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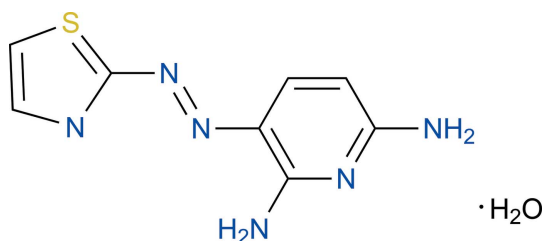
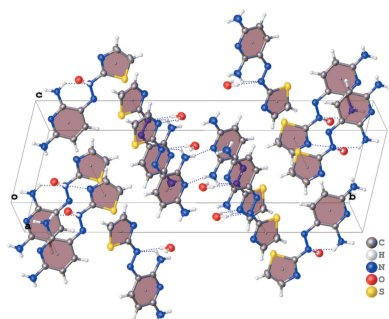
Crystal structure of 3-[2-(1,3-thiazol-2-yl)diazen-1-yl]pyridine-2,6-diamine monohydrate

Ratanon Chotima,^{a*} Bussaba Boonseng,^a Akkharadet Piyasaengthong,^b Apisit
Songsasen^b and Kittipong Chainok^c^aDepartment of Chemistry, Faculty of Science, Naresuan University, Muang, Phitsanulok 65000, Thailand, ^bDepartment of Chemistry, Faculty of Science, Kasetsart University, Chatuchak, Bangkok 10900, Thailand, and ^cMaterials and Textile Technology, Faculty of Science and Technology, Thammasat University, Khlong Luang, Pathum Thani 12121, Thailand.
*Correspondence e-mail: ratanonc@nu.ac.th

In the title hydrated azo compound, $C_8H_8N_6S \cdot H_2O$, the two aromatic groups are close to coplanar with the dihedral angle between the mean planes of the thiazole and pyridine rings being $2.9(2)^\circ$. The organic molecule adopts an *E* configuration with respect to the double bond of the azo bridge. In the crystal, molecules are linked by (amine) $N-H \cdots N$ (pyridine), (amine) $N-H \cdots O$ (water) and (water) $O-H \cdots N$ (thiazole) hydrogen bonds along with π - π interactions involving pairs of thiazole rings and pairs of pyridine rings. The plane-to-plane distance between two parallel molecules is $3.7856(4) \text{ \AA}$ and corresponds to the length of the *a* axis. In this way, a layer structure parallel to (010) is formed. The layers are linked by weak $C-H \cdots S$ hydrogen bonds, eventually resulting in a three-dimensional network.

1. Chemical context

Azo compounds are one of the most important organic dyes used in industrial applications to colour various consumer goods such as leather, plastics and cosmetics (Kaur *et al.*, 2018). The main characteristic of these compounds is the chromophore of the azo group ($-N=N-$), which is responsible for the color of the dyes. Compounds with an aromatic thiazolylazo moiety are a subclass of azo dyes, which contain the thiazole group on one side of the azo linkage and are important ligands in coordination chemistry (Kaim, 2001). In this regard, zinc complexes with polydentate chelating thiazolylazo ligands have been prepared as luminescence probes for selectively sensing phosphates (Hens *et al.*, 2015). Recently, Piyasaengthong *et al.* (2015) reported the synthesis of a gold(III) complex of 3-(2'-thiazolylazo)-2,6-diaminopyridine and investigated its pepsin inhibition.



We report here the crystal structure of 3-(2'-thiazolylazo)-2,6-diaminopyridine monohydrate, $C_8H_8N_6S \cdot H_2O$, (I), obtained through the diazotization of 2-aminothiazole

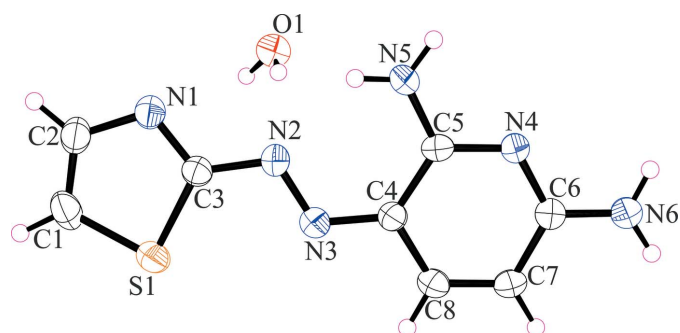


Figure 1
The molecular structure of the organic entity and the water molecule in compound (I), with the atom labelling and displacement ellipsoids drawn at the 50% probability level.

followed by a coupling reaction with 2,6-diaminopyridine (Montelongo *et al.*, 1982).

2. Structural commentary

The molecular entities of (I) with atom labelling are presented in Fig. 1. The organic molecule has an *E* configuration with respect to the azo bridge ($-\text{N}2=\text{N}3-$), and is essentially planar with an r.m.s deviation of the fitted non-hydrogen atoms being 0.033 Å. The amine N5 and N6 atoms are 0.044 (2) and -0.059 (3) Å, respectively, out of this plane. The thiazole ring (C1–C3, N1, S1) makes a dihedral angle of 2.9 (2)° with the pyridine ring (C4–C8, N4). An intramolecular N5–H5A···N2

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>
C2–H2···S1 ⁱ	0.93	3.02	3.665 (3)	128
N5–H5A···N2	0.86 (1)	2.03 (3)	2.645 (4)	128 (3)
N5–H5A···O1	0.86 (1)	2.59 (2)	3.314 (4)	143 (3)
N5–H5B···N4 ⁱⁱ	0.86 (1)	2.14 (1)	2.998 (4)	172 (3)
N6–H6A···O1 ⁱⁱⁱ	0.86 (1)	2.27 (2)	3.048 (4)	151 (4)
N6–H6B···O1 ⁱⁱⁱ	0.86 (1)	2.13 (1)	2.988 (4)	177 (4)
O1–H1A···N1	0.84 (1)	2.13 (3)	2.923 (4)	158 (6)
O1–H1B···N2 ^{iv}	0.84 (1)	2.31 (2)	3.143 (4)	170 (9)

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

hydrogen bond is observed (Table 1), showing an *S*(6) ring motif.

3. Supramolecular features

In the crystal of (I), extensive (amine)N–H···N(pyridine), (amine)N–H···O(water) and (water)O–H···N(thiazole) hydrogen bonds (Table 1) are present. Together with π – π interactions involving pairs of thiazole rings and pairs of pyridine rings with a plane-to-plane distance between two parallel molecules of 3.7856 (4) Å, a layered structure parallel to the *ac* plane is formed (Fig. 2). Weak C–H···S hydrogen bonds between adjacent thiazole rings further consolidate the crystal packing, thus generating a three-dimensional network.

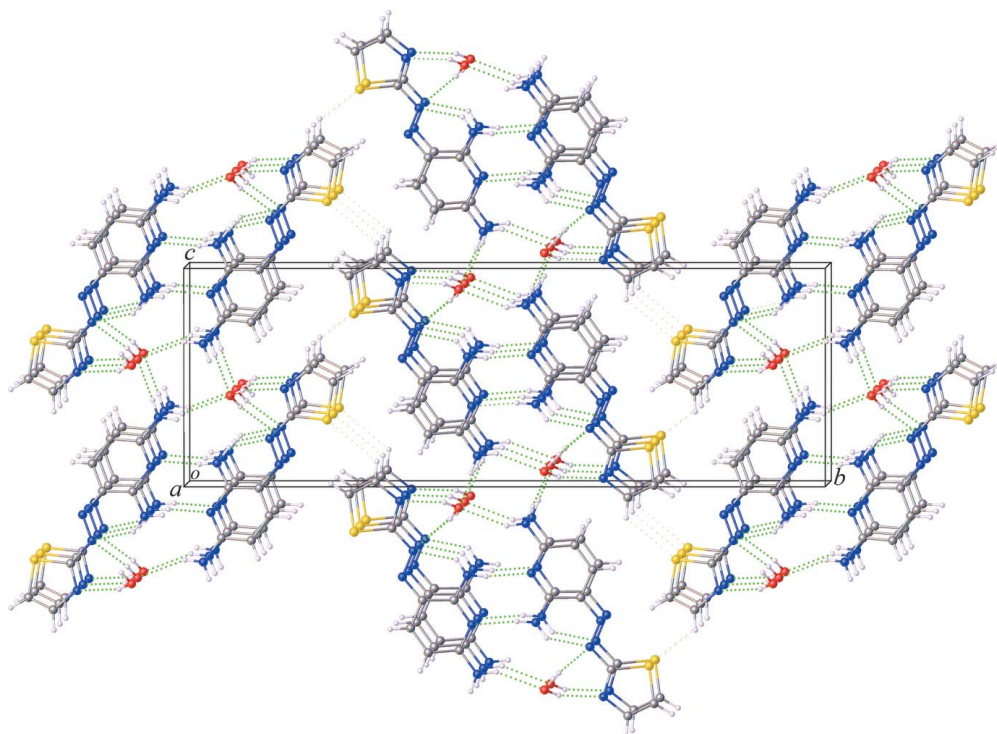


Figure 2
The unit-cell packing in (I), viewed approximately down [100]. The classical O–H···N, and N–H···O hydrogen bonds are shown as green dashed lines (see Table 1 for numerical details).

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₈ H ₈ N ₆ S·H ₂ O
<i>M_r</i>	238.28
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	3.7856 (4), 28.393 (3), 9.6324 (9)
β (°)	93.824 (3)
<i>V</i> (Å ³)	1033.02 (17)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.30
Crystal size (mm)	0.28 × 0.08 × 0.04
Data collection	
Diffractometer	Bruker D8 QUEST CMOS
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2016)
<i>T_{min}</i> , <i>T_{max}</i>	0.644, 0.745
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	11837, 2100, 1670
<i>R_{int}</i>	0.054
(sin θ/λ) _{max} (Å ⁻¹)	0.630
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.061, 0.121, 1.17
No. of reflections	2100
No. of parameters	169
No. of restraints	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.33, -0.26

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL2014* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

4. Database survey

A search of the Cambridge Structural Database (Groom *et al.*, 2016) for compounds with the (*E*)-2-(pyridin-3-ylidiaz-enyl)thiazole moiety gave no hits. However, structures of substituted thiazolylazo derivatives were found, for example, 5-(diethylamino)-2-(2-thiazolylazo)phenol (QAVNAD; Zhang *et al.*, 2005), 4-(2'-thiazolylazo)pyrocatechol (TZAZPC; Apinitis, 1978), 1-(2-thiazolylazo)-6-bromo-2-naphthol (TAZBRN10; Kurahashi *et al.*, 1976) and 1-(2-thiazolylazo)-2-naphthol (TAZNPL10; Kurahashi, 1976).

5. Synthesis and crystallization

2-Aminothiazole (1.0 g, 0.009 mol) was dissolved in 6 *M* hydrochloric acid (16 ml) with sodium nitrite (0.7 g, 0.01 mol). The mixture was stirred at a temperature between 268 and 273 K while a solution of 2,6-diaminopyridine (1.0 g, 0.009 mol) in 40 ml of 4 *M* hydrochloric acid was added. The reaction mixture was stirred for 1 h and then adjusted to pH

6.0 by 0.001 *M* sodium hydroxide. The red precipitate formed was filtered through suction and washed with water. Suitable crystals for X-ray analysis were grown by recrystallization using the vapor diffusion technique in a methanol-hexane mixture at 253 K [yield 1.12 g, 51%]. ¹H NMR (400 MHz, 298 K, C₂D₆OS): δ 6.10 (*d*, *m*-ArH py, 1H), 7.39 (*d*, thiazole-*H*, 1H), 7.55 (*d*, *p*-ArH py, 1H), 7.703 (*d*, thiazole-*H*, 1H). Mass spec. (ESI) *m/z* 220.9 (*M*⁺), 136.2, 108.3, 81.4. IR-KBr (cm⁻¹): 3335 (*w*), 3217 (*w*), 3082 (*w*), 1660 (*s*), 1631 (*s*), 1454 (*m*), 1292 (*s*), 1159 (*m*). Analysis calculated for C₈H₁₀N₆OS: C, 43.64; H, 3.66; N, 38.16; 14.56. Found: C, 43.80; H, 3.79; N, 38.45; S, 14.78.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms bonded to O and N atoms were located in difference-Fourier maps and refined with distance restraints of 0.84±0.02 Å with *U*_{iso}(H) = 1.5*U*_{eq}(O) and 0.86±0.02 Å with *U*_{iso}(H) = 1.2*U*_{eq}(N), respectively. The C-bound H atoms were included in calculated positions and treated as riding atoms: C–H = 0.93 Å with *U*_{iso}(H) = 1.2*U*_{eq}(C).

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Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINTE* (Bruker, 2016); data reduction: *SAINTE* (Bruker, 2016); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

3-[2-(1,3-Thiazol-2-yl)diazen-1-yl]pyridine-2,6-diamine monohydrate

Crystal data

$C_8H_8N_6S \cdot H_2O$

$M_r = 238.28$

Monoclinic, $P2_1/n$

$a = 3.7856$ (4) Å

$b = 28.393$ (3) Å

$c = 9.6324$ (9) Å

$\beta = 93.824$ (3)°

$V = 1033.02$ (17) Å³

$Z = 4$

$F(000) = 496$

$D_x = 1.532$ Mg m⁻³

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

Cell parameters from 4156 reflections

$\theta = 3.0$ – 26.6 °

$\mu = 0.30$ mm⁻¹

$T = 296$ K

Needle, dark orange

$0.28 \times 0.08 \times 0.04$ mm

Data collection

Bruker D8 QUEST CMOS
diffractometer

Radiation source: microfocus sealed x-ray tube,
Incoatec $I\mu$ s

GraphiteDouble Bounce Multilayer Mirror
monochromator

Detector resolution: 10.5 pixels mm⁻¹

ω and φ scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2016)

$T_{\min} = 0.644$, $T_{\max} = 0.745$

11837 measured reflections

2100 independent reflections

1670 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.054$

$\theta_{\max} = 26.6$ °, $\theta_{\min} = 3.6$ °

$h = -4 \rightarrow 4$

$k = -35 \rightarrow 35$

$l = -12 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.061$

$wR(F^2) = 0.121$

$S = 1.17$

2100 reflections

169 parameters

6 restraints

Primary atom site location: dual

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0131P)^2 + 1.7616P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.33 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$$

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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.1445 (2)	0.72666 (3)	0.18385 (9)	0.0377 (2)
N1	0.4021 (8)	0.65791 (9)	0.0492 (3)	0.0356 (6)
N2	0.2953 (7)	0.63596 (9)	0.2749 (3)	0.0317 (6)
N3	0.1805 (7)	0.65155 (9)	0.3905 (3)	0.0310 (6)
N4	0.2611 (7)	0.54434 (8)	0.6116 (3)	0.0299 (6)
N5	0.4246 (8)	0.55257 (10)	0.3899 (3)	0.0379 (7)
N6	0.1041 (9)	0.53404 (10)	0.8343 (3)	0.0437 (8)
C1	0.2378 (10)	0.73517 (12)	0.0133 (4)	0.0415 (8)
H1	0.2022	0.7632	-0.0355	0.050*
C2	0.3691 (10)	0.69560 (12)	-0.0395 (4)	0.0409 (8)
H2	0.4337	0.6939	-0.1308	0.049*
C3	0.2931 (8)	0.66920 (10)	0.1706 (3)	0.0303 (7)
C4	0.1707 (8)	0.62052 (10)	0.4978 (3)	0.0284 (7)
C5	0.2873 (8)	0.57206 (10)	0.4993 (3)	0.0279 (7)
C6	0.1248 (8)	0.56226 (10)	0.7246 (3)	0.0306 (7)
C7	0.0081 (9)	0.60975 (11)	0.7330 (3)	0.0342 (7)
H7	-0.0845	0.6212	0.8134	0.041*
C8	0.0359 (8)	0.63760 (11)	0.6209 (3)	0.0335 (7)
H8	-0.0357	0.6689	0.6250	0.040*
O1	0.7912 (8)	0.56959 (9)	0.0910 (3)	0.0489 (7)
H5A	0.471 (9)	0.5698 (10)	0.320 (2)	0.040 (10)*
H5B	0.504 (9)	0.5242 (6)	0.397 (4)	0.047 (11)*
H6A	0.166 (10)	0.5050 (5)	0.826 (4)	0.058 (12)*
H6B	0.022 (10)	0.5438 (12)	0.910 (2)	0.052 (12)*
H1A	0.647 (12)	0.5905 (15)	0.062 (6)	0.11 (2)*
H1B	0.936 (19)	0.584 (3)	0.145 (8)	0.23 (5)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0472 (5)	0.0283 (4)	0.0375 (5)	0.0039 (4)	0.0011 (4)	-0.0003 (3)
N1	0.0457 (16)	0.0316 (14)	0.0299 (15)	-0.0034 (12)	0.0044 (13)	-0.0004 (11)
N2	0.0362 (15)	0.0295 (13)	0.0295 (15)	0.0017 (11)	0.0028 (12)	0.0031 (11)
N3	0.0332 (14)	0.0286 (13)	0.0313 (15)	0.0013 (11)	0.0018 (12)	0.0008 (11)
N4	0.0342 (14)	0.0265 (13)	0.0292 (14)	0.0033 (11)	0.0048 (12)	0.0011 (10)
N5	0.0555 (19)	0.0264 (14)	0.0331 (16)	0.0100 (13)	0.0127 (14)	0.0034 (12)

N6	0.064 (2)	0.0359 (16)	0.0331 (17)	0.0112 (15)	0.0151 (15)	0.0028 (13)
C1	0.053 (2)	0.0324 (17)	0.037 (2)	-0.0067 (15)	-0.0083 (17)	0.0076 (14)
C2	0.054 (2)	0.0386 (18)	0.0298 (18)	-0.0102 (16)	0.0034 (16)	0.0041 (14)
C3	0.0321 (17)	0.0261 (15)	0.0323 (18)	-0.0027 (12)	0.0002 (14)	-0.0006 (12)
C4	0.0305 (16)	0.0259 (14)	0.0287 (16)	0.0015 (12)	0.0006 (13)	0.0007 (12)
C5	0.0273 (15)	0.0266 (15)	0.0300 (17)	0.0002 (12)	0.0028 (13)	-0.0027 (12)
C6	0.0309 (16)	0.0309 (16)	0.0301 (17)	0.0002 (13)	0.0033 (14)	0.0002 (12)
C7	0.0392 (18)	0.0327 (16)	0.0314 (18)	0.0054 (14)	0.0082 (15)	-0.0043 (13)
C8	0.0376 (18)	0.0272 (15)	0.0355 (19)	0.0065 (13)	0.0021 (15)	-0.0019 (13)
O1	0.0621 (18)	0.0385 (14)	0.0474 (16)	0.0045 (13)	0.0123 (14)	-0.0006 (12)

Geometric parameters (Å, °)

S1—C1	1.720 (4)	N6—H6A	0.863 (10)
S1—C3	1.733 (3)	N6—H6B	0.860 (10)
N1—C2	1.370 (4)	C1—H1	0.9300
N1—C3	1.305 (4)	C1—C2	1.342 (5)
N2—N3	1.300 (3)	C2—H2	0.9300
N2—C3	1.379 (4)	C4—C5	1.445 (4)
N3—C4	1.360 (4)	C4—C8	1.408 (4)
N4—C5	1.347 (4)	C6—C7	1.423 (4)
N4—C6	1.336 (4)	C7—H7	0.9300
N5—C5	1.326 (4)	C7—C8	1.348 (4)
N5—H5A	0.858 (10)	C8—H8	0.9300
N5—H5B	0.861 (10)	O1—H1A	0.841 (10)
N6—C6	1.333 (4)	O1—H1B	0.840 (10)
C1—S1—C3	88.47 (16)	N1—C3—N2	119.9 (3)
C3—N1—C2	110.2 (3)	N2—C3—S1	125.2 (2)
N3—N2—C3	113.9 (2)	N3—C4—C5	126.9 (3)
N2—N3—C4	117.2 (2)	N3—C4—C8	116.5 (3)
C6—N4—C5	119.0 (2)	C8—C4—C5	116.5 (3)
C5—N5—H5A	120 (2)	N4—C5—C4	121.7 (3)
C5—N5—H5B	119 (2)	N5—C5—N4	116.6 (3)
H5A—N5—H5B	121 (3)	N5—C5—C4	121.7 (3)
C6—N6—H6A	118 (3)	N4—C6—C7	123.0 (3)
C6—N6—H6B	122 (3)	N6—C6—N4	117.6 (3)
H6A—N6—H6B	120 (4)	N6—C6—C7	119.3 (3)
S1—C1—H1	124.8	C6—C7—H7	121.0
C2—C1—S1	110.4 (3)	C8—C7—C6	118.0 (3)
C2—C1—H1	124.8	C8—C7—H7	121.0
N1—C2—H2	122.0	C4—C8—H8	119.2
C1—C2—N1	116.0 (3)	C7—C8—C4	121.6 (3)
C1—C2—H2	122.0	C7—C8—H8	119.2
N1—C3—S1	114.9 (2)	H1A—O1—H1B	104 (7)
S1—C1—C2—N1	-0.1 (4)	C2—N1—C3—N2	178.4 (3)
N2—N3—C4—C5	2.5 (5)	C3—S1—C1—C2	0.0 (3)

N2—N3—C4—C8	-178.2 (3)	C3—N1—C2—C1	0.2 (5)
N3—N2—C3—S1	-1.5 (4)	C3—N2—N3—C4	179.2 (3)
N3—N2—C3—N1	-180.0 (3)	C5—N4—C6—N6	-179.6 (3)
N3—C4—C5—N4	-179.3 (3)	C5—N4—C6—C7	-0.7 (5)
N3—C4—C5—N5	0.5 (5)	C5—C4—C8—C7	-1.8 (5)
N3—C4—C8—C7	178.8 (3)	C6—N4—C5—N5	179.9 (3)
N4—C6—C7—C8	0.3 (5)	C6—N4—C5—C4	-0.3 (4)
N6—C6—C7—C8	179.3 (3)	C6—C7—C8—C4	1.0 (5)
C1—S1—C3—N1	0.1 (3)	C8—C4—C5—N4	1.4 (4)
C1—S1—C3—N2	-178.5 (3)	C8—C4—C5—N5	-178.8 (3)
C2—N1—C3—S1	-0.2 (4)		

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>
C2—H2 \cdots S1 ⁱ	0.93	3.02	3.665 (3)	128
N5—H5 <i>A</i> \cdots N2	0.86 (1)	2.03 (3)	2.645 (4)	128 (3)
N5—H5 <i>A</i> \cdots O1	0.86 (1)	2.59 (2)	3.314 (4)	143 (3)
N5—H5 <i>B</i> \cdots N4 ⁱⁱ	0.86 (1)	2.14 (1)	2.998 (4)	172 (3)
N6—H6 <i>A</i> \cdots O1 ⁱⁱ	0.86 (1)	2.27 (2)	3.048 (4)	151 (4)
N6—H6 <i>B</i> \cdots O1 ⁱⁱⁱ	0.86 (1)	2.13 (1)	2.988 (4)	177 (4)
O1—H1 <i>A</i> \cdots N1	0.84 (1)	2.13 (3)	2.923 (4)	158 (6)
O1—H1 <i>B</i> \cdots N2 ^{iv}	0.84 (1)	2.31 (2)	3.143 (4)	170 (9)

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