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Synthesis and crystal structure of 4,6-diamino-1-cyclohexyl-1,3,5-triazine-2(1*H*)-thione monohydrate

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In the crystal structure of the title compound, $C_9H_{15}N_5S{\cdot}H_2O$, the diaminotriazinethione (DTT) moiety and water molecules are hydrogen bonded to form ribbons. In the ribbon, each water molecule accepts a pair of $N—H\cdots O$ bonds from the DTT moieties of two adjacent molecules and donates one $O—H\cdots N$ bond to a third DTT moiety. The ribbons are stacked and linked through $O—H\cdots N$ interactions. The cyclohexane moieties are pendant to the ribbons forming a layer-like structure.

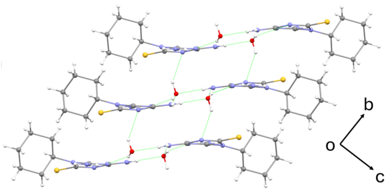
1. Chemical context

Triazines constitute one of the most noteworthy heterocyclic scaffolds for drug discovery as a result of their structural significance and broad-spectrum biological potencies (Kciuk *et al.*, 2023; Gornowicz *et al.*, 2020; Mohamed-Ezzat & Elgemeie, 2024*a*; Abdallah *et al.*, 2021). Numerous triazine-containing drugs for treatment of many diseases have been approved by the FDA, including decitabine, cycloguanil, altretamine, bimiralisib, almitrine, lamotrigine and triazavirin (Ali *et al.*, 2025).

The discovery of sulfur-based therapies has also been an important development of the pharmaceutical industry and sulfur-derived functional groups are present in a wide variety of natural products and pharmaceuticals. Sulfur continues to be the predominant heteroatom in many antimetabolic heterocycles and in a range of FDA-approved drugs (Mohamed-Ezzat *et al.*, 2022, 2023; Feng *et al.*, 2016; Elgemeie *et al.*, 1992, 1999).

The results presented here were obtained in continuation of our program in the synthesis of heterocycles utilizing cyanocarboimidodithioate as a key precursor. This highly reactive compound has been utilized effectively in the synthesis of various heterocycles (Elgemeie & Mohamed, 2014*a*,*b*; Elgemeie *et al.*, 2015; Mohamed-Ezzat & Elgemeie, 2023, 2024*a*; Mohamed-Ezzat *et al.*, 2024). We have also recently synthesized numerous triazines via novel approaches (Mohamed-Ezzat *et al.*, 2024*b*, 2025).

The incorporation of sulfur functionalities into molecules containing the triazine ring system combines two privileged scaffolds. Combination of the two important pharmacophores in the framework is a strategy for the development of potentially novel therapeutic agents. Herein, the novel triazinethione was synthesized via reaction of cyclohexyliso-



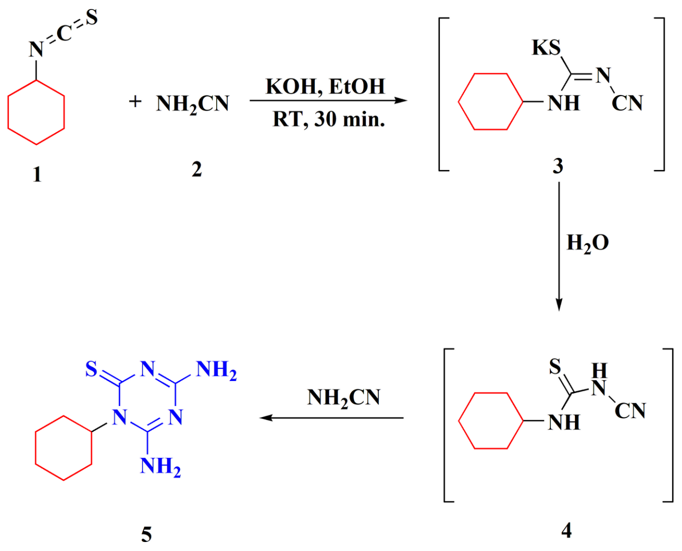
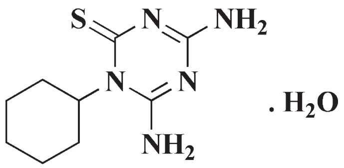


Figure 1
Reaction scheme showing the synthesis of compound **5**.

thiocyanate with cyanamide in the presence of potassium hydroxide at room temperature as depicted in Fig. 1.



2. Structural commentary

The compound crystallizes in the orthorhombic, *Pbca* space group. The asymmetric unit contains a molecule of 4,6-diamino-1-cyclohexyl-1,3,5-triazine-2(1*H*)-thione (**5**) and a water molecule (Fig. 2). The molecule of **5** consists of a cyclohexane ring (C1–C6) and a diaminotriazinethione (DTT) moiety (C7–C9, N1–N5, S1). In the molecule, the least-squares plane through the cyclohexane ring is twisted from the plane through the DTT moiety by a dihedral angle of 72.07 (10)°.

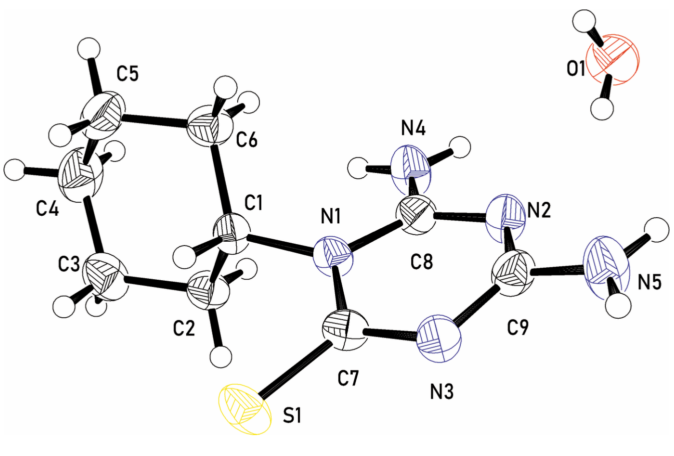


Figure 2
The asymmetric unit of the crystal structure of $\mathbf{5}\cdot H_2O$ showing displacement ellipsoids at the 50% probability level.

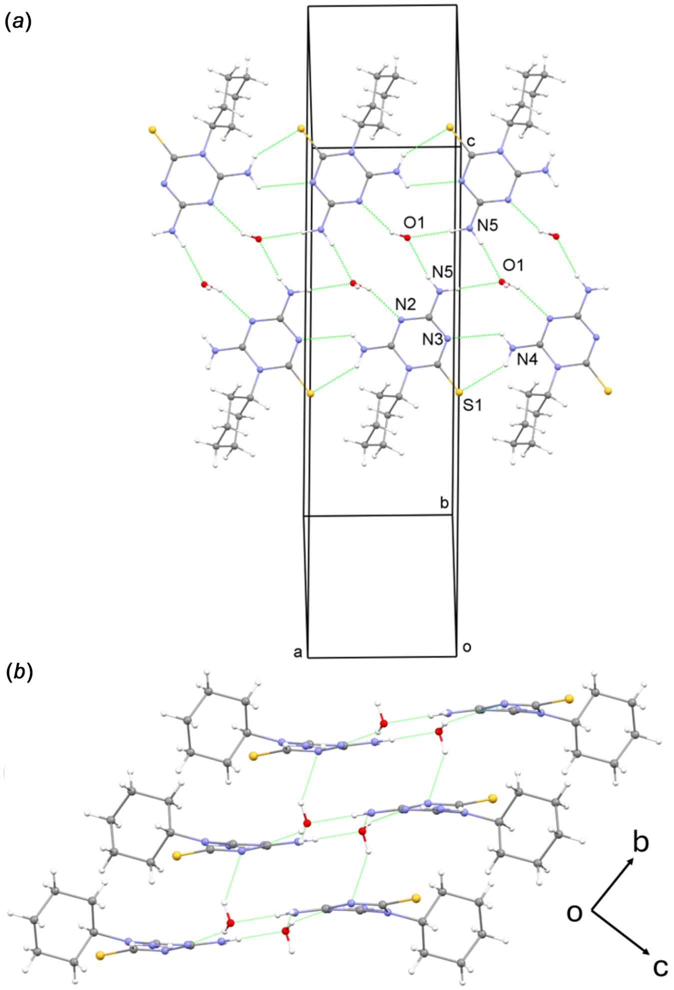


Figure 3
Segments of the crystal structure of $\mathbf{5}\cdot H_2O$ showing (*a*) a ribbon formed through hydrogen bonding and (*b*) the stacking of ribbons viewed down the *a* axis.

The cyclohexane ring is in a chair conformation. The triazine ring of the DTT moiety is slightly curved as indicated by displacement of atoms C9 and N1 to the same side of the ring, away from the plane through atoms C7, C8, N2, N3, by 0.125 (3) and 0.161 (3) Å, respectively.

3. Supramolecular features

In the crystal structure, the DTT moieties and water molecules are hydrogen bonded to form ribbons propagated in the [100] direction (Table 1, Fig. 3*a*). In the ribbon, each water molecule accepts a pair of N—H⋯O bonds from the DTT moieties of two adjacent molecules and donates one O—H⋯N bond to a third DTT moiety. Additional N—H⋯N and N—H⋯S hydrogen bonds also occur in the ribbon. The ribbons are stacked in the [010] direction in the crystal and they are linked through O—H⋯N interactions (Fig. 3*b*). Additionally, a weak O-H⋯S hydrogen bond connects ribbons in the *b*-axis

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*C*···N3^{i}	0.86 (3)	2.62 (3)	3.151 (3)	121 (2)
N4—H4*C*···O1	0.86 (3)	2.53 (3)	3.239 (3)	140 (2)
N4—H4*D*···S1^{i}	0.87 (3)	2.52 (3)	3.313 (2)	152 (2)
N5—H5*C*···O1^{ii}	0.89 (4)	2.09 (4)	2.967 (3)	167 (3)
N5—H5*D*···O1^{iii}	0.83 (3)	2.29 (3)	3.094 (3)	164 (3)
O1—H1*O*···N2	0.82 (4)	2.19 (3)	2.949 (3)	153 (3)
O1—H2*O*···N3^{iv}	0.85 (3)	2.61 (3)	3.325 (3)	142 (3)
O1—H2*O*···S1^{iv}	0.85 (3)	2.79 (3)	3.574 (2)	153 (3)

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

direction. The cyclohexane moieties are pendant to the ribbons and hence the structure is layer-like.

4. Database survey

A search of the CSD (version 6.00, November 2025; Groom *et al.*, 2016) for crystal structures containing the diaminotriazinethione moiety revealed 6-(benzylsulfanyl)-1,3,5-triazine-2,4-diamine (COFPEW; Liu *et al.*, 2024) and bis(4,6-diamino-2-thiono-1*H*-(1,3,5)triazinium) aquabis(oxalato-*O*,*O*′)dioxouranium(VI) *N*-cyanoguanidine (QELQAA, QELQAA01); Serezhkina *et al.*, 2007). COFPEW has three molecules in the asymmetric unit with the methylbenzene moieties linked to the DTT through the S atoms. The planes through the phenyl rings are twisted from the DTT planes by dihedral angles in the range 70–83°, comparable to that observed for the cyclohexane ring in the title compound. QELQAA(01) is a metal complex containing separate DTT units.

5. Synthesis and crystallization

The title compound was obtained, as depicted in Fig. 1, starting from the reaction of cyclohexylisothiocyanate (**1**) with cyanamide (**2**) in the presence of potassium hydroxide in ethanol at room temperature for 30 min. The reaction mixture was then poured into water and hydrolysed using hydrochloric acid to give the title compound **5** as colorless crystals of various shapes which were then crystallized from water to give needles.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The cyclohexane H atoms were inserted in idealized positions and refined using a riding model with $U_{\rm iso}$(H) = $U_{\rm eq}$(C).

Acknowledgements

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_9H_{15}N_5S \cdot H_2O$
M_r	243.33
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	293
a, *b*, *c* (Å)	7.0790 (4), 9.9029 (6), 33.0489 (19)
V (Å^3)	2316.8 (2)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	0.27
Crystal size (mm)	0.48 × 0.18 × 0.07
Data collection	
Diffractometer	SuperNova, Dual, Cu at home/near, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku, 2024)
$T_{\rm min}$, $T_{\rm max}$	0.545, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20982, 3038, 2038
$R_{\rm int}$	0.076
$(\sin \theta/\lambda)_{\rm max}$ (Å^{-1})	0.697
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.056, 0.136, 1.09
No. of reflections	3038
No. of parameters	167
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\rm max}$, $\Delta\rho_{\rm min}$ (e Å^{-3})	0.35, −0.23

Computer programs: *CrysAlis PRO* (Rigaku, 2024), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012).

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Synthesis and crystal structure of 4,6-diamino-1-cyclohexyl-1,3,5-triazine-2(1*H*)-thione monohydrate

Ebtsam A. Ahmed, Benson M. Kariuki, Reham A. Mohamed-Ezzat, Rasha A. Azzam and Galal H. Elgemeie

Computing details

4,6-Diamino-1-cyclohexyl-1,3,5-triazine-2(1*H*)-thione monohydrate

Crystal data

$C_9H_{15}N_5S{\cdot}H_2O$
$M_r = 243.33$
Orthorhombic, *Pbca*
$a = 7.0790$ (4) Å
$b = 9.9029$ (6) Å
$c = 33.0489$ (19) Å
$V = 2316.8$ (2) Å^3
$Z = 8$
$F(000) = 1040$
$D_x = 1.395$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5364 reflections
$\theta = 3.7–28.9°$
$\mu = 0.27$ mm^{-1}
$T = 293$ K
Needle, colourless
0.48 × 0.18 × 0.07 mm

Data collection

SuperNova, Dual, Cu at home/near, Atlas diffractometer
Detector resolution: 10.5082 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku, 2024)
$T_{\min} = 0.545$, $T_{\max} = 1.000$
20982 measured reflections
3038 independent reflections
2038 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.076$
$\theta_{\max} = 29.7°$, $\theta_{\min} = 3.1°$
$h = -9 \rightarrow 8$
$k = -12 \rightarrow 13$
$l = -43 \rightarrow 45$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.136$
$S = 1.09$
3038 reflections
167 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2 + 1.2175P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.35$ 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.

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

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
C1	0.3805 (3)	0.5848 (2)	0.34849 (6)	0.0293 (5)
H1	0.265632	0.575172	0.332190	0.035*
C2	0.4606 (3)	0.4428 (2)	0.35160 (7)	0.0353 (5)
H2A	0.373765	0.385546	0.366454	0.042*
H2B	0.579721	0.444867	0.366096	0.042*
C3	0.4910 (4)	0.3861 (3)	0.30934 (8)	0.0466 (6)
H3A	0.552642	0.298912	0.311366	0.056*
H3B	0.369353	0.372666	0.296438	0.056*
C4	0.6104 (4)	0.4792 (3)	0.28334 (8)	0.0537 (7)
H4A	0.737921	0.482095	0.294053	0.064*
H4B	0.616642	0.443384	0.256053	0.064*
C5	0.5306 (4)	0.6210 (3)	0.28206 (7)	0.0470 (6)
H5A	0.409229	0.619649	0.268428	0.056*
H5B	0.614785	0.678590	0.266612	0.056*
C6	0.5059 (3)	0.6795 (2)	0.32441 (7)	0.0378 (5)
H6A	0.627880	0.688390	0.337523	0.045*
H6B	0.448385	0.768242	0.322833	0.045*
C7	0.1215 (3)	0.6284 (2)	0.39842 (6)	0.0314 (5)
C8	0.4316 (3)	0.6997 (2)	0.41602 (6)	0.0320 (5)
C9	0.1762 (3)	0.7788 (2)	0.44935 (6)	0.0355 (5)
N1	0.3141 (2)	0.63940 (18)	0.38824 (5)	0.0297 (4)
N2	0.3644 (3)	0.7730 (2)	0.44638 (5)	0.0371 (5)
N3	0.0539 (3)	0.6996 (2)	0.42924 (6)	0.0364 (5)
N4	0.6155 (3)	0.6863 (2)	0.41318 (7)	0.0416 (5)
N5	0.1052 (4)	0.8655 (3)	0.47590 (7)	0.0531 (6)
S1	−0.02187 (9)	0.52678 (7)	0.37155 (2)	0.0437 (2)
H4C	0.687 (4)	0.731 (3)	0.4295 (7)	0.045 (7)*
H4D	0.678 (4)	0.637 (3)	0.3961 (8)	0.052 (8)*
H5C	0.185 (5)	0.915 (3)	0.4903 (10)	0.076 (10)*
H5D	−0.011 (4)	0.874 (3)	0.4776 (8)	0.046 (8)*
O1	0.6834 (3)	0.9457 (2)	0.47110 (6)	0.0525 (5)
H1O	0.582 (5)	0.905 (3)	0.4719 (9)	0.063*
H2O	0.654 (5)	0.993 (3)	0.4505 (9)	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0252 (12)	0.0335 (11)	0.0292 (10)	0.0015 (9)	0.0002 (9)	−0.0035 (8)
C2	0.0342 (13)	0.0314 (11)	0.0401 (13)	0.0003 (9)	0.0014 (10)	0.0002 (9)

C3	0.0475 (16)	0.0380 (13)	0.0544 (15)	0.0028 (12)	0.0037 (12)	−0.0124 (11)
C4	0.0534 (18)	0.0636 (18)	0.0442 (14)	0.0065 (14)	0.0130 (13)	−0.0130 (13)
C5	0.0467 (16)	0.0609 (17)	0.0334 (12)	−0.0022 (13)	0.0064 (11)	0.0032 (11)
C6	0.0360 (14)	0.0351 (12)	0.0423 (13)	0.0000 (10)	0.0045 (10)	0.0012 (10)
C7	0.0254 (12)	0.0305 (11)	0.0382 (12)	0.0011 (9)	0.0004 (9)	0.0015 (9)
C8	0.0290 (12)	0.0343 (12)	0.0327 (11)	−0.0013 (9)	−0.0012 (9)	0.0003 (9)
C9	0.0302 (13)	0.0441 (13)	0.0321 (11)	0.0000 (10)	0.0042 (9)	−0.0020 (10)
N1	0.0207 (9)	0.0341 (10)	0.0341 (9)	−0.0015 (8)	−0.0004 (7)	−0.0044 (7)
N2	0.0288 (11)	0.0491 (12)	0.0332 (10)	−0.0004 (9)	−0.0001 (8)	−0.0080 (9)
N3	0.0257 (10)	0.0453 (11)	0.0382 (10)	−0.0032 (8)	0.0042 (8)	−0.0079 (9)
N4	0.0243 (11)	0.0550 (14)	0.0455 (12)	0.0014 (10)	−0.0041 (9)	−0.0145 (10)
N5	0.0295 (14)	0.0732 (17)	0.0567 (14)	−0.0022 (12)	0.0078 (11)	−0.0297 (12)
S1	0.0250 (3)	0.0452 (4)	0.0609 (4)	−0.0053 (3)	0.0014 (3)	−0.0173 (3)
O1	0.0395 (12)	0.0657 (14)	0.0522 (11)	−0.0120 (9)	−0.0087 (9)	0.0006 (9)

Geometric parameters (Å, º)

C1—N1	1.496 (3)	C6—H6B	0.9700
C1—C6	1.517 (3)	C7—N3	1.328 (3)
C1—C2	1.519 (3)	C7—N1	1.408 (3)
C1—H1	0.9800	C7—S1	1.683 (2)
C2—C3	1.520 (3)	C8—N4	1.312 (3)
C2—H2A	0.9700	C8—N2	1.326 (3)
C2—H2B	0.9700	C8—N1	1.375 (3)
C3—C4	1.517 (4)	C9—N5	1.327 (3)
C3—H3A	0.9700	C9—N2	1.337 (3)
C3—H3B	0.9700	C9—N3	1.344 (3)
C4—C5	1.515 (4)	N4—H4C	0.86 (3)
C4—H4A	0.9700	N4—H4D	0.87 (3)
C4—H4B	0.9700	N5—H5C	0.89 (4)
C5—C6	1.525 (3)	N5—H5D	0.83 (3)
C5—H5A	0.9700	O1—H1O	0.82 (4)
C5—H5B	0.9700	O1—H2O	0.85 (3)
C6—H6A	0.9700		
N1—C1—C6	114.88 (17)	H5A—C5—H5B	107.9
N1—C1—C2	113.10 (17)	C1—C6—C5	108.28 (19)
C6—C1—C2	112.89 (18)	C1—C6—H6A	110.0
N1—C1—H1	104.9	C5—C6—H6A	110.0
C6—C1—H1	104.9	C1—C6—H6B	110.0
C2—C1—H1	104.9	C5—C6—H6B	110.0
C1—C2—C3	109.42 (19)	H6A—C6—H6B	108.4
C1—C2—H2A	109.8	N3—C7—N1	119.42 (19)
C3—C2—H2A	109.8	N3—C7—S1	120.31 (17)
C1—C2—H2B	109.8	N1—C7—S1	120.28 (16)
C3—C2—H2B	109.8	N4—C8—N2	117.7 (2)
H2A—C2—H2B	108.2	N4—C8—N1	120.5 (2)
C4—C3—C2	112.0 (2)	N2—C8—N1	121.7 (2)

C4—C3—H3A	109.2	N5—C9—N2	117.0 (2)
C2—C3—H3A	109.2	N5—C9—N3	117.4 (2)
C4—C3—H3B	109.2	N2—C9—N3	125.5 (2)
C2—C3—H3B	109.2	C8—N1—C7	117.35 (18)
H3A—C3—H3B	107.9	C8—N1—C1	123.59 (17)
C5—C4—C3	111.8 (2)	C7—N1—C1	119.05 (17)
C5—C4—H4A	109.3	C8—N2—C9	115.88 (19)
C3—C4—H4A	109.3	C7—N3—C9	117.17 (19)
C5—C4—H4B	109.3	C8—N4—H4C	119.0 (17)
C3—C4—H4B	109.3	C8—N4—H4D	127.5 (19)
H4A—C4—H4B	107.9	H4C—N4—H4D	114 (3)
C4—C5—C6	111.7 (2)	C9—N5—H5C	118 (2)
C4—C5—H5A	109.3	C9—N5—H5D	118.9 (19)
C6—C5—H5A	109.3	H5C—N5—H5D	123 (3)
C4—C5—H5B	109.3	H1O—O1—H2O	95 (3)
C6—C5—H5B	109.3		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*C*···N3^{i}	0.86 (3)	2.62 (3)	3.151 (3)	121 (2)
N4—H4*C*···O1	0.86 (3)	2.53 (3)	3.239 (3)	140 (2)
N4—H4*D*···S1^{i}	0.87 (3)	2.52 (3)	3.313 (2)	152 (2)
N5—H5*C*···O1^{ii}	0.89 (4)	2.09 (4)	2.967 (3)	167 (3)
N5—H5*D*···O1^{iii}	0.83 (3)	2.29 (3)	3.094 (3)	164 (3)
O1—H1*O*···N2	0.82 (4)	2.19 (3)	2.949 (3)	153 (3)
O1—H2*O*···N3^{iv}	0.85 (3)	2.61 (3)	3.325 (3)	142 (3)
O1—H2*O*···S1^{iv}	0.85 (3)	2.79 (3)	3.574 (2)	153 (3)

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+1, −*y*+2, −*z*+1; (iii) *x*−1, *y*, *z*; (iv) −*x*+1/2, *y*+1/2, *z*.