)

C1—C2	1.381 (2)	C10—H10	0.9300
C1—C6	1.386 (2)	C9—C8	1.444 (2)
C1—S1	1.7498 (17)	C8—C7	1.356 (2)
C2—C3	1.384 (3)	C8—C15	1.468 (2)
C2—H2	0.9300	C7—N1	1.3913 (18)
C3—C4	1.375 (3)	C7—H7	0.9300
C3—H3	0.9300	C15—O3	1.227 (2)
C4—C5	1.364 (3)	C15—C16	1.490 (2)
C4—H4	0.9300	C16—C21	1.379 (2)
C5—C6	1.376 (3)	C16—C17	1.387 (2)
C5—H5	0.9300	C21—C20	1.385 (3)
C6—H6	0.9300	C21—H21	0.9300
C14—C13	1.387 (2)	C20—C19	1.385 (3)
C14—C9	1.397 (2)	C20—H20	0.9300
C14—N1	1.4152 (19)	C19—C18	1.369 (3)
C13—C12	1.370 (2)	C19—H19	0.9300
C13—H13	0.9300	C18—C17	1.361 (3)
C12—C11	1.388 (3)	C18—H18	0.9300
C12—H12	0.9300	C17—H17	0.9300
C11—C10	1.366 (3)	N1—S1	1.6677 (12)
C11—H11	0.9300	O1—S1	1.4195 (11)
C10—C9	1.399 (2)	O2—S1	1.4195 (11)
C2—C1—C6	121.26 (17)	C7—C8—C9	107.38 (13)
C2—C1—S1	119.33 (14)	C7—C8—C15	127.21 (15)
C6—C1—S1	119.39 (12)	C9—C8—C15	125.29 (15)
C1—C2—C3	118.46 (19)	C8—C7—N1	109.68 (13)
C1—C2—H2	120.8	C8—C7—H7	125.2
C3—C2—H2	120.8	N1—C7—H7	125.2
C4—C3—C2	120.39 (18)	O3—C15—C8	119.99 (16)
C4—C3—H3	119.8	O3—C15—C16	119.61 (14)
C2—C3—H3	119.8	C8—C15—C16	120.39 (14)
C5—C4—C3	120.5 (2)	C21—C16—C17	118.93 (18)
C5—C4—H4	119.7	C21—C16—C15	123.05 (15)

C3—C4—H4	119.7	C17—C16—C15	117.84 (17)
C4—C5—C6	120.5 (2)	C16—C21—C20	120.24 (18)
C4—C5—H5	119.8	C16—C21—H21	119.9
C6—C5—H5	119.8	C20—C21—H21	119.9
C5—C6—C1	118.91 (18)	C21—C20—C19	119.5 (2)
C5—C6—H6	120.5	C21—C20—H20	120.2
C1—C6—H6	120.5	C19—C20—H20	120.2
C13—C14—C9	122.50 (15)	C18—C19—C20	120.2 (2)
C13—C14—N1	130.70 (14)	C18—C19—H19	119.9
C9—C14—N1	106.78 (13)	C20—C19—H19	119.9
C12—C13—C14	117.03 (16)	C17—C18—C19	120.1 (2)
C12—C13—H13	121.5	C17—C18—H18	120.0
C14—C13—H13	121.5	C19—C18—H18	120.0
C13—C12—C11	121.58 (17)	C18—C17—C16	121.0 (2)
C13—C12—H12	119.2	C18—C17—H17	119.5
C11—C12—H12	119.2	C16—C17—H17	119.5
C10—C11—C12	121.37 (17)	C7—N1—C14	108.35 (12)
C10—C11—H11	119.3	C7—N1—S1	123.27 (10)
C12—C11—H11	119.3	C14—N1—S1	126.91 (10)
C11—C10—C9	118.68 (17)	O2—S1—O1	120.91 (7)
C11—C10—H10	120.7	O2—S1—N1	105.43 (7)
C9—C10—H10	120.7	O1—S1—N1	106.66 (7)
C14—C9—C10	118.82 (15)	O2—S1—C1	108.92 (7)
C14—C9—C8	107.78 (14)	O1—S1—C1	109.22 (7)
C10—C9—C8	133.37 (15)	N1—S1—C1	104.41 (7)

C6—C1—C2—C3	−0.4 (3)	C8—C15—C16—C21	−42.0 (2)
S1—C1—C2—C3	178.44 (13)	O3—C15—C16—C17	−35.9 (2)
C1—C2—C3—C4	0.2 (3)	C8—C15—C16—C17	142.89 (16)
C2—C3—C4—C5	0.2 (3)	C17—C16—C21—C20	1.0 (3)
C3—C4—C5—C6	−0.5 (3)	C15—C16—C21—C20	−174.08 (16)
C4—C5—C6—C1	0.3 (3)	C16—C21—C20—C19	−1.4 (3)
C2—C1—C6—C5	0.2 (3)	C21—C20—C19—C18	1.1 (3)
S1—C1—C6—C5	−178.69 (14)	C20—C19—C18—C17	−0.4 (4)
C9—C14—C13—C12	0.7 (2)	C19—C18—C17—C16	0.0 (3)
N1—C14—C13—C12	178.95 (15)	C21—C16—C17—C18	−0.3 (3)
C14—C13—C12—C11	−1.5 (3)	C15—C16—C17—C18	175.06 (18)
C13—C12—C11—C10	1.0 (3)	C8—C7—N1—C14	1.51 (16)
C12—C11—C10—C9	0.3 (3)	C8—C7—N1—S1	168.55 (10)
C13—C14—C9—C10	0.5 (2)	C13—C14—N1—C7	−179.63 (15)
N1—C14—C9—C10	−178.11 (13)	C9—C14—N1—C7	−1.22 (16)
C13—C14—C9—C8	179.08 (14)	C13—C14—N1—S1	13.9 (2)
N1—C14—C9—C8	0.51 (16)	C9—C14—N1—S1	−167.65 (10)
C11—C10—C9—C14	−1.0 (2)	C7—N1—S1—O2	33.46 (13)
C11—C10—C9—C8	−179.16 (16)	C14—N1—S1—O2	−161.98 (12)
C14—C9—C8—C7	0.40 (16)	C7—N1—S1—O1	163.18 (12)
C10—C9—C8—C7	178.74 (17)	C14—N1—S1—O1	−32.27 (14)
C14—C9—C8—C15	176.58 (14)	C7—N1—S1—C1	−81.25 (13)

C10—C9—C8—C15	−5.1 (3)	C14—N1—S1—C1	83.30 (13)
C9—C8—C7—N1	−1.18 (17)	C2—C1—S1—O2	155.20 (12)
C15—C8—C7—N1	−177.26 (14)	C6—C1—S1—O2	−25.92 (15)
C7—C8—C15—O3	161.36 (17)	C2—C1—S1—O1	21.21 (15)
C9—C8—C15—O3	−14.1 (2)	C6—C1—S1—O1	−159.91 (13)
C7—C8—C15—C16	−17.5 (2)	C2—C1—S1—N1	−92.56 (13)
C9—C8—C15—C16	167.13 (14)	C6—C1—S1—N1	86.32 (14)
O3—C15—C16—C21	139.19 (18)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C16–C21 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1	0.93	2.59	2.934 (2)	103
C10—H10···O3	0.93	2.57	3.068 (3)	114
C13—H13···O1	0.93	2.42	2.999 (2)	120
C6—H6···O2^{i}	0.93	2.58	3.493 (2)	167
C7—H7···O2^{i}	0.93	2.54	3.429 (2)	160
C4—H4···*Cg*1^{ii}	0.93	2.98	3.774 (3)	144

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