

7-Chloro-3-(4-methylbenzenesulfonyl)pyrrolo[1,2-c]pyrimidine

Easha Narayan,^a Liangfeng Fu,^a Gordon W. Gribble,^{a*} Manpreet Kaur^b and Jerry P. Jasinski^{b*}

^aDepartment of Chemistry, Dartmouth College, Hanover, NH 03755, USA, and ^bDepartment of Chemistry, Keene State College, 229 Main Street, Keene, NH 03435, USA. *Correspondence e-mail: Gordon.W.Gribble@dartmouth.edu, jjasinski@keene.edu

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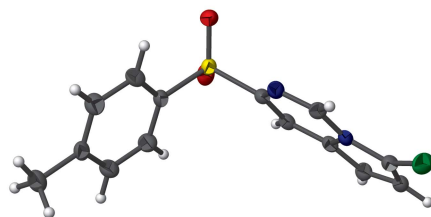
Keywords: crystal structure; weak intermolecular interactions; pyrrolo[1,2-c]pyrimidine and pyrimidine rings; π - π stacking.

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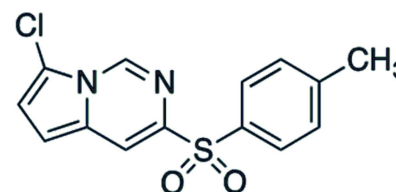
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, C₁₄H₁₁ClN₂O₂S, the dihedral angle between the pyrrolo[1,2-c]pyrimidine ring system (r.m.s. deviation = 0.008 Å) and the benzene ring is 80.2 (9)°. In the crystal, inversion dimers linked by pairs of C—H···O interactions generate R₂²(16) loops. Several aromatic π - π stacking interactions between the pyrrolo[1,2-c]pyrimidine rings, as well as separately between the pyrrolo and pyrimidine groups [shortest centroid-centroid separation = 3.5758 (14) Å], help to consolidate the packing.

3D view



Chemical scheme



Structure description

Pyrrolo[1,2-c]pyrimidines are a class of fused heterocycles of interest for their biological activity, electrochemical properties, and as components of natural products (Tatu *et al.*, 2018). As part of our studies in this area, we now report the crystal structure of the title compound, C₁₄H₁₁N₂O₂SCl (Fig. 1). We believe that this is the first crystal structure to be reported of a pyrrolo[1,2-c]pyrimidine and one of the few unsymmetrical 'diaryl sulfones' to be described.

The dihedral angle between the C1–C7/N1/N2 pyrrolo[1,2-c]pyrimidine ring system (r.m.s. deviation = 0.008 Å) and the C8–C13 benzene ring is 80.2 (9)°. The rings adopt a typical diaryl sulfone 'open-book' conformation with respect to the sulfonyl group (Koch & Moffitt, 1951; Sime & Woodhouse, 1974; Bocelli & Rizzoli, 1990; Colquhoun, 1997; Colquhoun *et al.*, 2002; Rudolph *et al.*, 2010; Benhalima *et al.*, 2012). Notably, the torsion angles differ from the ideal 90°. Thus, the torsion angles in the title compound reveal that the *p*-*d* π overlap in the benzene ring between C8 and S1 [torsion angle C1–S1–C8–C9 = 105.19 (19)°], is favored over the *p*-*d* π overlap in the pyrrolo[1,2-c]pyrimidine ring between C1 and S1 [C8–S1–C1–C2 = 110.70 (18)°], probably because the benzene ring

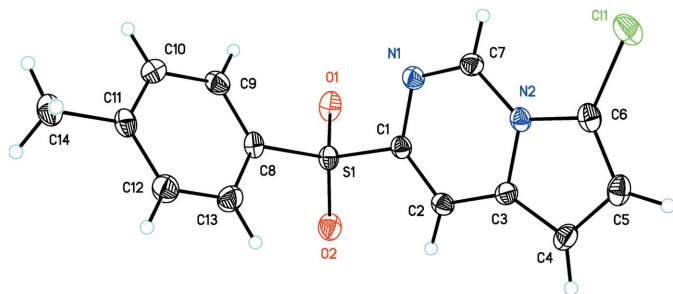


Figure 1
The molecular structure of the title compound, showing 50% probability ellipsoids.

is electron-rich relative to the pyrrolo[1,2-*c*]pyrimidine ring. Consistent with this notion is the observation that the S1–C8 bond length [1.767 (2) Å] is slightly shorter than S1–C1 [1.773 (2) Å]. The O1–S1–O2 bond angle of 119.68 (11)° agrees with the literature values for diaryl sulfones (Sime & Woodhouse, 1974; Colquhoun, 1997; Colquhoun *et al.*, 2002; Rudolph *et al.*, 2010; Benhalima *et al.*, 2012). Likewise, the C1–S1–C8 bond angle of 105.03 (10)° is consistent with the literature data (Sime & Woodhouse, 1974; Bocelli & Rizzoli, 1990; Colquhoun *et al.*, 2002).

In the crystal, a weak C14–H14B···O2 hydrogen bond (Table 1) links two molecules together in a ring face–ring face arrangement (Fig. 2). This packing motif was also observed by Sime & Woodhouse (1974) in the crystal structure of diphenyl sulfone and by Colquhoun *et al.* (2002) in the crystal structure of poly(1,4-phenylenesulfone). Several aromatic π – π stacking interactions between the pyrrolo[1,2-*c*]pyrimidine rings as well as separately between the pyrrolo and pyrimidine groups (Table 2) are observed and help to consolidate the packing.

Synthesis and crystallization

A stirred solution of 5-chloropyrrole-2-carbaldehyde (Leen *et al.*, 2011) (0.023 g, 0.18 mmol) in dioxane (10 ml) was cooled in an ice bath and toluenesulfonylmethyl isocyanide (TosMIC) (0.046 g, 0.26 mmol) and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) (0.04 ml) were added. The solution was then stirred for 20 h at 52°C. The reaction was quenched with 1M hydrochloric

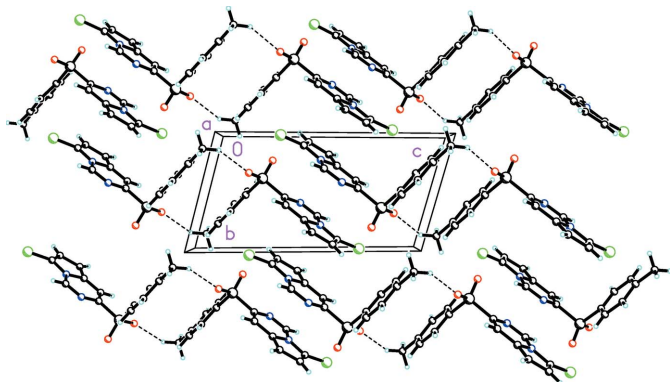


Figure 2
Packing diagram of the title compound viewed along the *a* axis direction showing inversion dimers linked by pairs of weak C–H···O interactions.

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

<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>
C14–H14B···O2 ⁱ	0.96	2.49	3.329 (3)	146

Symmetry code: (i) $-x + 1, -y + 1, -z + 2$.

Table 2
 π – π distances (Å) and angles (°) for the title compound.

C_g(I)–*C_g(J)* is the distance between ring centroids, α is dihedral angle between planes *C_g(I)* and *C_g(J)* and slippage is the distance between *C_g(I)* and perpendicular the projection of *C_g(J)* on ring *I*. *C_g(1)*, *C_g(2)* and *C_g(4)* are the centroids N2/C3–C6, N1/C1/C2/C3/N2/C7 and C1–C7/N1/N2 rings, respectively.

<i>C_g(I)</i> ^a	<i>C_g(J)</i> ^b	<i>d</i> [<i>C_g(I)</i> ··· <i>C_g(J)</i>]	α	slippage
<i>C_g(1)</i>	<i>C_g(1)</i> ⁱ	3.5758 (14)	0.00 (13)	1.169
<i>C_g(1)</i>	<i>C_g(2)</i> ⁱ	3.6261 (14)	0.73 (12)	1.348
<i>C_g(1)</i>	<i>C_g(2)</i> ⁱⁱ	3.6495 (14)	0.73 (12)	1.092
<i>C_g(1)</i>	<i>C_g(4)</i> ⁱ	3.4423 (13)	0.42 (11)	0.699
<i>C_g(1)</i>	<i>C_g(4)</i> ⁱⁱ	3.8876 (13)	0.42 (11)	1.738
<i>C_g(2)</i>	<i>C_g(2)</i> ⁱⁱ	3.9724 (13)	0.00 (10)	1.932
<i>C_g(2)</i>	<i>C_g(4)</i> ⁱⁱ	3.6901 (12)	0.32 (9)	1.233
<i>C_g(4)</i>	<i>C_g(4)</i> ⁱ	3.7241 (11)	0.00 (7)	1.586
<i>C_g(4)</i>	<i>C_g(4)</i> ⁱⁱ	3.6280 (11)	0.00 (7)	1.010

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

acid (25 ml) and extracted with ethyl acetate (50 ml). The organic layer was washed once each with 1 M hydrochloric acid (20 ml), saturated aqueous sodium bicarbonate solution (20 ml), and brine (20 ml). The organic layer was dried over anhydrous sodium sulfate, filtered over glass wool and concentrated *in vacuo*. The resulting crude product was purified by flash chromatography using 6:1 hexane:ethyl acetate. Evaporation of the solvent afforded 0.036 g (66%) of 7-chloro-3-tosylpyrrolo[1,2-*c*]pyrimidine as a light-yellow solid: mp 181–184°C; ¹H NMR (500 MHz, CDCl₃) δ 8.77 (*s*, 1H), 8.24 (*d*, *J* = 1 Hz, 1H), 7.95 (*d*, *J* = 8 Hz, 2H), 7.33 (*d*, *J* = 8 Hz, 2H), 6.92 (*d*, *J* = 4 Hz, 1H), 6.84 (*d*, *J* = 4 Hz, 1H), 2.42 (*s*, 3H); ¹³C NMR (500 MHz, CDCl₃) δ 144.8, 141.2, 136.4, 135.9, 130.0, 129.60, 128.9, 116.9, 115.0, 110.7, 106.2, 21.8; HRMS *m/z* calculated for C₁₄H₁₂N₂O₂SCl: 307.0308, found: 307.0303. Colorless prisms suitable for X-ray crystal structure determination were recrystallized from ethanol solution. The reaction scheme is shown in Fig. 3.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

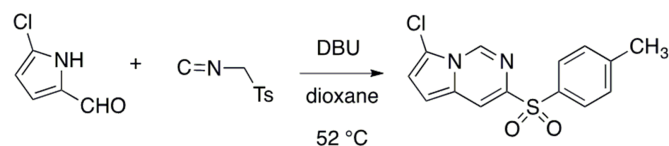


Figure 3
Reaction scheme.

Table 3

Experimental details.

Crystal data	
Chemical formula	C ₁₄ H ₁₁ ClN ₂ O ₂ S
<i>M</i> _r	306.76
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	173
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.2285 (5), 7.2385 (5), 13.7586 (11)
α , β , γ (°)	102.192 (7), 99.616 (6), 104.149 (6)
<i>V</i> (Å ³)	663.91 (9)
<i>Z</i>	2
Radiation type	Cu <i>K</i> α
μ (mm ⁻¹)	4.05
Crystal size (mm)	0.16 × 0.13 × 0.08
Data collection	
Diffractometer	Rigaku Oxford Diffraction Eos, Gemini
Absorption correction	Multi-scan
<i>T</i> _{min} , <i>T</i> _{max}	0.748, 1.000
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	3839, 2498, 2177
<i>R</i> _{int}	0.036
(sin θ / λ) _{max} (Å ⁻¹)	0.614
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.043, 0.114, 1.04
No. of reflections	2498
No. of parameters	183
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.53, -0.31

Computer programs: *CrysAlis PRO* (Rigaku OD, 2019), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

Funding information

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References

- Benhalima, A., Hudon, F., Koulibaly, F., Tessier, C. & Brisson, J. (2012). *Can. J. Chem.* **90**, 880–890.
- Bocelli, G. & Rizzoli, C. (1990). *Acta Cryst.* **C46**, 2259–2260.
- Colquhoun, H. M. (1997). *Polymer*, **38**, 991–994.
- Colquhoun, H. M., Aldred, P. L., Kohnke, F. H., Herbertson, P. L., Baxter, I. & Williams, D. J. (2002). *Macromolecules*, **35**, 1685–1690.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Koch, H. P. & Moffitt, W. E. (1951). *Trans. Faraday Soc.* **47**, 7–15.
- Leen, V., Leemans, T., Boens, N. & Dehaen, W. (2011). *Eur. J. Org. Chem.* pp. 4386–4396.
- Rigaku OD (2019). *CrysAlis PRO*. Rigaku Americas, The Woodlands, TX, USA.
- Rudolph, F. A. M., Fuller, A. L., Slawin, A. M. Z., Bühl, M., Aitken, R. A. & Woollins, J. D. (2010). *J. Chem. Crystallogr.* **40**, 253–265.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
- Sime, J. G. & Woodhouse, D. I. (1974). *J. Cryst. Mol. Struct.* **4**, 269–285.
- Tatu, M. L., Harja, F., Ungureanu, E. M., Georgescu, E. & Popa, M. M. (2018). *Rev. Chim.* **69**, 499–506.

full crystallographic data

IUCrData (2020). 5, x200382 [https://doi.org/10.1107/S241431462000382X]

7-Chloro-3-(4-methylbenzenesulfonyl)pyrrolo[1,2-c]pyrimidine

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7-Chloro-3-(4-methylbenzenesulfonyl)pyrrolo[1,2-c]pyrimidine

Crystal data

$C_{14}H_{11}ClN_2O_2S$	$Z = 2$
$M_r = 306.76$	$F(000) = 316$
Triclinic, $P\bar{1}$	$D_x = 1.535 \text{ Mg m}^{-3}$
$a = 7.2285 (5) \text{ \AA}$	Cu $K\alpha$ radiation, $\lambda = 1.54184 \text{ \AA}$
$b = 7.2385 (5) \text{ \AA}$	Cell parameters from 1885 reflections
$c = 13.7586 (11) \text{ \AA}$	$\theta = 6.5\text{--}71.4^\circ$
$\alpha = 102.192 (7)^\circ$	$\mu = 4.05 \text{ mm}^{-1}$
$\beta = 99.616 (6)^\circ$	$T = 173 \text{ K}$
$\gamma = 104.149 (6)^\circ$	Prism, colourless
$V = 663.91 (9) \text{ \AA}^3$	$0.16 \times 0.13 \times 0.08 \text{ mm}$

Data collection

Rigaku-Oxford Diffraction Eos, Gemini diffractometer	2498 independent reflections
Radiation source: fine-focus sealed X-ray tube	2177 reflections with $I > 2\sigma(I)$
Detector resolution: $16.0416 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.036$
ω scans	$\theta_{\text{max}} = 71.2^\circ$, $\theta_{\text{min}} = 3.4^\circ$
Absorption correction: multi-scan	$h = -5 \rightarrow 8$
$T_{\text{min}} = 0.748$, $T_{\text{max}} = 1.000$	$k = -8 \rightarrow 8$
3839 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.114$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.53 \text{ e \AA}^{-3}$
2498 reflections	$\Delta\rho_{\text{min}} = -0.31 \text{ e \AA}^{-3}$
183 parameters	Extinction correction: SHELXL-2018/1
0 restraints	(Sheldrick 2015),
Primary atom site location: dual	$Fc^* = kFc[1 + 0.001x Fc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Hydrogen site location: inferred from neighbouring sites	Extinction coefficient: 0.0018 (6)

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. All of the H atoms were placed in their calculated positions and then refined with atom-H lengths of 0.93 Å (CH); 0.96 Å (CH₃) using the riding model with U_{iso} (H) = 1.2 (CH) or 1.5 times U_{eq} (CH₃) of the parent atom. The idealized methyl group was refined as a rotating group.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.01870 (9)	0.02376 (9)	0.27155 (4)	0.03578 (19)
S1	0.40553 (8)	0.62315 (7)	0.76558 (4)	0.02404 (18)
O1	0.5458 (3)	0.7802 (2)	0.74516 (13)	0.0334 (4)
O2	0.2700 (3)	0.6692 (3)	0.82618 (13)	0.0340 (4)
N1	0.3648 (3)	0.4137 (3)	0.57537 (14)	0.0250 (4)
N2	0.0639 (3)	0.2272 (3)	0.46404 (13)	0.0216 (4)
C1	0.2605 (3)	0.4612 (3)	0.64732 (16)	0.0221 (4)
C2	0.0627 (3)	0.3971 (3)	0.63311 (16)	0.0231 (4)
H2	0.001144	0.434521	0.685034	0.028*
C3	-0.0462 (3)	0.2721 (3)	0.53723 (17)	0.0228 (4)
C4	-0.2410 (3)	0.1749 (3)	0.49171 (18)	0.0282 (5)
H4	-0.346453	0.178047	0.521972	0.034*
C5	-0.2517 (3)	0.0705 (3)	0.39148 (18)	0.0289 (5)
H5	-0.365477	-0.008063	0.343710	0.035*
C6	-0.0663 (3)	0.1047 (3)	0.37665 (16)	0.0257 (5)
C7	0.2645 (3)	0.3009 (3)	0.48672 (16)	0.0235 (4)
H7	0.331004	0.268421	0.436325	0.028*
C8	0.5354 (3)	0.4809 (3)	0.82241 (16)	0.0253 (4)
C9	0.7327 (4)	0.5134 (3)	0.82356 (17)	0.0293 (5)
H9	0.796540	0.608266	0.794615	0.035*
C10	0.8339 (4)	0.4003 (4)	0.86927 (19)	0.0316 (5)
H10	0.966752	0.421378	0.871207	0.038*
C11	0.7390 (4)	0.2571 (3)	0.91184 (16)	0.0269 (5)
C12	0.5414 (4)	0.2299 (4)	0.90997 (19)	0.0331 (5)
H12	0.476588	0.134692	0.938446	0.040*
C13	0.4392 (4)	0.3421 (4)	0.86641 (19)	0.0326 (5)
H13	0.307487	0.324508	0.866706	0.039*
C14	0.8477 (4)	0.1336 (4)	0.95979 (18)	0.0335 (5)
H14A	0.794694	-0.002190	0.921296	0.050*
H14B	0.833361	0.145628	1.028789	0.050*
H14C	0.984104	0.178670	0.959859	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0431 (4)	0.0340 (3)	0.0238 (3)	0.0029 (2)	0.0081 (2)	0.0033 (2)
S1	0.0260 (3)	0.0219 (3)	0.0216 (3)	0.0068 (2)	0.0011 (2)	0.00387 (19)
O1	0.0329 (9)	0.0238 (8)	0.0372 (9)	0.0025 (7)	-0.0034 (7)	0.0107 (7)
O2	0.0357 (9)	0.0376 (9)	0.0269 (8)	0.0160 (7)	0.0033 (7)	0.0016 (7)
N1	0.0239 (9)	0.0272 (9)	0.0235 (9)	0.0050 (7)	0.0050 (7)	0.0091 (7)
N2	0.0240 (9)	0.0212 (8)	0.0200 (8)	0.0054 (7)	0.0031 (7)	0.0089 (7)

C1	0.0240 (10)	0.0209 (10)	0.0214 (10)	0.0054 (8)	0.0040 (8)	0.0080 (8)
C2	0.0271 (11)	0.0234 (10)	0.0228 (10)	0.0108 (8)	0.0080 (8)	0.0090 (8)
C3	0.0220 (10)	0.0247 (10)	0.0263 (10)	0.0093 (8)	0.0067 (8)	0.0124 (8)
C4	0.0207 (10)	0.0310 (12)	0.0338 (12)	0.0076 (9)	0.0030 (9)	0.0128 (9)
C5	0.0276 (11)	0.0257 (11)	0.0302 (11)	0.0044 (9)	-0.0018 (9)	0.0109 (9)
C6	0.0309 (11)	0.0210 (10)	0.0230 (10)	0.0050 (8)	0.0021 (9)	0.0070 (8)
C7	0.0230 (10)	0.0236 (10)	0.0244 (10)	0.0056 (8)	0.0069 (8)	0.0077 (8)
C8	0.0275 (11)	0.0241 (10)	0.0216 (10)	0.0063 (8)	-0.0004 (8)	0.0065 (8)
C9	0.0342 (12)	0.0299 (11)	0.0278 (11)	0.0096 (9)	0.0111 (9)	0.0124 (9)
C10	0.0262 (11)	0.0391 (13)	0.0331 (11)	0.0120 (10)	0.0091 (9)	0.0124 (10)
C11	0.0331 (12)	0.0260 (11)	0.0193 (9)	0.0095 (9)	0.0011 (8)	0.0038 (8)
C12	0.0322 (12)	0.0326 (12)	0.0360 (12)	0.0064 (10)	0.0074 (10)	0.0161 (10)
C13	0.0248 (11)	0.0350 (12)	0.0375 (12)	0.0047 (9)	0.0054 (9)	0.0145 (10)
C14	0.0435 (14)	0.0328 (12)	0.0275 (11)	0.0179 (11)	0.0058 (10)	0.0088 (9)

Geometric parameters (Å, °)

C11—C6	1.711 (2)	C2—C3	1.407 (3)
S1—O1	1.4370 (18)	C3—C4	1.380 (3)
S1—O2	1.4429 (18)	C4—C5	1.405 (3)
S1—C1	1.773 (2)	C5—C6	1.360 (3)
S1—C8	1.767 (2)	C8—C9	1.384 (3)
N1—C1	1.378 (3)	C8—C13	1.384 (3)
N1—C7	1.294 (3)	C9—C10	1.399 (3)
N2—C3	1.417 (3)	C10—C11	1.390 (3)
N2—C6	1.371 (3)	C11—C12	1.389 (4)
N2—C7	1.373 (3)	C11—C14	1.507 (3)
C1—C2	1.358 (3)	C12—C13	1.384 (4)
O1—S1—O2	119.68 (11)	C3—C4—C5	107.8 (2)
O1—S1—C1	108.51 (10)	C6—C5—C4	108.0 (2)
O1—S1—C8	107.90 (11)	N2—C6—C11	119.51 (18)
O2—S1—C1	106.24 (11)	C5—C6—C11	130.89 (18)
O2—S1—C8	108.56 (11)	C5—C6—N2	109.6 (2)
C8—S1—C1	105.03 (10)	N1—C7—N2	122.67 (19)
C7—N1—C1	116.87 (19)	C9—C8—S1	119.13 (17)
C6—N2—C3	107.32 (18)	C13—C8—S1	119.48 (18)
C6—N2—C7	131.24 (19)	C13—C8—C9	121.4 (2)
C7—N2—C3	121.44 (18)	C8—C9—C10	118.5 (2)
N1—C1—S1	114.68 (16)	C11—C10—C9	121.1 (2)
C2—C1—S1	119.95 (16)	C10—C11—C14	121.0 (2)
C2—C1—N1	125.37 (19)	C12—C11—C10	118.8 (2)
C1—C2—C3	117.78 (19)	C12—C11—C14	120.2 (2)
C2—C3—N2	115.87 (19)	C13—C12—C11	121.1 (2)
C4—C3—N2	107.3 (2)	C8—C13—C12	119.2 (2)
C4—C3—C2	136.8 (2)		
S1—C1—C2—C3	178.70 (15)	C3—C4—C5—C6	-0.2 (3)

S1—C8—C9—C10	179.69 (17)	C4—C5—C6—C11	-179.09 (17)
S1—C8—C13—C12	179.40 (19)	C4—C5—C6—N2	0.2 (2)
O1—S1—C1—N1	44.81 (18)	C6—N2—C3—C2	179.87 (17)
O1—S1—C1—C2	-134.12 (16)	C6—N2—C3—C4	0.0 (2)
O1—S1—C8—C9	-10.4 (2)	C6—N2—C7—N1	-178.8 (2)
O1—S1—C8—C13	168.42 (19)	C7—N1—C1—S1	-177.86 (15)
O2—S1—C1—N1	174.70 (15)	C7—N1—C1—C2	1.0 (3)
O2—S1—C1—C2	-4.23 (19)	C7—N2—C3—C2	0.5 (3)
O2—S1—C8—C9	-141.51 (19)	C7—N2—C3—C4	-179.37 (18)
O2—S1—C8—C13	37.3 (2)	C7—N2—C6—C11	-1.5 (3)
N1—C1—C2—C3	-0.1 (3)	C7—N2—C6—C5	179.1 (2)
N2—C3—C4—C5	0.2 (2)	C8—S1—C1—N1	-70.37 (17)
C1—S1—C8—C9	105.19 (19)	C8—S1—C1—C2	110.70 (18)
C1—S1—C8—C13	-76.0 (2)	C8—C9—C10—C11	0.6 (4)
C1—N1—C7—N2	-1.1 (3)	C9—C8—C13—C12	-1.8 (4)
C1—C2—C3—N2	-0.6 (3)	C9—C10—C11—C12	-1.1 (4)
C1—C2—C3—C4	179.2 (2)	C9—C10—C11—C14	179.2 (2)
C2—C3—C4—C5	-179.7 (2)	C10—C11—C12—C13	0.2 (4)
C3—N2—C6—C11	179.28 (14)	C11—C12—C13—C8	1.2 (4)
C3—N2—C6—C5	-0.1 (2)	C13—C8—C9—C10	0.9 (3)
C3—N2—C7—N1	0.4 (3)	C14—C11—C12—C13	179.9 (2)

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>
C14—H14B \cdots O2 ⁱ	0.96	2.49	3.329 (3)	146

Symmetry code: (i) $-x+1, -y+1, -z+2$.