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5-Cyclopropyl-1-[(4-methylbenzene)sulfonyl]-indole-2-carbaldehyde

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Keywords: single-crystal X-ray diffraction; indole derivative; crystal structure; Hirshfeld surface analysis; π–π stacking interactions; C—H···O hydrogen bonding.

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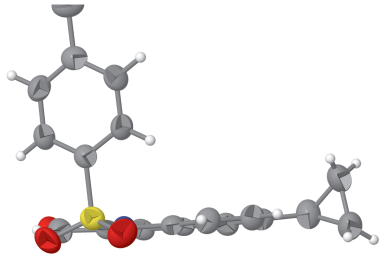
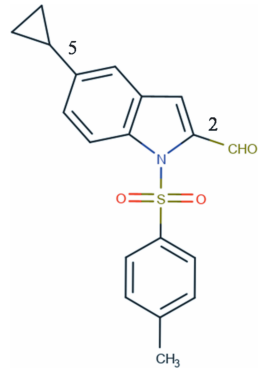
Structural data: full structural data are available from iucrdata.iucr.org

The crystal structure of the title compound, $C_{19}H_{17}NO_3S$, was determined by single-crystal X-ray diffraction. The compound crystallizes in the monoclinic crystal system with space group $P2_1/c$. The indole ring is essentially planar, with cyclopropyl, aldehyde and *p*-toluenesulfonyl groups attached at the C5, C2 and N1 positions, respectively. The aldehyde substituent is nearly coplanar with the indole ring, while the cyclopropyl and *p*-tolyl rings are almost perpendicular to it. The crystal packing is mainly influenced by slipped π–π stacking interactions, along with weak C—H···O interactions involving the sulfonyl oxygen atoms. Hirshfeld surface analysis shows that H···H (46.6%), O···H/H···O (23.5%), C···H/H···C (16.0%) and C···C (8.0%) contacts make the major contributions to the crystal packing.

3D view



Chemical scheme



Structure description

Indole derivatives continue to attract considerable attention because of their diverse biological activities and their widespread occurrence in natural products and therapeutic agents (Sundberg, 2012; Gribble, 2016; Kumar *et al.*, 2022). Owing to their structural versatility, indole-based compounds have become privileged scaffolds in medicinal chemistry, and structural modification of the groups attached to the indole nucleus can influence molecular conformation, intermolecular interactions and physicochemical properties (Sravanthi & Manju, 2016; Zeng *et al.*, 2024; Yang *et al.*, 2026; Drăgoi *et al.*, 2026). Among indole-incorporated small organic molecules (SOMs), those containing a

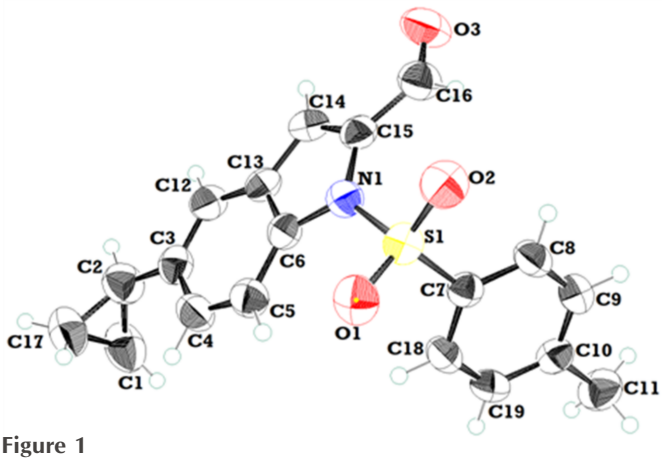


Figure 1
Molecular structure of the title compound showing the atom-numbering scheme with displacement ellipsoids drawn at the 50% probability level

cyclopropane ring have attracted attention for tuning the ADMET properties of drug candidates (Foote *et al.*, 2013; Tran & Henary, 2022; Hassam *et al.*, 2012). In view of the interest in cyclopropyl- and indole-containing SOMs, we determined the solid-state structure of the title compound (Fig. 1) and describe its structural features here.

The molecular structure of the title compound is shown in Fig. 2. The compound crystallizes in the monoclinic space group $P2_1/c$, with one molecule in the asymmetric unit. The molecule consists of an indole ring substituted by a cyclopropyl group at the C5 position, an aldehyde group at C2, and a *p*-toluenesulfonyl (tosyl) group attached to atom N1. The indole ring system is essentially planar with an r.m.s. deviation of 0.019 Å, whereas the overall molecular conformation is non-coplanar because of the orientation of the substituent groups. The sulfur atom adopts the expected distorted tetrahedral geometry, being coordinated by two oxygen atoms, one nitrogen atom and one carbon atom. The S1—O1 [1.421 (2) Å], S1—O2 [1.422 (2) Å] and S1—N1 [1.684 (3) Å] bond lengths are typical of aromatic sulfonamide derivatives. Likewise, the widened O1—S1—O2 angle of 120.73 (15)° is characteristic of sulfonyl-containing compounds and is consistent with the geometry commonly observed for aromatic sulfonamides.

Least-squares plane analysis shows that the aldehyde group is nearly coplanar with the indole ring system, with a dihedral angle of 3.1 (4)°. In contrast, the cyclopropyl and *p*-tolyl rings are oriented nearly perpendicular to the indole plane, with dihedral angles of 87.0 (3) and 84.49 (9)°, respectively. The cyclopropyl ring shows the expected angular compression associated with a strained three-membered ring. The torsion angles about the *N*-sulfonyl linkage [S1—N1—C6—C13 = −169.3 (2)° and S1—N1—C15—C14 = 169.2 (2)°] indicate an extended conformation of the *N*-sulfonyl group. In the crystal structure (Fig. 3), no classical hydrogen bonds are present because the molecule lacks N—H and O—H donor groups. Instead, the crystal packing involves weak C—H···O interactions, with the sulfonyl oxygen atoms acting as acceptors, together with slipped π–π stacking interactions between neighbouring aromatic rings [$Cg1\cdots Cg2$ = 3.9655 (18) Å, perpendicular distance = 3.627 Å, interplanar angle = 1.10° and slippage = 1.603 Å and $Cg3\cdots Cg4$ = 3.7798 (18) Å, perpendicular distance = 3.576 Å, interplanar angle = 0.02° and slippage = 1.223 Å where *Cg*1 and *Cg*2 are the centroids of the C7–C10/C18/C19 ring and its syemmetry-generated counterpart at $(x, \frac{1}{2}-y, -\frac{1}{2}+z)$ and *Cg*2 and *Cg*3 are the centroids of the C3–C6/C12/C13 ring and its symmetry-generated counterpart at $(1-x, -y, -z)$].

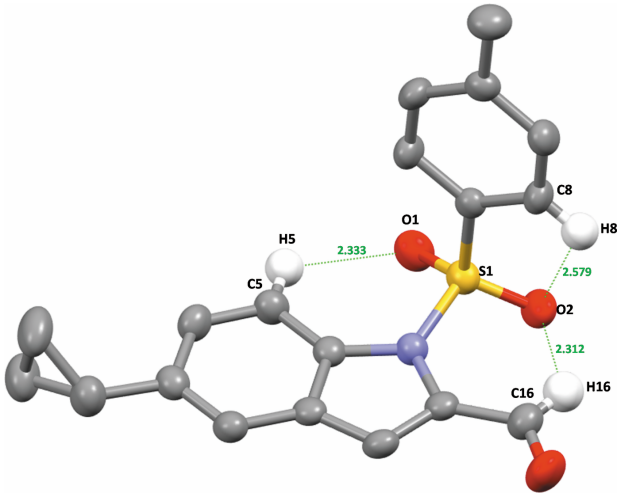


Figure 2
Molecular structure of title compound showing the intramolecular weak C—H···O interactions involving the sulfonyl oxygen atoms, which contribute to conformational stabilization. The atomic labelling scheme is shown for clarity.

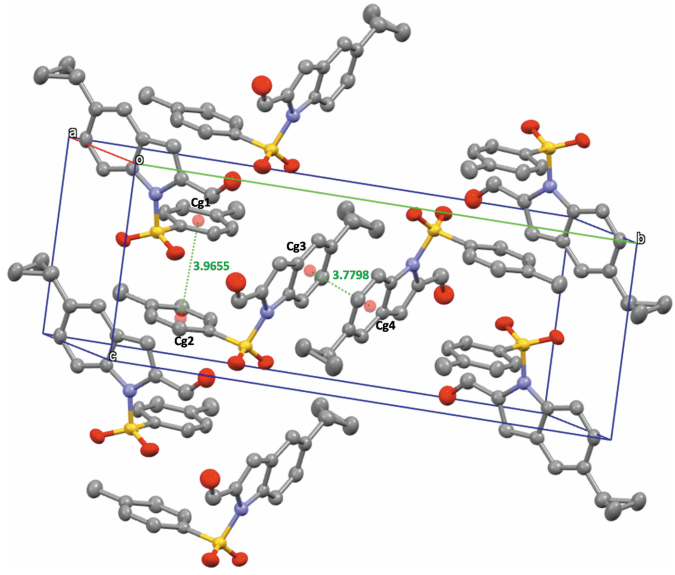


Figure 3
Crystal packing of the title compound showing significant slipped π–π stacking interactions between neighboring aromatic rings contributing to supramolecular assembly and molecular packing [centroid–centroid distances $Cg1\cdots Cg2$ = 3.9655 (18) and $Cg3\cdots Cg4$ = 3.7798 (18) Å where *Cg*1 and *Cg*2 are the centroids of the C7–C10/C18/C19 ring and its syemmetry-generated counterpart at $(x, \frac{1}{2}-y, -\frac{1}{2}+z)$ and *Cg*2 and *Cg*3 are the centroids of the C3–C6/C12/C13 ring and its symmetry-generated counterpart at $(1-x, -y, -z)$]. Hydrogen atoms are omitted for clarity.

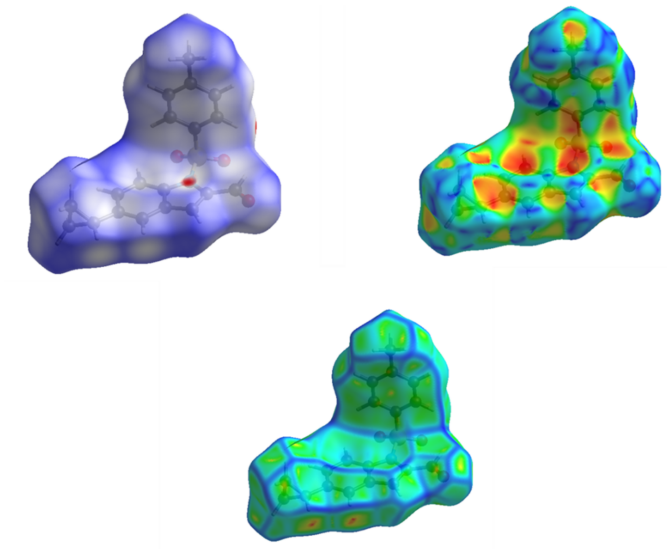


Figure 4
Hirshfeld surface analysis of title compound showing (*a*) d_{norm} surface highlighting close inter/intra molecular contacts as red patches, (*b*) shape-index map illustrating complementary red and blue triangular regions associated with slipped aromatic π–π stacking interactions and (*c*) curvedness surface showing flat aromatic regions characteristic of stacking interactions

The intermolecular contacts were further analysed using Hirshfeld surface analysis. The d_{norm} surface (Fig. 4) shows prominent red regions corresponding to close C—H···O contacts, while the shape-index surface indicates slipped π–π stacking interactions. The corresponding two-dimensional fingerprint plots (Fig. 5) show that H···H contacts contribute 46.6% to the Hirshfeld surface, followed by O···H/H···O (23.5%), C···H/H···C (16.0%) and C···C (8.0%). These contacts represent the major contributions to the crystal packing.

A comparison with the related structure of 3-methyl-1-tosyl-1*H*-indole-2-carbaldehyde (Pradeep *et al.*, 2013) shows that both compounds have a non-coplanar arrangement associated with the *N*-tosyl substituent. However, the title compound adopts a more extended conformation about the *N*-sulfonyl linkage, which may be associated with the presence of the cyclopropyl substituent at the C5 position. Although *N*-tosyl cyclopropyl-substituted indole derivatives have been reported in the patent literature (World Intellectual Property Organization, 2011), closely related crystal structures have not been reported. The present structure therefore adds to the available crystallographic data for cyclopropyl-substituted *N*-tosyl indole derivatives.

Synthesis and crystallization

Ethyl 5-*cyclo*propyl-1-tosyl-1*H*-indole-2-carboxylate (5.0 g, 13.03 mmol) was dissolved in 2-methyltetrahydrofuran (50 ml) and cooled to 0°C under a nitrogen atmosphere. Lithium aluminium hydride (1.2 g, 32.60 mmol, 2.5 equiv.) was added portion wise over 1 h with continuous stirring. The reaction mixture was maintained at 0°C for an additional 1 h until the reduction was complete, as monitored by thin-layer chromatography (TLC). The excess lithium aluminium hydride was carefully quenched with saturated aqueous potassium sodium tartrate solution, followed by the addition of ethyl acetate. The reaction mixture was allowed to warm to room temperature, and the organic layer was separated, washed with saturated potassium sodium tartrate solution and brine, dried over anhydrous sodium sulfate, and concentrated under reduced pressure to afford crude (5-*cyclo*propyl-1-tosyl-1*H*-indol-2-yl) methanol, which was used directly in the subsequent oxidation step without further purification. The crude alcohol (3.5 g, 10.26 mmol) was dissolved in dichloromethane (35 ml) and cooled to 0°C. Dess–Martin periodinane (8.7 g, 20.52 mmol, 2.0 equiv.) was added portionwise over 30 min, and the reaction mixture was stirred at 0°C for 3 h. Upon completion of the reaction (TLC), the precipitated by-product was removed by filtration, and the filtrate was concentrated under reduced pressure. The residue was purified by silica-gel column chromatography to afford the title compound, 5-cyclopropyl-1-[(4-methylbenzene)sulfonyl]indole-2-carbaldehyde, as a white solid in 92% yield (3.2 g). Crystals suitable for single-crystal X-ray diffraction analysis were obtained by slow evaporation of an ethyl acetate/hexane (9:1 *v*/*v*) solution of the purified compound at room temperature over several days..

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{17}NO_3S$
M_r	339.39
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	273
a, b, c (Å)	9.9586 (4), 21.0209 (9), 7.9204 (3)
β (°)	99.126 (2)
V (Å^3)	1637.06 (11)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.22
Crystal size (mm)	0.32 × 0.06 × 0.05
Data collection	
Diffractometer	Bruker D8 Quest ECO
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.680, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	83410, 4049, 2668
R_{int}	0.064
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.065, 0.184, 1.06
No. of reflections	4049
No. of parameters	218
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.41, −0.23

Computer programs: *APEX4* and *SAINT* (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystal data, data collection, and structure refinement details are given in Table 1.

Acknowledgements

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full crystallographic data

IUCrData (2026). **11**, x260927 [https://doi.org/10.1107/S2414314626009272]

5-Cyclopropyl-1-[(4-methylbenzene)sulfonyl]indole-2-carbaldehyde

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5-Cyclopropyl-1-[(4-methylbenzene)sulfonyl]indole-2-carbaldehyde

Crystal data

$C_{19}H_{17}NO_3S$
M_r = 339.39
Monoclinic, $P2_1/c$
a = 9.9586 (4) Å
b = 21.0209 (9) Å
c = 7.9204 (3) Å
β = 99.126 (2)°
V = 1637.06 (11) Å^3
Z = 4
$F(000)$ = 712
D_x = 1.377 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9880 reflections
θ = 2.3–23.3°
μ = 0.22 mm^{-1}
T = 273 K
Needle, colourless
0.32 × 0.06 × 0.05 mm

Data collection

Bruker D8 Quest ECO diffractometer
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.680, T_{max} = 0.746
83410 measured reflections
4049 independent reflections
2668 reflections with $I > 2\sigma(I)$
R_{int} = 0.064
θ_{max} = 28.3°, θ_{min} = 2.8°
h = −13→13
k = −27→27
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.184
S = 1.06
4049 reflections
218 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2 + 1.6942P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The structure was solved by direct methods and refined by full-matrix least-squares on (F^2). All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed in calculated positions and refined using a riding model.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.34851 (8)	0.64905 (4)	0.12355 (9)	0.0496 (2)
O1	0.2746 (3)	0.59482 (11)	0.0534 (3)	0.0642 (6)
O2	0.4513 (2)	0.67646 (12)	0.0409 (3)	0.0647 (6)
O3	0.7097 (3)	0.73354 (14)	0.4654 (4)	0.0819 (8)
N1	0.4263 (2)	0.62609 (12)	0.3185 (3)	0.0488 (6)
C1	0.1366 (5)	0.4586 (2)	0.8626 (6)	0.0876 (13)
H1A	0.065643	0.479533	0.783852	0.105*
H1B	0.123379	0.459031	0.981323	0.105*
C2	0.2763 (4)	0.46231 (19)	0.8264 (5)	0.0709 (10)
H2	0.345081	0.462744	0.929707	0.085*
C3	0.3137 (3)	0.50271 (15)	0.6843 (4)	0.0534 (8)
C4	0.2355 (3)	0.50178 (15)	0.5196 (5)	0.0581 (8)
H4	0.161396	0.474363	0.499190	0.070*
C5	0.2635 (3)	0.53947 (15)	0.3878 (4)	0.0554 (8)
H5	0.210914	0.537331	0.279871	0.066*
C6	0.3733 (3)	0.58092 (13)	0.4215 (4)	0.0452 (7)
C7	0.2339 (3)	0.70821 (14)	0.1642 (3)	0.0434 (6)
C8	0.2692 (3)	0.77164 (15)	0.1546 (4)	0.0527 (8)
H8	0.353357	0.783046	0.127150	0.063*
C9	0.1777 (3)	0.81772 (15)	0.1863 (4)	0.0560 (8)
H9	0.200572	0.860374	0.178169	0.067*
C10	0.0530 (3)	0.80202 (15)	0.2298 (4)	0.0501 (7)
C11	−0.0452 (4)	0.85274 (18)	0.2633 (5)	0.0729 (10)
H11A	0.003942	0.890643	0.302204	0.109*
H11B	−0.095984	0.838329	0.349431	0.109*
H11C	−0.106534	0.861729	0.159851	0.109*
C12	0.4228 (3)	0.54307 (16)	0.7145 (4)	0.0537 (8)
H12	0.476977	0.543870	0.821508	0.064*
C13	0.4530 (3)	0.58307 (14)	0.5844 (4)	0.0459 (7)
C14	0.5534 (3)	0.63084 (16)	0.5795 (4)	0.0516 (7)
H14	0.620262	0.642139	0.670245	0.062*
C15	0.5361 (3)	0.65718 (14)	0.4221 (4)	0.0477 (7)
C16	0.6178 (3)	0.70994 (17)	0.3694 (5)	0.0623 (9)
H16	0.597420	0.725422	0.258265	0.075*
C17	0.2027 (4)	0.40283 (19)	0.8008 (6)	0.0802 (12)
H17A	0.229813	0.368677	0.881351	0.096*
H17B	0.172129	0.389161	0.684055	0.096*
C18	0.1090 (3)	0.69125 (15)	0.2069 (4)	0.0538 (8)
H18	0.085492	0.648608	0.213329	0.065*
C19	0.0200 (3)	0.73828 (16)	0.2397 (5)	0.0570 (8)
H19	−0.063568	0.726965	0.268957	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0553 (5)	0.0524 (5)	0.0420 (4)	0.0031 (3)	0.0110 (3)	−0.0025 (3)
O1	0.0828 (17)	0.0564 (14)	0.0514 (13)	−0.0019 (12)	0.0040 (12)	−0.0114 (11)
O2	0.0645 (14)	0.0806 (16)	0.0544 (13)	0.0058 (12)	0.0261 (11)	0.0075 (12)
O3	0.0610 (15)	0.0894 (19)	0.095 (2)	−0.0249 (15)	0.0098 (14)	−0.0019 (16)
N1	0.0475 (14)	0.0501 (14)	0.0489 (14)	−0.0005 (11)	0.0076 (11)	0.0024 (11)
C1	0.096 (3)	0.070 (3)	0.110 (3)	−0.005 (2)	0.056 (3)	0.005 (2)
C2	0.073 (2)	0.073 (2)	0.067 (2)	−0.009 (2)	0.0125 (19)	0.0067 (19)
C3	0.0576 (19)	0.0488 (17)	0.0557 (18)	0.0072 (14)	0.0145 (15)	0.0011 (14)
C4	0.0556 (19)	0.0484 (17)	0.072 (2)	−0.0089 (15)	0.0136 (16)	−0.0055 (16)
C5	0.0571 (19)	0.0522 (18)	0.0548 (18)	−0.0033 (15)	0.0028 (15)	−0.0014 (15)
C6	0.0446 (15)	0.0412 (15)	0.0506 (16)	0.0060 (12)	0.0104 (13)	−0.0029 (12)
C7	0.0435 (15)	0.0478 (16)	0.0381 (14)	−0.0008 (13)	0.0038 (11)	0.0004 (12)
C8	0.0483 (17)	0.0512 (17)	0.0603 (19)	−0.0093 (14)	0.0140 (14)	0.0033 (14)
C9	0.0591 (19)	0.0427 (17)	0.066 (2)	−0.0051 (14)	0.0088 (16)	0.0034 (14)
C10	0.0479 (16)	0.0542 (18)	0.0459 (16)	0.0042 (14)	0.0007 (13)	−0.0024 (13)
C11	0.063 (2)	0.069 (2)	0.086 (3)	0.0138 (18)	0.0095 (19)	−0.007 (2)
C12	0.0467 (16)	0.0608 (19)	0.0535 (18)	0.0041 (15)	0.0073 (14)	0.0036 (15)
C13	0.0384 (15)	0.0511 (16)	0.0494 (16)	0.0096 (12)	0.0105 (12)	−0.0016 (13)
C14	0.0362 (14)	0.0627 (19)	0.0552 (18)	0.0026 (14)	0.0049 (13)	−0.0035 (15)
C15	0.0376 (15)	0.0506 (17)	0.0557 (17)	0.0064 (13)	0.0100 (13)	−0.0019 (14)
C16	0.0531 (19)	0.065 (2)	0.070 (2)	−0.0043 (17)	0.0148 (17)	0.0002 (18)
C17	0.097 (3)	0.058 (2)	0.093 (3)	−0.006 (2)	0.039 (2)	0.003 (2)
C18	0.0489 (17)	0.0434 (16)	0.070 (2)	−0.0089 (13)	0.0128 (15)	0.0018 (15)
C19	0.0381 (15)	0.060 (2)	0.073 (2)	−0.0063 (14)	0.0110 (15)	0.0036 (16)

Geometric parameters (Å, º)

S1—O1	1.421 (2)	C7—C18	1.386 (4)
S1—O2	1.422 (2)	C8—H8	0.9300
S1—N1	1.684 (3)	C8—C9	1.380 (4)
S1—C7	1.752 (3)	C9—H9	0.9300
O3—C16	1.201 (4)	C9—C10	1.380 (4)
N1—C6	1.409 (4)	C10—C11	1.499 (5)
N1—C15	1.418 (4)	C10—C19	1.385 (4)
C1—H1A	0.9700	C11—H11A	0.9600
C1—H1B	0.9700	C11—H11B	0.9600
C1—C2	1.467 (5)	C11—H11C	0.9600
C1—C17	1.467 (6)	C12—H12	0.9300
C2—H2	0.9800	C12—C13	1.399 (4)
C2—C3	1.503 (5)	C13—C14	1.422 (4)
C2—C17	1.447 (5)	C14—H14	0.9300
C3—C4	1.409 (5)	C14—C15	1.350 (4)
C3—C12	1.370 (5)	C15—C16	1.474 (5)
C4—H4	0.9300	C16—H16	0.9300
C4—C5	1.374 (5)	C17—H17A	0.9700

C5—H5	0.9300	C17—H17B	0.9700
C5—C6	1.390 (4)	C18—H18	0.9300
C6—C13	1.404 (4)	C18—C19	1.380 (4)
C7—C8	1.384 (4)	C19—H19	0.9300
O1—S1—O2	120.73 (15)	C8—C9—H9	119.2
O1—S1—N1	105.26 (14)	C8—C9—C10	121.6 (3)
O1—S1—C7	109.21 (14)	C10—C9—H9	119.2
O2—S1—N1	106.15 (14)	C9—C10—C11	120.8 (3)
O2—S1—C7	109.53 (15)	C9—C10—C19	118.4 (3)
N1—S1—C7	104.68 (13)	C19—C10—C11	120.8 (3)
C6—N1—S1	124.3 (2)	C10—C11—H11A	109.5
C6—N1—C15	107.5 (2)	C10—C11—H11B	109.5
C15—N1—S1	126.8 (2)	C10—C11—H11C	109.5
H1A—C1—H1B	115.0	H11A—C11—H11B	109.5
C2—C1—H1A	117.9	H11A—C11—H11C	109.5
C2—C1—H1B	117.9	H11B—C11—H11C	109.5
C2—C1—C17	59.1 (3)	C3—C12—H12	120.0
C17—C1—H1A	117.9	C3—C12—C13	120.1 (3)
C17—C1—H1B	117.9	C13—C12—H12	120.0
C1—C2—H2	113.4	C6—C13—C14	107.2 (3)
C1—C2—C3	122.1 (4)	C12—C13—C6	120.1 (3)
C3—C2—H2	113.4	C12—C13—C14	132.8 (3)
C17—C2—C1	60.4 (3)	C13—C14—H14	125.4
C17—C2—H2	113.4	C15—C14—C13	109.1 (3)
C17—C2—C3	124.3 (4)	C15—C14—H14	125.4
C4—C3—C2	121.3 (3)	N1—C15—C16	126.3 (3)
C12—C3—C2	120.2 (3)	C14—C15—N1	108.6 (3)
C12—C3—C4	118.4 (3)	C14—C15—C16	125.1 (3)
C3—C4—H4	118.4	O3—C16—C15	122.1 (4)
C5—C4—C3	123.1 (3)	O3—C16—H16	119.0
C5—C4—H4	118.4	C15—C16—H16	119.0
C4—C5—H5	121.2	C1—C17—H17A	117.7
C4—C5—C6	117.6 (3)	C1—C17—H17B	117.7
C6—C5—H5	121.2	C2—C17—C1	60.4 (3)
C5—C6—N1	131.8 (3)	C2—C17—H17A	117.7
C5—C6—C13	120.6 (3)	C2—C17—H17B	117.7
C13—C6—N1	107.5 (3)	H17A—C17—H17B	114.8
C8—C7—S1	119.7 (2)	C7—C18—H18	120.3
C8—C7—C18	120.4 (3)	C19—C18—C7	119.3 (3)
C18—C7—S1	119.9 (2)	C19—C18—H18	120.3
C7—C8—H8	120.5	C10—C19—H19	119.4
C9—C8—C7	119.0 (3)	C18—C19—C10	121.2 (3)
C9—C8—H8	120.5	C18—C19—H19	119.4
S1—N1—C6—C5	9.9 (5)	C4—C5—C6—N1	−178.3 (3)
S1—N1—C6—C13	−169.3 (2)	C4—C5—C6—C13	0.9 (4)
S1—N1—C15—C14	169.2 (2)	C5—C6—C13—C12	0.3 (4)

S1—N1—C15—C16	−10.2 (4)	C5—C6—C13—C14	−178.3 (3)
S1—C7—C8—C9	179.8 (2)	C6—N1—C15—C14	2.2 (3)
S1—C7—C18—C19	179.6 (3)	C6—N1—C15—C16	−177.1 (3)
O1—S1—N1—C6	−31.3 (3)	C6—C13—C14—C15	0.4 (3)
O1—S1—N1—C15	163.8 (2)	C7—S1—N1—C6	83.8 (3)
O1—S1—C7—C8	−149.7 (2)	C7—S1—N1—C15	−81.1 (3)
O1—S1—C7—C18	30.7 (3)	C7—C8—C9—C10	1.0 (5)
O2—S1—N1—C6	−160.3 (2)	C7—C18—C19—C10	0.4 (5)
O2—S1—N1—C15	34.8 (3)	C8—C7—C18—C19	0.0 (5)
O2—S1—C7—C8	−15.4 (3)	C8—C9—C10—C11	−179.8 (3)
O2—S1—C7—C18	165.0 (2)	C8—C9—C10—C19	−0.6 (5)
N1—S1—C7—C8	98.0 (3)	C9—C10—C19—C18	−0.1 (5)
N1—S1—C7—C18	−81.6 (3)	C11—C10—C19—C18	179.1 (3)
N1—C6—C13—C12	179.7 (3)	C12—C3—C4—C5	0.0 (5)
N1—C6—C13—C14	1.0 (3)	C12—C13—C14—C15	−178.1 (3)
N1—C15—C16—O3	−179.8 (3)	C13—C14—C15—N1	−1.6 (3)
C1—C2—C3—C4	−46.6 (5)	C13—C14—C15—C16	177.8 (3)
C1—C2—C3—C12	131.3 (4)	C14—C15—C16—O3	1.0 (5)
C2—C3—C4—C5	177.8 (3)	C15—N1—C6—C5	177.3 (3)
C2—C3—C12—C13	−176.6 (3)	C15—N1—C6—C13	−2.0 (3)
C3—C2—C17—C1	−110.6 (5)	C17—C1—C2—C3	114.1 (4)
C3—C4—C5—C6	−1.0 (5)	C17—C2—C3—C4	27.3 (5)
C3—C12—C13—C6	−1.4 (4)	C17—C2—C3—C12	−154.9 (4)
C3—C12—C13—C14	176.8 (3)	C18—C7—C8—C9	−0.7 (5)
C4—C3—C12—C13	1.3 (5)		