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2-Chloromethyl-3-methyl-1-phenylsulfonyl-1*H*-indole

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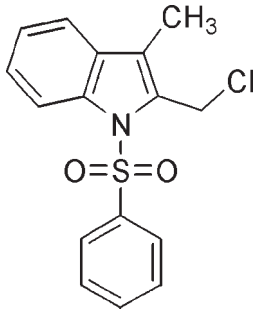
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.120; data-to-parameter ratio = 20.3.

In the title compound, $C_{16}H_{14}ClNO_2S$, the phenyl ring makes a dihedral angle of 78.1 (1)° with the indole ring system. The molecular structure is stabilized by weak intramolecular C—H···O interactions. The crystal structure exhibits weak intermolecular C—H···O, C—H···π and π–π [centroid–centroid distances = 3.620 (1)–3.794 (1) Å] interactions.

Related literature

For the biological activity of indole derivatives, see: Okabe & Adachi (1998); Schollmeyer *et al.* (1995). For related crystal structures, see: Chakkaravarthi *et al.* (2007, 2008).



Experimental

Crystal data

$C_{16}H_{14}ClNO_2S$
M_r = 319.79
Monoclinic, $P2_1/c$
a = 7.9769 (6) Å
b = 10.8064 (9) Å
c = 17.3418 (12) Å
β = 97.500 (2)°
V = 1482.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 295 K
0.30 × 0.28 × 0.26 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.889, T_{max} = 0.903
17616 measured reflections
3885 independent reflections
3201 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.120
S = 1.04
3885 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1	0.93	2.51	2.886 (3)	104
C13—H13···O1	0.93	2.47	3.033 (2)	119
C15—H15*B*···O2	0.97	2.31	2.853 (3)	114
C16—H16*A*···*Cg*2^{ii}	0.96	2.94	3.777 (2)	146
C16—H16*B*···*Cg*3^{iii}	0.96	2.92	3.781 (3)	149

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x+1, -y, -z+1$. *Cg*2 and *Cg*3 are the centroids of the C1–C6 and C9–C14 rings, respectively.

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 IIT, Madras, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2470).

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Acta Cryst. (2009). E**65**, o2733 [https://doi.org/10.1107/S1600536809041191]

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S1. Comment

The indole derivatives are found to possess antibacterial (Okabe & Adachi, 1998) and antitumour (Schollmeyer *et al.*, 1995) activities. In continuation of our studies in indole derivatives, we present the crystal structure of the title compound (I). The geometric parameters of (I) (Fig. 1) agree with those in the reported structures (Chakkaravarthi *et al.*, 2007, 2008).

The plane of the phenyl ring forms a dihedral angle of 78.1 (1)° with the indole ring system. The torsion angles O2—S1—N1—C7 and O1—S1—N1—C14 [-22.9 (2)° and 54.5 (1)°, respectively] indicate the *syn*-conformation of the sulfonyl moiety. The sum of bond angles around N1 [355.6 (1)°] indicates that N1 is sp^2-hybridized.

The molecular packing is stabilized by weak intramolecular C—H···O interactions and the crystal packing of I (Fig. 2) exhibit weak intermolecular C—H···O, C—H···π (see Table 1) and π–π [*Cg*1···*Cg*1(-*x*, -*y*, 1 - *z*) distance of 3.620 (1) Å and *Cg*1···*Cg*3 (-*x*, -*y*, 1 - *z*) distance of 3.794 (1) Å interactions. *Cg*1 and *Cg*3 are the centroids of the N1/C7–C9/C14 and C9–C14 rings, respectively.

S2. Experimental

A mixture of 1-phenylsulfonyl-2,3-dimethylindole (5 g, 17.5 mmol) and finely powdered NCS (2.56 g, 19.17 mmol) in dry CCl_4 (80 ml) containing catalytic amount of benzoyl peroxide (0.1 g) was refluxed for 1 h and cooled. The floated succinimide was filtered off and washed with CCl_4 (15 ml). The solvent was then removed completely under vacuo and recrystallized from $CDCl_3$.

S3. Refinement

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 = 0.97 Å and U_{iso}(H) = 1.5U_{eq}(C) for methylene, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl.

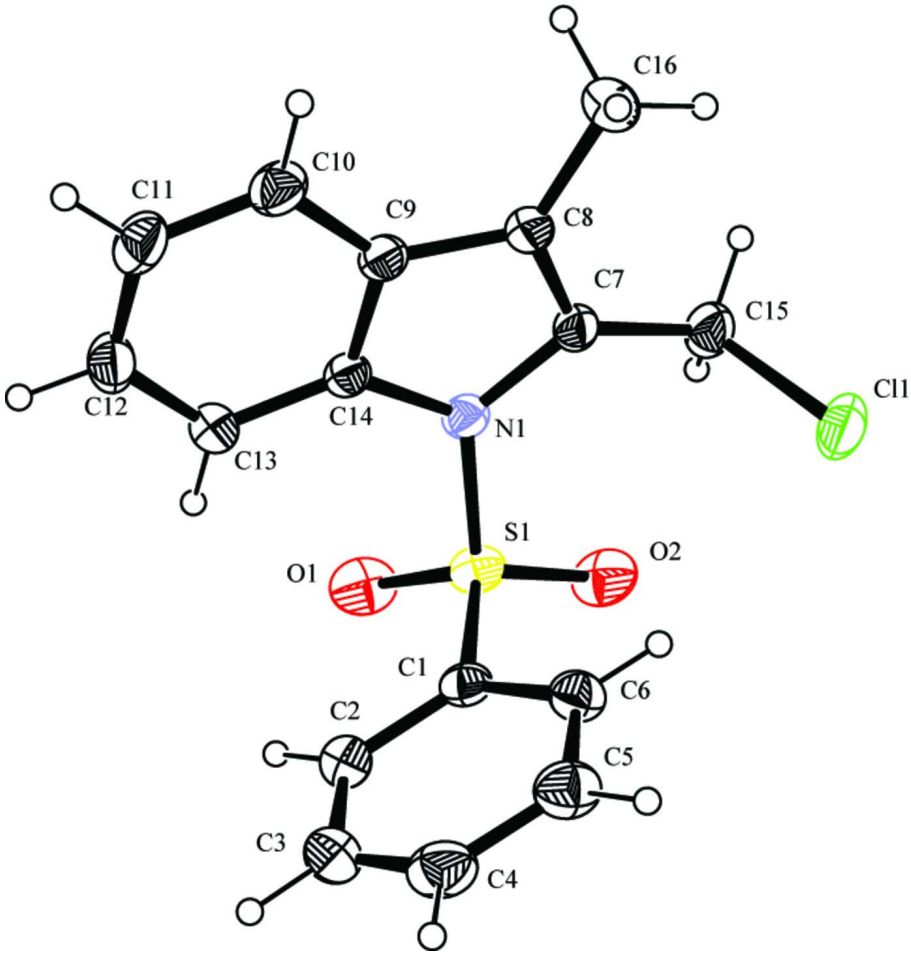

Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

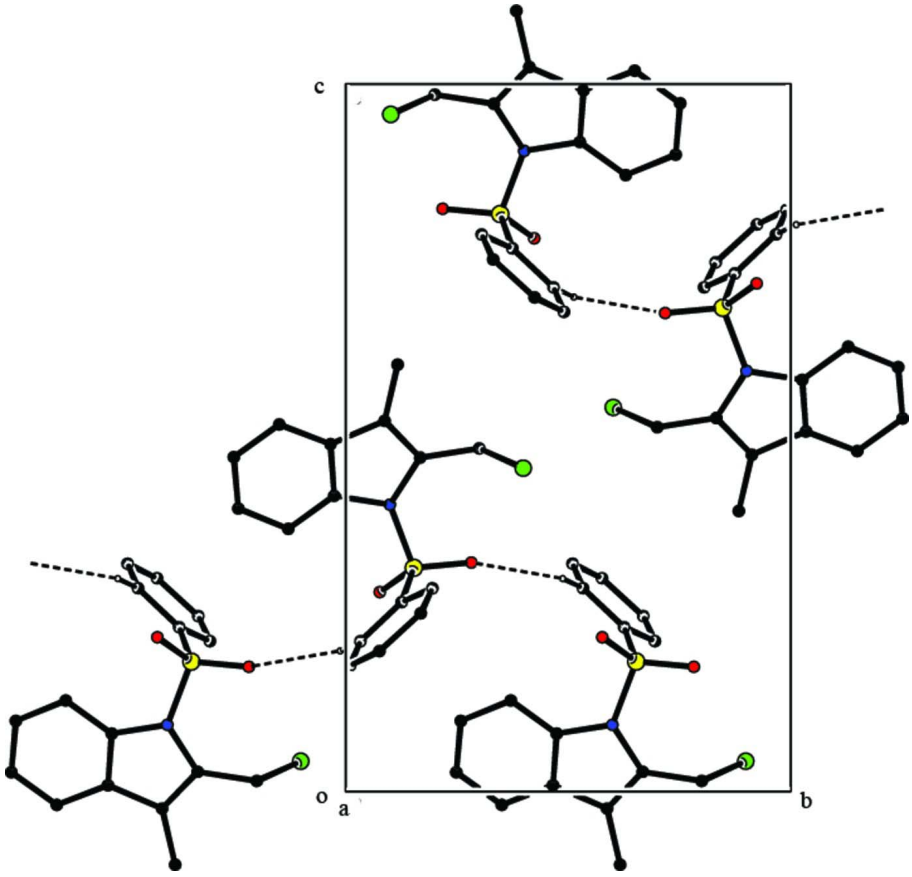

Figure 2

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

2-Chloromethyl-3-methyl-1-phenylsulfonyl-1*H*-indole

Crystal data

$C_{16}H_{14}ClNO_2S$
$M_r = 319.79$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.9769\ (6)$ Å
$b = 10.8064\ (9)$ Å
$c = 17.3418\ (12)$ Å
$\beta = 97.500\ (2)°$
$V = 1482.1\ (2)$ Å^3
$Z = 4$
$F(000) = 664$
$D_x = 1.433$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8432 reflections
$\theta = 2.2–28.8°$
$\mu = 0.40$ mm^{-1}
$T = 295$ K
Block, colourless
0.30 × 0.28 × 0.26 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)
$T_{min} = 0.889$, $T_{max} = 0.903$
17616 measured reflections
3885 independent reflections
3201 reflections with $I > 2\sigma(I)$

R_{int} = 0.024
θ_{max} = 28.9°, θ_{min} = 2.2°
h = −10→10
k = −14→14
l = −13→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.120
S = 1.04
3885 reflections
191 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
$w = 1/[\sigma^2(F_o^2) + (0.0606P)^2 + 0.5623P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2222 (2)	0.12567 (15)	0.26775 (9)	0.0376 (3)
C2	0.2156 (3)	0.03299 (18)	0.21251 (11)	0.0510 (4)
H2	0.1172	−0.0125	0.1989	0.061*
C3	0.3596 (3)	0.0096 (2)	0.17795 (12)	0.0633 (6)
H3	0.3576	−0.0519	0.1403	0.076*
C4	0.5042 (3)	0.0757 (2)	0.19847 (13)	0.0602 (5)
H4	0.6006	0.0573	0.1758	0.072*
C5	0.5086 (3)	0.1686 (2)	0.25200 (12)	0.0554 (5)
H5	0.6069	0.2145	0.2647	0.067*
C6	0.3671 (2)	0.19466 (18)	0.28736 (10)	0.0460 (4)
H6	0.3695	0.2578	0.3239	0.055*
C7	0.1768 (2)	0.16719 (15)	0.47207 (10)	0.0391 (3)
C8	0.2587 (2)	0.08731 (16)	0.52391 (9)	0.0408 (4)
C9	0.2430 (2)	−0.03433 (15)	0.49110 (9)	0.0371 (3)
C10	0.3019 (3)	−0.14938 (18)	0.51880 (11)	0.0498 (4)
H10	0.3646	−0.1568	0.5677	0.060*
C11	0.2658 (3)	−0.25159 (18)	0.47269 (13)	0.0543 (5)
H11	0.3054	−0.3288	0.4904	0.065*
C12	0.1713 (3)	−0.24139 (17)	0.40010 (12)	0.0503 (4)
H12	0.1491	−0.3121	0.3700	0.060*
C13	0.1090 (2)	−0.12916 (16)	0.37131 (10)	0.0426 (4)
H13	0.0446	−0.1229	0.3227	0.051*
C14	0.14676 (19)	−0.02597 (15)	0.41808 (9)	0.0343 (3)
C15	0.1467 (3)	0.29996 (17)	0.48501 (12)	0.0530 (5)
H15A	0.1376	0.3130	0.5396	0.064*
H15B	0.0398	0.3236	0.4555	0.064*
C16	0.3463 (3)	0.1166 (2)	0.60340 (11)	0.0604 (5)
H16A	0.3348	0.2033	0.6137	0.091*
H16B	0.4640	0.0960	0.6062	0.091*
H16C	0.2963	0.0694	0.6414	0.091*
N1	0.10231 (17)	0.09922 (13)	0.40560 (7)	0.0370 (3)

O1	−0.08880 (16)	0.07654 (16)	0.28192 (8)	0.0602 (4)
O2	0.0208 (2)	0.28227 (14)	0.32369 (9)	0.0621 (4)
S1	0.04580 (5)	0.15288 (4)	0.31625 (2)	0.04245 (13)
Cl1	0.31210 (9)	0.39887 (5)	0.45712 (4)	0.07026 (19)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0415 (8)	0.0392 (8)	0.0318 (7)	0.0045 (6)	0.0032 (6)	0.0087 (6)
C2	0.0614 (11)	0.0464 (10)	0.0462 (9)	−0.0100 (9)	0.0108 (8)	−0.0018 (8)
C3	0.0900 (16)	0.0496 (12)	0.0557 (12)	−0.0003 (11)	0.0294 (11)	−0.0080 (9)
C4	0.0614 (12)	0.0649 (13)	0.0592 (12)	0.0082 (10)	0.0270 (10)	0.0068 (10)
C5	0.0454 (9)	0.0698 (14)	0.0519 (10)	−0.0043 (9)	0.0090 (8)	0.0039 (9)
C6	0.0467 (9)	0.0519 (10)	0.0389 (8)	−0.0010 (8)	0.0040 (7)	−0.0004 (7)
C7	0.0465 (9)	0.0336 (8)	0.0401 (8)	−0.0044 (7)	0.0162 (7)	−0.0023 (6)
C8	0.0469 (9)	0.0415 (9)	0.0347 (7)	−0.0092 (7)	0.0082 (6)	−0.0005 (6)
C9	0.0391 (8)	0.0374 (8)	0.0349 (7)	−0.0027 (6)	0.0058 (6)	0.0039 (6)
C10	0.0539 (10)	0.0460 (10)	0.0470 (9)	0.0006 (8)	−0.0025 (8)	0.0117 (8)
C11	0.0630 (12)	0.0355 (9)	0.0649 (12)	0.0069 (8)	0.0097 (9)	0.0094 (8)
C12	0.0585 (11)	0.0359 (9)	0.0579 (11)	−0.0027 (8)	0.0130 (9)	−0.0072 (8)
C13	0.0474 (9)	0.0413 (9)	0.0392 (8)	−0.0026 (7)	0.0057 (7)	−0.0033 (7)
C14	0.0355 (7)	0.0338 (8)	0.0344 (7)	0.0006 (6)	0.0081 (6)	0.0029 (6)
C15	0.0683 (12)	0.0373 (9)	0.0588 (11)	−0.0017 (9)	0.0279 (9)	−0.0040 (8)
C16	0.0773 (14)	0.0624 (13)	0.0397 (9)	−0.0185 (11)	0.0007 (9)	−0.0052 (9)
N1	0.0423 (7)	0.0337 (7)	0.0354 (6)	0.0033 (5)	0.0070 (5)	0.0039 (5)
O1	0.0372 (6)	0.0834 (11)	0.0567 (8)	0.0000 (7)	−0.0064 (6)	0.0106 (7)
O2	0.0714 (10)	0.0515 (9)	0.0644 (9)	0.0286 (7)	0.0124 (7)	0.0183 (7)
S1	0.0366 (2)	0.0485 (3)	0.0416 (2)	0.01086 (17)	0.00270 (15)	0.01142 (17)
Cl1	0.0967 (4)	0.0386 (3)	0.0815 (4)	−0.0169 (3)	0.0344 (3)	−0.0031 (2)

Geometric parameters (Å, º)

C1—C6	1.380 (3)	C10—C11	1.372 (3)
C1—C2	1.382 (3)	C10—H10	0.9300
C1—S1	1.7559 (17)	C11—C12	1.385 (3)
C2—C3	1.387 (3)	C11—H11	0.9300
C2—H2	0.9300	C12—C13	1.379 (3)
C3—C4	1.364 (3)	C12—H12	0.9300
C3—H3	0.9300	C13—C14	1.389 (2)
C4—C5	1.365 (3)	C13—H13	0.9300
C4—H4	0.9300	C14—N1	1.408 (2)
C5—C6	1.382 (3)	C15—Cl1	1.812 (2)
C5—H5	0.9300	C15—H15A	0.9700
C6—H6	0.9300	C15—H15B	0.9700
C7—C8	1.352 (2)	C16—H16A	0.9600
C7—N1	1.429 (2)	C16—H16B	0.9600
C7—C15	1.477 (2)	C16—H16C	0.9600
C8—C9	1.431 (2)	N1—S1	1.6607 (13)

C8—C16	1.496 (2)	O1—S1	1.4216 (15)
C9—C10	1.392 (2)	O2—S1	1.4206 (15)
C9—C14	1.395 (2)		

C6—C1—C2	121.15 (17)	C12—C11—H11	119.5
C6—C1—S1	119.29 (13)	C13—C12—C11	121.79 (18)
C2—C1—S1	119.53 (14)	C13—C12—H12	119.1
C1—C2—C3	118.21 (19)	C11—C12—H12	119.1
C1—C2—H2	120.9	C12—C13—C14	117.02 (17)
C3—C2—H2	120.9	C12—C13—H13	121.5
C4—C3—C2	120.80 (19)	C14—C13—H13	121.5
C4—C3—H3	119.6	C13—C14—C9	121.98 (15)
C2—C3—H3	119.6	C13—C14—N1	130.59 (15)
C3—C4—C5	120.56 (19)	C9—C14—N1	107.42 (13)
C3—C4—H4	119.7	C7—C15—Cl1	113.22 (13)
C5—C4—H4	119.7	C7—C15—H15A	108.9
C4—C5—C6	120.1 (2)	Cl1—C15—H15A	108.9
C4—C5—H5	119.9	C7—C15—H15B	108.9
C6—C5—H5	119.9	Cl1—C15—H15B	108.9
C1—C6—C5	119.14 (18)	H15A—C15—H15B	107.7
C1—C6—H6	120.4	C8—C16—H16A	109.5
C5—C6—H6	120.4	C8—C16—H16B	109.5
C8—C7—N1	108.80 (14)	H16A—C16—H16B	109.5
C8—C7—C15	126.40 (17)	C8—C16—H16C	109.5
N1—C7—C15	124.29 (16)	H16A—C16—H16C	109.5
C7—C8—C9	108.21 (15)	H16B—C16—H16C	109.5
C7—C8—C16	127.22 (17)	C14—N1—C7	107.46 (13)
C9—C8—C16	124.53 (17)	C14—N1—S1	120.74 (11)
C10—C9—C14	119.47 (16)	C7—N1—S1	127.36 (12)
C10—C9—C8	132.44 (16)	O2—S1—O1	120.13 (10)
C14—C9—C8	108.08 (14)	O2—S1—N1	106.45 (8)
C11—C10—C9	118.82 (17)	O1—S1—N1	106.64 (8)
C11—C10—H10	120.6	O2—S1—C1	109.81 (9)
C9—C10—H10	120.6	O1—S1—C1	108.11 (9)
C10—C11—C12	120.91 (18)	N1—S1—C1	104.57 (7)
C10—C11—H11	119.5		

C6—C1—C2—C3	1.0 (3)	C10—C9—C14—N1	179.02 (15)
S1—C1—C2—C3	−176.87 (15)	C8—C9—C14—N1	−0.22 (18)
C1—C2—C3—C4	0.5 (3)	C8—C7—C15—Cl1	91.1 (2)
C2—C3—C4—C5	−1.8 (4)	N1—C7—C15—Cl1	−98.03 (19)
C3—C4—C5—C6	1.6 (3)	C13—C14—N1—C7	−179.07 (16)
C2—C1—C6—C5	−1.2 (3)	C9—C14—N1—C7	1.18 (17)
S1—C1—C6—C5	176.64 (15)	C13—C14—N1—S1	−21.1 (2)
C4—C5—C6—C1	−0.1 (3)	C9—C14—N1—S1	159.16 (11)
N1—C7—C8—C9	1.60 (19)	C8—C7—N1—C14	−1.75 (17)
C15—C7—C8—C9	173.60 (16)	C15—C7—N1—C14	−173.96 (15)
N1—C7—C8—C16	−176.32 (18)	C8—C7—N1—S1	−157.84 (13)

C15—C7—C8—C16	−4.3 (3)	C15—C7—N1—S1	30.0 (2)
C7—C8—C9—C10	−179.98 (19)	C14—N1—S1—O2	−176.12 (13)
C16—C8—C9—C10	−2.0 (3)	C7—N1—S1—O2	−22.86 (16)
C7—C8—C9—C14	−0.87 (19)	C14—N1—S1—O1	54.50 (14)
C16—C8—C9—C14	177.12 (17)	C7—N1—S1—O1	−152.24 (14)
C14—C9—C10—C11	1.1 (3)	C14—N1—S1—C1	−59.89 (14)
C8—C9—C10—C11	−179.89 (19)	C7—N1—S1—C1	93.37 (15)
C9—C10—C11—C12	−0.6 (3)	C6—C1—S1—O2	43.32 (16)
C10—C11—C12—C13	−0.3 (3)	C2—C1—S1—O2	−138.81 (15)
C11—C12—C13—C14	0.6 (3)	C6—C1—S1—O1	176.10 (14)
C12—C13—C14—C9	−0.1 (2)	C2—C1—S1—O1	−6.02 (17)
C12—C13—C14—N1	−179.82 (17)	C6—C1—S1—N1	−70.55 (15)
C10—C9—C14—C13	−0.8 (2)	C2—C1—S1—N1	107.33 (15)
C8—C9—C14—C13	180.00 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1	0.93	2.51	2.886 (3)	104
C13—H13···O1	0.93	2.47	3.033 (2)	119
C15—H15*B*···O2	0.97	2.31	2.853 (3)	114
C2—H2···O2^{i}	0.93	2.48	3.314 (2)	149
C16—H16*A*···*Cg*2^{ii}	0.96	2.94	3.777 (2)	146
C16—H16*B*···*Cg*3^{iii}	0.96	2.92	3.781 (3)	149

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