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Crystal structure of 1-[(6-chloropyridin-3-yl)sulfonyl]-1,2,3,4-tetrahydroquinoline

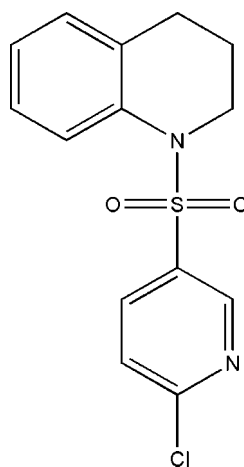
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The tetrahydropyridine ring of the quinoline system in the title compound, C₁₄H₁₃ClN₂O₂S, adopts a half-chair conformation with the bond-angle sum at the N atom being 350.0°. The dihedral angle between the least-squares planes of the two aromatic rings is 50.13 (11)°. In the crystal, inversion dimers linked by pairs of C—H...O hydrogen bonds generate *R*₂²(10) loops. Additional intermolecular C—H...O hydrogen bonds generate *C*(7) chains along [100].

1. Chemical context

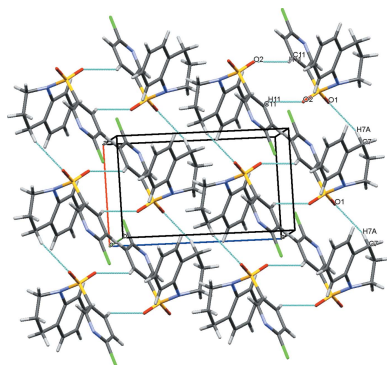
1,2,3,4-Tetrahydroquinoline derivatives play a vital role in developing pharmacological agents and they have been considered as potential drugs (White *et al.*, 1994; Kokwaro & Taylor, 1990; Omura & Nakagawa, 1981) and also antagonists for *N*-methyl-*D*-aspartate (NMDA) receptors at the glycine recognition site (Cai *et al.*, 1996).



Recently, we have synthesized a series of 1,2,3,4-tetrahydroquinoline derivatives and a few molecules in fact exhibit pharmacological activity (unpublished results). In a continuation of our work on the derivatives of 1,2,3,4-tetrahydroquinolines (Jeyaseelan *et al.*, 2014, 2015*a,b*), we report herein the synthesis and crystal structure of 1-[(6-chloropyridin-3-yl)sulfonyl]-1,2,3,4-tetrahydroquinoline, (I).

2. Structural commentary

The molecular structure of compound (I) is shown in Fig. 1. The dihedral angle between the planes of the aromatic rings is



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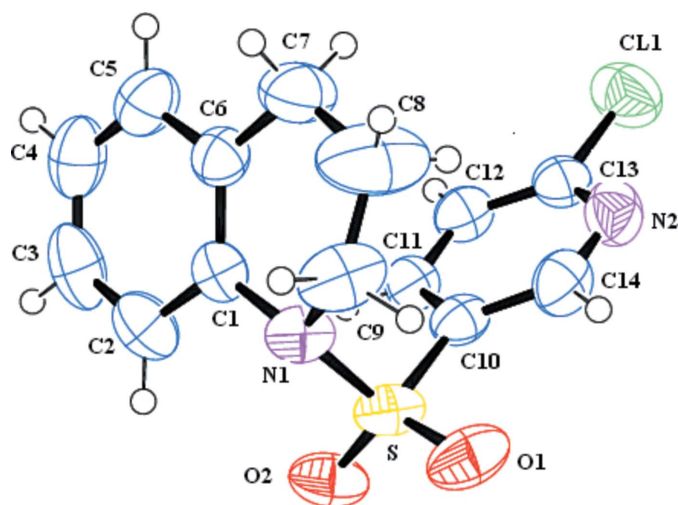


Figure 1
The molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level.

50.13 (11)°. In comparison, the dihedral angle in the 1-tosyl-1,2,3,4-tetrahydroquinoline, (II), is 47.74 (9)° (Jeyaseelan *et al.*, 2014), and in 1-benzylsulfonyl-1,2,3,4-tetrahydroquinoline, (III), it is 74.15 (10)° (Jeyaseelan *et al.*, 2015*b*). In the structures of compounds (II), (III) and 1-methanesulfonyl-1,2,3,4-tetrahydroquinoline, (IV) (Jeyaseelan *et al.*, 2015*a*), the tetrahydropyridine (C1/C6–C9/N1) ring is in a half-chair conformation, with the methylene C9 atom as the flap. However, the bond-angle sums at the N atom in (I), (II), (III) and (IV) differ somehow, with values of 350.0, 350.2, 354.61 and 347.9°, respectively.

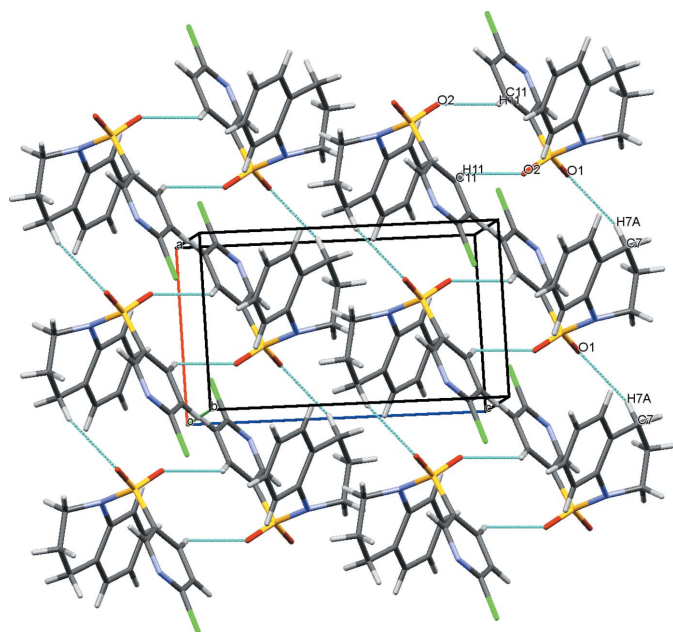


Figure 2
The molecular packing of the title compound. Dashed lines indicate the pairs of C–H...O hydrogen bonds which link the molecules into inversion dimers with $R_2^2(10)$ ring motifs and forming $C(7)$ chains along [100].

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C11-H11\cdots O2^i$	0.93	2.60	3.309 (3)	134
$C7-H7A\cdots O1^{ii}$	0.97	2.66	3.586 (5)	160

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

3. Supramolecular features

In the crystal, inversion dimers linked by pairs of $C11-H11\cdots O2$ hydrogen bonds generate $R_2^2(10)$ loops. In addition, molecules are linked by $C7-H7A\cdots O1$ hydrogen bonds, generating $C(7)$ chains along [100], as shown in Fig. 2. Numerical values of these interactions are compiled in Table 1.

4. Synthesis and crystallization

To an ice-cold solution of 1,2,3,4-tetrahydroquinoline (1.332 g, 10 mmol) and triethylamine (1.518 g, 15 mmol) in dichloromethane (50 ml), a solution of 6-chloropyridine-3-sulfonyl chloride (2.332 g, 11 mmol) in dichloromethane (20 ml) was added dropwise and stirred for 30 min. The reaction mixture was diluted with dichloromethane (150 ml), the organic layer washed with aqueous 5% NaHCO_3 solution and brine, and dried over anhydrous Na_2SO_4 . The solvent was evaporated under reduced pressure to give 1-[(6-chloropyridin-3-yl)sulfonyl]-1,2,3,4-tetrahydroquinoline, (I). The product was

Table 2
Experimental details.

Crystal data	
Chemical formula	$\text{C}_{14}\text{H}_{13}\text{ClN}_2\text{O}_2\text{S}$
M_r	308.77
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	296
a, b, c (Å)	6.5661 (10), 10.2595 (18), 11.3490 (19)
α, β, γ (°)	69.101 (7), 88.219 (7), 77.238 (7)
V (Å ³)	695.6 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.43
Crystal size (mm)	0.23 × 0.18 × 0.16
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Bruker, 2013)
$T_{\min}, T_{\max}$	0.912, 0.934
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9865, 2454, 1980
R_{int}	0.053
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.050, 0.146, 1.09
No. of reflections	2454
No. of parameters	181
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.59, -0.43

Computer programs: APEX2 and SAINT (Bruker, 2013), SHELXS97 (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2015), ORTEP-3 for Windows (Farrugia, 2012) and Mercury (Macrae *et al.*, 2008).

recrystallized from a mixture of dichloromethane and *n*-hexane (1:1 *v/v*) to obtain crystals suitable for X-ray diffraction studies.

5. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were positioned with idealized geometry using a riding-model approximation, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic H atoms and with C—H = 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for methylene H atoms.

Acknowledgements

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Crystal structure of 1-[(6-chloropyridin-3-yl)sulfonyl]-1,2,3,4-tetrahydroquinoline

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Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015).

1-[(6-Chloropyridin-3-yl)sulfonyl]-1,2,3,4-tetrahydroquinoline

Crystal data

$C_{14}H_{13}ClN_2O_2S$

$M_r = 308.77$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 6.5661$ (10) Å

$b = 10.2595$ (18) Å

$c = 11.3490$ (19) Å

$\alpha = 69.101$ (7)°

$\beta = 88.219$ (7)°

$\gamma = 77.238$ (7)°

$V = 695.6$ (2) Å³

$Z = 2$

$F(000) = 320$

prism

$D_x = 1.474$ Mg m⁻³

Melting point: 413 K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1980 reflections

$\theta = 1.9$ – 25.0°

$\mu = 0.43$ mm⁻¹

$T = 296$ K

Prism, colourless

$0.23 \times 0.18 \times 0.16$ mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 2.01 pixels mm⁻¹

phi and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2013)

$T_{\min} = 0.912$, $T_{\max} = 0.934$

9865 measured reflections

2454 independent reflections

1980 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.053$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 1.9^\circ$

$h = -7 \rightarrow 7$

$k = -12 \rightarrow 12$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.146$

$S = 1.09$

2454 reflections

181 parameters

0 restraints

0 constraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0677P)^2 + 0.3614P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 0.59 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.43 \text{ e } \text{\AA}^{-3}$$

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.3014 (3)	0.1696 (3)	0.3092 (2)	0.0753 (7)
S	0.40371 (11)	0.28345 (8)	0.24768 (6)	0.0562 (3)
Cl1	1.24374 (14)	0.01308 (10)	0.08760 (9)	0.0853 (3)
C10	0.6392 (4)	0.2111 (3)	0.1933 (2)	0.0479 (6)
N1	0.4673 (3)	0.3394 (2)	0.35739 (19)	0.0532 (6)
O2	0.3005 (3)	0.4047 (2)	0.14401 (19)	0.0712 (6)
C11	0.7513 (4)	0.2997 (3)	0.1091 (2)	0.0504 (6)
H11	0.6991	0.3983	0.0764	0.060*
N2	0.9018 (4)	0.0058 (3)	0.2047 (2)	0.0657 (7)
C1	0.5901 (4)	0.4468 (3)	0.3217 (2)	0.0479 (6)
C13	1.0055 (4)	0.0935 (3)	0.1264 (2)	0.0545 (7)
C6	0.7874 (4)	0.4136 (3)	0.3794 (3)	0.0542 (7)
C12	0.9387 (4)	0.2403 (3)	0.0750 (3)	0.0545 (7)
H12	1.0188	0.2965	0.0190	0.065*
C14	0.7193 (5)	0.0656 (3)	0.2371 (3)	0.0615 (8)
H14	0.6417	0.0064	0.2921	0.074*
C2	0.5110 (5)	0.5812 (3)	0.2320 (3)	0.0678 (8)
H2	0.3760	0.6042	0.1966	0.081*
C5	0.9038 (5)	0.5175 (4)	0.3419 (3)	0.0690 (8)
H5	1.0362	0.4975	0.3798	0.083*
C9	0.5138 (5)	0.2322 (4)	0.4875 (3)	0.0733 (10)
H9A	0.4544	0.2766	0.5470	0.088*
H9B	0.4466	0.1542	0.4963	0.088*
C3	0.6339 (7)	0.6804 (3)	0.1957 (3)	0.0812 (10)
H3	0.5830	0.7694	0.1335	0.097*
C4	0.8292 (6)	0.6494 (4)	0.2502 (3)	0.0766 (10)
H4	0.9112	0.7169	0.2255	0.092*
C7	0.8693 (6)	0.2732 (4)	0.4825 (4)	0.0796 (10)
H7A	0.9980	0.2263	0.4563	0.096*
H7B	0.9042	0.2917	0.5566	0.096*
C8	0.7326 (7)	0.1753 (5)	0.5187 (4)	0.124 (2)
H8A	0.7792	0.1037	0.4804	0.149*

H8B 0.7507 0.1261 0.6095 0.149*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0680 (14)	0.0963 (16)	0.0687 (13)	−0.0494 (13)	0.0085 (11)	−0.0202 (12)
S	0.0469 (4)	0.0698 (5)	0.0465 (4)	−0.0217 (3)	−0.0027 (3)	−0.0090 (3)
Cl1	0.0736 (6)	0.0948 (7)	0.0859 (6)	0.0056 (5)	−0.0027 (5)	−0.0446 (5)
C10	0.0520 (15)	0.0511 (15)	0.0373 (12)	−0.0186 (12)	−0.0063 (11)	−0.0069 (11)
N1	0.0489 (12)	0.0633 (14)	0.0406 (11)	−0.0183 (11)	0.0032 (9)	−0.0072 (10)
O2	0.0547 (12)	0.0850 (15)	0.0553 (11)	−0.0067 (11)	−0.0148 (9)	−0.0068 (11)
C11	0.0571 (16)	0.0441 (14)	0.0429 (13)	−0.0133 (12)	−0.0019 (12)	−0.0056 (11)
N2	0.0813 (19)	0.0509 (14)	0.0591 (15)	−0.0116 (13)	−0.0060 (13)	−0.0140 (12)
C1	0.0511 (15)	0.0463 (14)	0.0435 (13)	−0.0087 (12)	0.0095 (11)	−0.0146 (11)
C13	0.0566 (16)	0.0595 (17)	0.0472 (14)	−0.0088 (13)	−0.0096 (12)	−0.0203 (13)
C6	0.0566 (16)	0.0517 (16)	0.0551 (15)	−0.0155 (13)	0.0029 (13)	−0.0184 (13)
C12	0.0561 (16)	0.0596 (17)	0.0482 (14)	−0.0218 (14)	0.0053 (12)	−0.0149 (13)
C14	0.078 (2)	0.0509 (17)	0.0508 (15)	−0.0255 (16)	0.0011 (14)	−0.0056 (13)
C2	0.0673 (19)	0.0558 (18)	0.0628 (18)	−0.0001 (15)	0.0048 (15)	−0.0088 (14)
C5	0.070 (2)	0.070 (2)	0.077 (2)	−0.0312 (17)	0.0105 (16)	−0.0290 (17)
C9	0.079 (2)	0.093 (2)	0.0399 (15)	−0.0443 (19)	0.0005 (14)	−0.0004 (15)
C3	0.105 (3)	0.0411 (16)	0.081 (2)	−0.0057 (18)	0.025 (2)	−0.0101 (15)
C4	0.098 (3)	0.060 (2)	0.084 (2)	−0.0356 (19)	0.033 (2)	−0.0315 (18)
C7	0.066 (2)	0.068 (2)	0.086 (2)	−0.0170 (17)	−0.0195 (17)	−0.0029 (17)
C8	0.110 (3)	0.118 (3)	0.089 (3)	−0.050 (3)	−0.042 (3)	0.047 (3)

Geometric parameters ($\text{\AA}$, $^\circ$)

O1—S	1.428 (2)	C6—C5	1.385 (4)
S—O2	1.423 (2)	C6—C7	1.492 (4)
S—O1	1.428 (2)	C12—H12	0.9300
S—N1	1.644 (2)	C14—H14	0.9300
S—C10	1.756 (3)	C2—C3	1.378 (5)
Cl1—C13	1.723 (3)	C2—H2	0.9300
C10—C14	1.376 (4)	C5—C4	1.374 (5)
C10—C11	1.383 (3)	C5—H5	0.9300
N1—C1	1.443 (3)	C9—C8	1.430 (5)
N1—C9	1.484 (3)	C9—H9A	0.9700
C11—C12	1.358 (4)	C9—H9B	0.9700
C11—H11	0.9300	C3—C4	1.362 (5)
N2—C13	1.314 (4)	C3—H3	0.9300
N2—C14	1.325 (4)	C4—H4	0.9300
C1—C2	1.386 (4)	C7—C8	1.437 (5)
C1—C6	1.387 (4)	C7—H7A	0.9700
C13—C12	1.378 (4)	C8—H8A	0.9700
O2—S—O1	120.12 (13)	C3—C2—C1	119.5 (3)
O2—S—N1	108.30 (13)	C3—C2—H2	120.2

O1—S—N1	106.51 (12)	C1—C2—H2	120.2
O2—S—C10	106.62 (12)	C4—C5—C6	121.9 (3)
O1—S—C10	107.97 (14)	C4—C5—H5	119.1
N1—S—C10	106.63 (12)	C6—C5—H5	119.1
C14—C10—C11	118.8 (3)	C8—C9—N1	113.3 (3)
C14—C10—S	120.6 (2)	C8—C9—H9A	108.9
C11—C10—S	120.6 (2)	N1—C9—H9A	108.9
C1—N1—C9	115.2 (2)	C8—C9—H9B	108.9
C1—N1—S	117.64 (16)	N1—C9—H9B	108.9
C9—N1—S	117.2 (2)	H9A—C9—H9B	107.7
C12—C11—C10	118.9 (3)	C4—C3—C2	120.7 (3)
C12—C11—H11	120.6	C4—C3—H3	119.6
C10—C11—H11	120.6	C2—C3—H3	119.6
C13—N2—C14	116.3 (2)	C3—C4—C5	119.4 (3)
C2—C1—C6	120.7 (3)	C3—C4—H4	120.3
C2—C1—N1	120.4 (3)	C5—C4—H4	120.3
C6—C1—N1	118.8 (2)	C8—C7—C6	116.5 (3)
N2—C13—C12	125.4 (3)	C8—C7—H7A	108.2
N2—C13—C11	115.3 (2)	C6—C7—H7A	108.2
C12—C13—C11	119.2 (2)	C8—C7—H7B	108.2
C5—C6—C1	117.8 (3)	C6—C7—H7B	108.2
C5—C6—C7	120.7 (3)	H7A—C7—H7B	107.3
C1—C6—C7	121.5 (2)	C9—C8—C7	118.0 (4)
C11—C12—C13	117.4 (3)	C9—C8—H8A	107.8
C11—C12—H12	121.3	C7—C8—H8A	107.8
C13—C12—H12	121.3	C9—C8—H8B	107.8
N2—C14—C10	123.1 (3)	C7—C8—H8B	107.8
N2—C14—H14	118.4	H8A—C8—H8B	107.1
C10—C14—H14	118.4		
O2—S—C10—C14	−145.4 (2)	C9—N1—C1—C6	27.0 (4)
O2—S—C10—C14	−145.4 (2)	S—N1—C1—C6	−117.9 (2)
O1—S—C10—C14	−15.0 (3)	C14—N2—C13—C12	−1.0 (4)
O1—S—C10—C14	−15.0 (3)	C14—N2—C13—C11	179.2 (2)
O1—S—C10—C14	−15.0 (3)	C2—C1—C6—C5	−1.8 (4)
N1—S—C10—C14	99.1 (2)	N1—C1—C6—C5	178.8 (2)
O2—S—C10—C11	37.0 (2)	C2—C1—C6—C7	175.7 (3)
O2—S—C10—C11	37.0 (2)	N1—C1—C6—C7	−3.7 (4)
O1—S—C10—C11	167.3 (2)	C10—C11—C12—C13	0.4 (4)
O1—S—C10—C11	167.3 (2)	N2—C13—C12—C11	0.9 (4)
O1—S—C10—C11	167.3 (2)	C11—C13—C12—C11	−179.2 (2)
N1—S—C10—C11	−78.6 (2)	C13—N2—C14—C10	−0.3 (4)
O2—S—N1—C1	−54.9 (2)	C11—C10—C14—N2	1.5 (4)
O2—S—N1—C1	−54.9 (2)	S—C10—C14—N2	−176.1 (2)
O1—S—N1—C1	174.7 (2)	C6—C1—C2—C3	3.1 (4)
O1—S—N1—C1	174.7 (2)	N1—C1—C2—C3	−177.6 (3)
O1—S—N1—C1	174.7 (2)	C1—C6—C5—C4	−0.3 (5)
C10—S—N1—C1	59.5 (2)	C7—C6—C5—C4	−177.8 (3)

O2—S—N1—C9	161.0 (2)	C1—N1—C9—C8	−46.6 (5)
O2—S—N1—C9	161.0 (2)	S—N1—C9—C8	98.4 (4)
O1—S—N1—C9	30.5 (2)	C1—C2—C3—C4	−2.3 (5)
O1—S—N1—C9	30.5 (2)	C2—C3—C4—C5	0.2 (5)
O1—S—N1—C9	30.5 (2)	C6—C5—C4—C3	1.1 (5)
C10—S—N1—C9	−84.6 (2)	C5—C6—C7—C8	177.1 (4)
C14—C10—C11—C12	−1.6 (4)	C1—C6—C7—C8	−0.3 (6)
S—C10—C11—C12	176.12 (19)	N1—C9—C8—C7	43.5 (6)
C9—N1—C1—C2	−152.4 (3)	C6—C7—C8—C9	−20.5 (7)
S—N1—C1—C2	62.8 (3)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C11—H11 $\cdots$ O2 ⁱ	0.93	2.60	3.309 (3)	134
C7—H7A $\cdots$ O1 ⁱⁱ	0.97	2.66	3.586 (5)	160

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