

(Z)-3-(1-Chloroprop-1-enyl)-2-methyl-1-phenylsulfonyl-1H-indole

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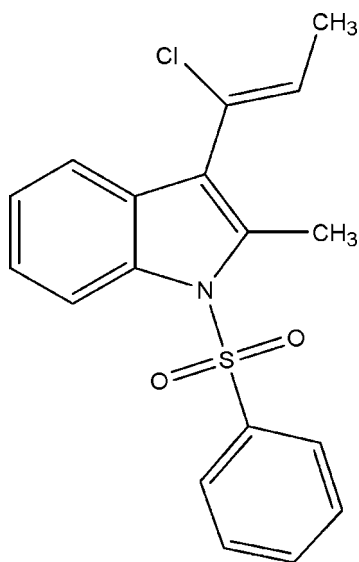
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.042; wR factor = 0.118; data-to-parameter ratio = 22.4.

In the title compound, $\text{C}_{18}\text{H}_{16}\text{ClNO}_2\text{S}$, the indole ring system forms a dihedral angle of $75.07(8)^\circ$ with the phenyl ring. The molecular structure is stabilized by a weak intramolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bond. In the crystal, molecules are linked by weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a chain along $[10\bar{1}]$. $\text{C}-\text{H}\cdots\pi$ interactions are also observed, leading to a three-dimensional network.

Related literature

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



Experimental

Crystal data

$\text{C}_{18}\text{H}_{16}\text{ClNO}_2\text{S}$	$V = 1685.7(2) \text{ \AA}^3$
$M_r = 345.83$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 12.5204(10) \text{ \AA}$	$\mu = 0.36 \text{ mm}^{-1}$
$b = 10.4962(7) \text{ \AA}$	$T = 295 \text{ K}$
$c = 12.983(1) \text{ \AA}$	$0.28 \times 0.24 \times 0.18 \text{ mm}$
$\beta = 98.892(2)^\circ$	

Data collection

Bruker Kappa APEXII diffractometer	20036 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	4705 independent reflections
$T_{\min} = 0.906$, $T_{\max} = 0.938$	3357 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.032$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$	210 parameters
$wR(F^2) = 0.118$	H-atom parameters constrained
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.26 \text{ e \AA}^{-3}$
4705 reflections	$\Delta\rho_{\text{min}} = -0.38 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

$Cg1$ is the centroid of the N1/C7/C12–C14 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C8}-\text{H8}\cdots\text{O1}$	0.93	2.39	2.973(2)	120
$\text{C10}-\text{H10}\cdots\text{O2}^i$	0.93	2.49	3.364(2)	157
$\text{C5}-\text{H5}\cdots\text{Cg1}^{ii}$	0.93	2.82	3.477(2)	128

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $x - \frac{3}{2}, -y - \frac{1}{2}, z - \frac{3}{2}$.

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.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5320).

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supplementary materials

Acta Cryst. (2013). E69, o1781 [doi:10.1107/S1600536813030730]

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1. Comment

The indole derivatives are known to exhibit anti-bacterial and anti-tumour activities (Okabe & Adachi, 1998; Schollmeyer *et al.*, 1995). We herein report the crystal structure of the title compound (I), (Fig. 1). The geometric parameters of (I) are comparable with the reported similar structures (Chakkaravarthi *et al.*, 2007, 2008). The phenyl ring forms a dihedral angle of 75.07 (8)° with the indole ring system. The five-membered (N1/C7/C12–C14) and six-membered (C7–C12) rings in the indole ring system are planar, with a dihedral angle of 0.38 (9)° between these rings. The bond angles around N1 (351.5°) indicate the sp^2 hybridization of N1 atom. The molecular structure is stabilized by a weak intramolecular C—H···O (Table 1) hydrogen bond. The crystal structure exhibits weak intermolecular C—H···O (Fig. 2) and C—H··· π (Table 1) interactions.

2. Experimental

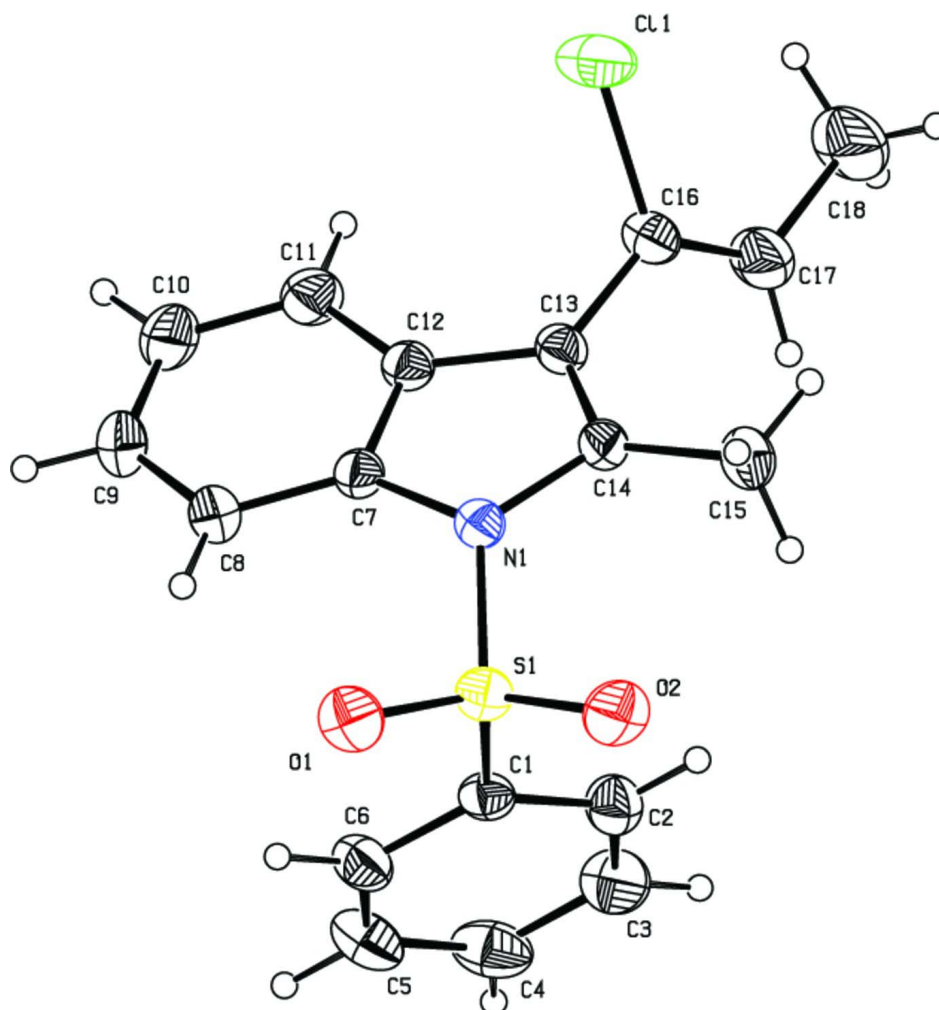
To a solution of 2-methyl-1-(phenylsulfonyl)-1H-indole (1 g, 3.69 mmol) in dry dichloromethane (20 ml), AlCl₃ (1.47 g, 11.07 mmol) and propionic anhydride (0.71 ml, 5.53 mmol) were added at 0 °C and stirred for 3 h. Then, the reaction mixture was washed with saturated NaHCO₃ (2 × 10 ml) solution, followed by water (3 × 10 ml) and dried (Na₂SO₄). Removal of the solvent followed a column chromatographic purification (Silica gel; hexane-ethyl acetate, 95:5) afforded the title compound, suitable for X-Ray diffraction quality crystals.

3. Refinement

H atoms were positioned geometrically and refined using riding model, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for CH, and C—H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for CH₃.

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); 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.

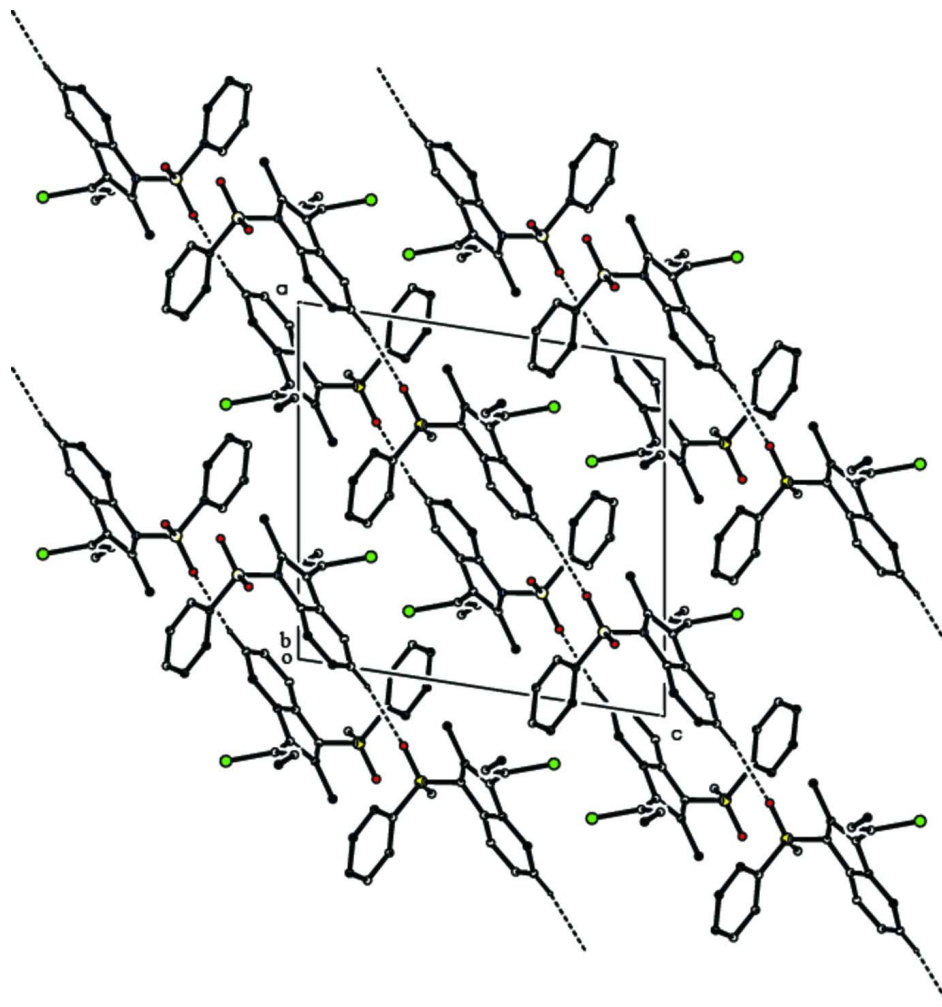


Figure 2

A packing diagram of the title compound, view down the *b* axis. Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involving hydrogen bonding have been omitted.

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Crystal data

$C_{18}H_{16}ClNO_2S$

$M_r = 345.83$

Monoclinic, $P2_1/n$

Hall symbol: $-P 2_1/n$

$a = 12.5204 (10) \text{ \AA}$

$b = 10.4962 (7) \text{ \AA}$

$c = 12.983 (1) \text{ \AA}$

$\beta = 98.892 (2)^\circ$

$V = 1685.7 (2) \text{ \AA}^3$

$Z = 4$

$F(000) = 720$

$D_x = 1.363 \text{ Mg m}^{-3}$

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

Cell parameters from 6694 reflections

$\theta = 2.1\text{--}27.9^\circ$

$\mu = 0.36 \text{ mm}^{-1}$

$T = 295 \text{ K}$

Block, colourless

$0.28 \times 0.24 \times 0.18 \text{ mm}$

Data collection

Bruker Kappa APEXII diffractometer	20036 measured reflections
Radiation source: fine-focus sealed tube	4705 independent reflections
Graphite monochromator	3357 reflections with $I > 2\sigma(I)$
ω and φ scan	$R_{\text{int}} = 0.032$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 29.6^\circ$, $\theta_{\text{min}} = 2.1^\circ$
$T_{\text{min}} = 0.906$, $T_{\text{max}} = 0.938$	$h = -17 \rightarrow 17$
	$k = -14 \rightarrow 8$
	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.118$	$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 0.5443P]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
4705 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
210 parameters	$\Delta\rho_{\text{max}} = 0.26 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.38 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.59725 (13)	0.25271 (15)	0.25702 (12)	0.0409 (4)
C2	0.61126 (16)	0.36677 (19)	0.20771 (15)	0.0538 (4)
H2	0.6791	0.4046	0.2140	0.065*
C3	0.52304 (19)	0.4234 (2)	0.14909 (17)	0.0662 (6)
H3	0.5310	0.5006	0.1159	0.079*
C4	0.42317 (19)	0.3664 (2)	0.13940 (17)	0.0677 (6)
H4	0.3641	0.4048	0.0990	0.081*
C5	0.41016 (17)	0.2544 (2)	0.18844 (18)	0.0658 (6)
H5	0.3421	0.2170	0.1817	0.079*
C6	0.49712 (15)	0.19547 (18)	0.24823 (16)	0.0532 (4)
H6	0.4883	0.1188	0.2818	0.064*
C7	0.64323 (12)	0.27161 (16)	0.50763 (12)	0.0387 (3)
C8	0.56922 (15)	0.17868 (18)	0.52523 (15)	0.0506 (4)
H8	0.5671	0.0997	0.4925	0.061*
C9	0.49922 (17)	0.2087 (2)	0.59334 (17)	0.0616 (5)
H9	0.4485	0.1487	0.6068	0.074*
C10	0.50223 (17)	0.3261 (2)	0.64240 (17)	0.0643 (6)
H10	0.4534	0.3435	0.6877	0.077*
C11	0.57600 (16)	0.4172 (2)	0.62521 (15)	0.0548 (5)
H11	0.5778	0.4958	0.6585	0.066*
C12	0.64785 (13)	0.38933 (16)	0.55705 (13)	0.0402 (4)

C13	0.73423 (13)	0.46134 (16)	0.52297 (13)	0.0404 (4)
C14	0.77940 (13)	0.39021 (16)	0.45452 (13)	0.0403 (4)
C15	0.87719 (15)	0.4191 (2)	0.40629 (17)	0.0599 (5)
H15A	0.9096	0.4967	0.4352	0.090*
H15B	0.8568	0.4287	0.3323	0.090*
H15C	0.9282	0.3506	0.4203	0.090*
C16	0.77116 (14)	0.58673 (17)	0.56392 (14)	0.0474 (4)
C17	0.7704 (2)	0.6928 (2)	0.51122 (18)	0.0678 (6)
H17	0.7463	0.6881	0.4399	0.081*
C18	0.8047 (3)	0.8218 (2)	0.5545 (2)	0.0989 (10)
H18A	0.7573	0.8856	0.5198	0.148*
H18B	0.8775	0.8386	0.5434	0.148*
H18C	0.8014	0.8234	0.6278	0.148*
N1	0.72580 (10)	0.26962 (13)	0.44364 (10)	0.0389 (3)
O1	0.68061 (11)	0.05793 (12)	0.36391 (11)	0.0580 (3)
O2	0.80267 (11)	0.20029 (14)	0.28742 (11)	0.0606 (4)
S1	0.70889 (3)	0.18303 (4)	0.33504 (3)	0.04316 (13)
Cl1	0.81805 (5)	0.58714 (5)	0.69822 (4)	0.07334 (19)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0475 (9)	0.0363 (9)	0.0386 (8)	0.0013 (7)	0.0059 (7)	-0.0079 (6)
C2	0.0581 (11)	0.0478 (11)	0.0547 (11)	-0.0050 (8)	0.0061 (9)	0.0042 (8)
C3	0.0830 (16)	0.0484 (12)	0.0628 (13)	0.0038 (10)	-0.0028 (11)	0.0088 (9)
C4	0.0729 (14)	0.0563 (13)	0.0647 (13)	0.0113 (11)	-0.0182 (11)	-0.0081 (10)
C5	0.0532 (12)	0.0609 (14)	0.0768 (15)	-0.0059 (9)	-0.0107 (10)	-0.0115 (11)
C6	0.0562 (11)	0.0432 (10)	0.0575 (11)	-0.0082 (8)	0.0008 (9)	-0.0047 (8)
C7	0.0361 (8)	0.0442 (9)	0.0353 (8)	-0.0018 (6)	0.0041 (6)	0.0017 (6)
C8	0.0532 (10)	0.0487 (11)	0.0502 (10)	-0.0107 (8)	0.0086 (8)	0.0016 (8)
C9	0.0551 (11)	0.0723 (14)	0.0602 (12)	-0.0187 (10)	0.0178 (9)	0.0050 (10)
C10	0.0534 (11)	0.0863 (16)	0.0586 (12)	-0.0065 (10)	0.0260 (10)	-0.0055 (11)
C11	0.0534 (11)	0.0625 (12)	0.0507 (11)	-0.0006 (9)	0.0147 (8)	-0.0114 (9)
C12	0.0381 (8)	0.0443 (9)	0.0372 (8)	-0.0003 (6)	0.0030 (6)	0.0004 (6)
C13	0.0393 (8)	0.0400 (9)	0.0403 (8)	-0.0028 (6)	0.0009 (6)	0.0010 (6)
C14	0.0367 (8)	0.0443 (9)	0.0392 (8)	-0.0053 (6)	0.0032 (6)	0.0018 (6)
C15	0.0452 (10)	0.0750 (14)	0.0617 (12)	-0.0163 (9)	0.0151 (9)	-0.0058 (10)
C16	0.0464 (9)	0.0449 (10)	0.0484 (10)	-0.0041 (7)	-0.0008 (7)	-0.0033 (7)
C17	0.0869 (16)	0.0502 (13)	0.0620 (13)	-0.0157 (10)	-0.0022 (11)	0.0037 (9)
C18	0.147 (3)	0.0493 (15)	0.094 (2)	-0.0298 (15)	-0.0015 (18)	0.0022 (12)
N1	0.0374 (7)	0.0413 (8)	0.0381 (7)	-0.0024 (5)	0.0059 (5)	-0.0021 (5)
O1	0.0720 (9)	0.0340 (7)	0.0679 (9)	0.0075 (6)	0.0105 (7)	-0.0009 (6)
O2	0.0519 (8)	0.0711 (10)	0.0631 (9)	0.0087 (6)	0.0228 (6)	-0.0116 (7)
S1	0.0456 (2)	0.0383 (2)	0.0463 (2)	0.00578 (16)	0.00928 (17)	-0.00582 (17)
Cl1	0.1009 (4)	0.0574 (3)	0.0532 (3)	-0.0016 (3)	-0.0152 (3)	-0.0087 (2)

Geometric parameters (\AA , $^\circ$)

C1—C6	1.379 (2)	C11—C12	1.387 (2)
C1—C2	1.382 (2)	C11—H11	0.9300

C1—S1	1.7541 (17)	C12—C13	1.444 (2)
C2—C3	1.376 (3)	C13—C14	1.350 (2)
C2—H2	0.9300	C13—C16	1.467 (2)
C3—C4	1.374 (3)	C14—N1	1.429 (2)
C3—H3	0.9300	C14—C15	1.490 (2)
C4—C5	1.359 (3)	C15—H15A	0.9600
C4—H4	0.9300	C15—H15B	0.9600
C5—C6	1.382 (3)	C15—H15C	0.9600
C5—H5	0.9300	C16—C17	1.306 (3)
C6—H6	0.9300	C16—Cl1	1.7517 (18)
C7—C8	1.388 (2)	C17—C18	1.502 (3)
C7—C12	1.389 (2)	C17—H17	0.9300
C7—N1	1.4229 (19)	C18—H18A	0.9600
C8—C9	1.374 (3)	C18—H18B	0.9600
C8—H8	0.9300	C18—H18C	0.9600
C9—C10	1.385 (3)	N1—S1	1.6634 (14)
C9—H9	0.9300	O1—S1	1.4251 (14)
C10—C11	1.371 (3)	O2—S1	1.4207 (13)
C10—H10	0.9300		
C6—C1—C2	121.21 (17)	C7—C12—C13	107.68 (14)
C6—C1—S1	119.95 (14)	C14—C13—C12	108.79 (15)
C2—C1—S1	118.82 (14)	C14—C13—C16	126.44 (15)
C3—C2—C1	118.84 (19)	C12—C13—C16	124.58 (15)
C3—C2—H2	120.6	C13—C14—N1	108.47 (14)
C1—C2—H2	120.6	C13—C14—C15	128.24 (16)
C4—C3—C2	120.3 (2)	N1—C14—C15	122.86 (15)
C4—C3—H3	119.9	C14—C15—H15A	109.5
C2—C3—H3	119.9	C14—C15—H15B	109.5
C5—C4—C3	120.5 (2)	H15A—C15—H15B	109.5
C5—C4—H4	119.8	C14—C15—H15C	109.5
C3—C4—H4	119.8	H15A—C15—H15C	109.5
C4—C5—C6	120.6 (2)	H15B—C15—H15C	109.5
C4—C5—H5	119.7	C17—C16—C13	126.77 (18)
C6—C5—H5	119.7	C17—C16—Cl1	119.57 (15)
C1—C6—C5	118.62 (19)	C13—C16—Cl1	113.66 (13)
C1—C6—H6	120.7	C16—C17—C18	126.4 (2)
C5—C6—H6	120.7	C16—C17—H17	116.8
C8—C7—C12	122.00 (15)	C18—C17—H17	116.8
C8—C7—N1	130.50 (16)	C17—C18—H18A	109.5
C12—C7—N1	107.49 (13)	C17—C18—H18B	109.5
C9—C8—C7	116.92 (18)	H18A—C18—H18B	109.5
C9—C8—H8	121.5	C17—C18—H18C	109.5
C7—C8—H8	121.5	H18A—C18—H18C	109.5
C8—C9—C10	121.70 (18)	H18B—C18—H18C	109.5
C8—C9—H9	119.2	C7—N1—C14	107.56 (13)
C10—C9—H9	119.2	C7—N1—S1	119.61 (11)
C11—C10—C9	121.08 (18)	C14—N1—S1	124.33 (11)
C11—C10—H10	119.5	O2—S1—O1	119.18 (8)

C9—C10—H10	119.5	O2—S1—N1	107.08 (8)
C10—C11—C12	118.48 (18)	O1—S1—N1	106.54 (8)
C10—C11—H11	120.8	O2—S1—C1	109.51 (8)
C12—C11—H11	120.8	O1—S1—C1	109.14 (8)
C11—C12—C7	119.81 (16)	N1—S1—C1	104.32 (7)
C11—C12—C13	132.51 (17)		
C6—C1—C2—C3	0.1 (3)	C14—C13—C16—C17	66.3 (3)
S1—C1—C2—C3	-178.03 (16)	C12—C13—C16—C17	-119.2 (2)
C1—C2—C3—C4	-0.5 (3)	C14—C13—C16—C11	-114.73 (18)
C2—C3—C4—C5	0.7 (4)	C12—C13—C16—C11	59.8 (2)
C3—C4—C5—C6	-0.4 (3)	C13—C16—C17—C18	177.7 (2)
C2—C1—C6—C5	0.2 (3)	C11—C16—C17—C18	-1.3 (4)
S1—C1—C6—C5	178.30 (15)	C8—C7—N1—C14	-179.54 (17)
C4—C5—C6—C1	0.0 (3)	C12—C7—N1—C14	-0.88 (17)
C12—C7—C8—C9	0.7 (3)	C8—C7—N1—S1	31.1 (2)
N1—C7—C8—C9	179.20 (18)	C12—C7—N1—S1	-150.22 (12)
C7—C8—C9—C10	-0.1 (3)	C13—C14—N1—C7	1.30 (18)
C8—C9—C10—C11	-0.4 (4)	C15—C14—N1—C7	174.34 (16)
C9—C10—C11—C12	0.2 (3)	C13—C14—N1—S1	148.83 (12)
C10—C11—C12—C7	0.4 (3)	C15—C14—N1—S1	-38.1 (2)
C10—C11—C12—C13	-179.39 (19)	C7—N1—S1—O2	179.44 (12)
C8—C7—C12—C11	-0.9 (3)	C14—N1—S1—O2	35.51 (15)
N1—C7—C12—C11	-179.69 (16)	C7—N1—S1—O1	-51.99 (14)
C8—C7—C12—C13	178.96 (16)	C14—N1—S1—O1	164.08 (13)
N1—C7—C12—C13	0.17 (18)	C7—N1—S1—C1	63.40 (14)
C11—C12—C13—C14	-179.51 (19)	C14—N1—S1—C1	-80.53 (14)
C7—C12—C13—C14	0.65 (19)	C6—C1—S1—O2	143.30 (15)
C11—C12—C13—C16	5.2 (3)	C2—C1—S1—O2	-38.55 (16)
C7—C12—C13—C16	-174.67 (15)	C6—C1—S1—O1	11.19 (17)
C12—C13—C14—N1	-1.20 (18)	C2—C1—S1—O1	-170.66 (13)
C16—C13—C14—N1	174.01 (15)	C6—C1—S1—N1	-102.37 (15)
C12—C13—C14—C15	-173.75 (18)	C2—C1—S1—N1	75.78 (15)
C16—C13—C14—C15	1.5 (3)		

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the N1/C7/C12—C14 ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C8—H8...O1	0.93	2.39	2.973 (2)	120
C10—H10...O2 ⁱ	0.93	2.49	3.364 (2)	157
C5—H5...Cg1 ⁱⁱ	0.93	2.82	3.477 (2)	128

Symmetry codes: (i) $x-1/2, -y+1/2, z+1/2$; (ii) $x-3/2, -y-1/2, z-3/2$.