Crystal structures and Hirshfeld surface analyses of 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-N-(pyridin-2-yl)acetamide and 2-[(4,6-diaminopyrimidin-2-yl)-sulfanyl]-N-(pyrazin-2-yl)acetamide

Manisha Choudhury,[a] Vijayan Viswanathan,[a] Ajay Kumar Timiri,[b] Barij Nayan Sinha,[b] Venkatesan Jayaprakash[b] and Devadasan Velmurugan[a]*

[a]Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, and [b]Department of Pharmaceutical Science and Technology, Birla Institute of Technology, Mesta, Ranchi 835215, Jharkhand, India. *Correspondence e-mail: shirai2011@gmail.com

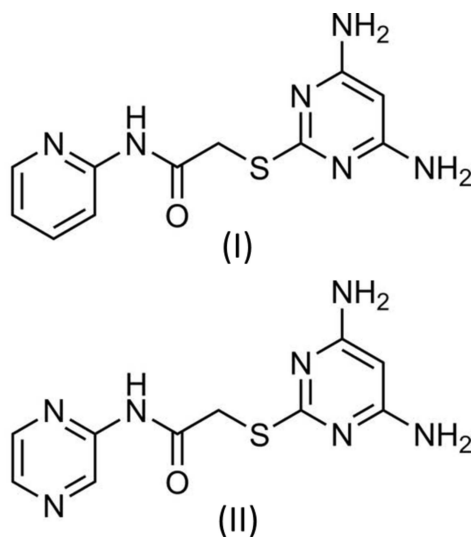In the title compounds, $C_{11}H_{12}N_6OS$ (I) and $C_{10}H_{11}N_7OS$ (II), the diamino-pyrimidine ring makes dihedral angles of 71.10 (9)° with the pyridine ring in (I) and 62.93 (15)° with the pyrazine ring in (II). The ethanamine group, $-CH_2-C(=O)-NH-$ lies in the plane of the pyridine and pyrazine rings in compounds (I) and (II), respectively. In both compounds, there is an intramolecular N—H$\cdots$N hydrogen bond forming an $S(7)$ ring motif and a short C—H$\cdots$O interaction forming an $S(6)$ loop. In the crystals of both compounds, molecules are linked by pairs of N—H$\cdots$N hydrogen bonds, forming inversion dimers with $R_2^2(8)$ ring motifs. In (I), the dimers are linked by N—H$\cdots$O and N—H$\cdots$N hydrogen bonds, forming layers parallel to ($1\overline{1}\overline{1}$). The layers are linked by offset π–π interactions [intercentroid distance = 3.777 (1) Å], forming a three-dimensional supramolecular structure. In (II), the dimers are linked by N—H$\cdots$O, N—H$\cdots$N and C—H$\cdots$O hydrogen bonds, also forming a three-dimensional supramolecular structure.

1. Chemical context

An important property of diaminopyrimidine derivatives is their inhibition potential against cancer targets. Because of the limited capacity of drugs that can cure cancer, there is always an urgent requirement for new chemotherapeutics. 2,4-Di-aminopyrimidine derivatives combined with arylthiazole derivatives have shown to possess significant anti-proliferation properties against breast cancer cell lines (Zhou *et al.*, 2015). 2,4-Diaminopyrimidine derivatives have shown significant inhibitory activity against influenza viruses (Kimura *et al.*, 2006). A series of 2,4- diaminopyrimidine derivatives were evaluated against Bacillus anthracis, which showed inhibition (Nammalwar *et al.*, 2012). Dihydrofolate reductase inhibitor drugs such as pyrimethamine, trimetrexate and piritrexim (Nelson & Rosowsky, 2001) and the antibiotics iclaprim and trimethoprim all include diaminopyrimidine as the fundamental structural motif. Diaminopyrimidine derivatives have also shown anti-retroviral activity (Hocková *et al.*, 2004), antibacterial (Kandeel *et al.*, 1994) and potential anti-microbial properties (Holla *et al.*, 2006). As part of our own studies in this area, we report herein on the syntheses, crystal structures and Hirshfeld surface analyses of the title compounds, 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-N-(pyridin-2-yl)acet-amide (I) and 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-N-(pyrazin-2-yl)acetamide (II).

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

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
N5—H5$\cdots$N3	0.86 (2)	2.18 (2)	2.975 (2)	154 (2)
C8—H8$\cdots$O1	0.93	2.31	2.894 (2)	121
N2—H2B$\cdots$N4^{i}	0.88 (2)	2.20 (2)	3.082 (2)	178 (2)
N1—H1A$\cdots$N6^{ii}	0.86 (2)	2.38 (2)	3.174 (2)	155 (2)
N2—H2A$\cdots$O1^{iii}	0.86 (2)	2.13 (2)	2.956 (2)	159 (2)

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

Table 2
Hydrogen-bond geometry (Å, °) for (II).

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
N5—H5$\cdots$N3	0.82 (3)	2.25 (3)	2.993 (4)	151 (3)
C8—H8$\cdots$O1	0.93	2.24	2.854 (4)	123
N2—H2B$\cdots$N4^{i}	1.00 (3)	2.11 (3)	3.092 (4)	169 (3)
N1—H1A$\cdots$O1^{ii}	0.86 (3)	2.06 (4)	2.904 (4)	167 (3)
N2—H2A$\cdots$N7^{iii}	0.85 (3)	2.41 (3)	3.235 (4)	164 (3)
C9—H9$\cdots$O1^{iv}	0.93	2.56	3.368 (4)	145

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $x-1, y, z$; (iv) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

2. Structural commentary

The molecular structure of compounds (I) and (II) are shown in the Figs. 1 and 2, respectively. Compound (I) crystallizes in the triclinic space group $P\bar{1}$ and compound (II) crystallizes in the monoclinic space group $P2_1/c$. In both the compounds, there is an intramolecular N—H$\cdots$N hydrogen bond forming an $S(7)$ ring motif and a short C—H$\cdots$O interaction forming an $S(6)$ loop; see Tables 1 and 2 for details of the hydrogen bonding. The nitrogen atoms N1 and N2 lie in the plane of the pyrimidine ring to which they are attached [deviations are -0.0269 (17) and 0.0521 (16) Å, respectively, for compound (I), and 0.0350 (28) and 0.0284 (28) Å, respectively, for compound (II)]. The diaminopyrimidine ring makes a dihedral angle of 71.10 (9)° with the pyridine ring in compound (I) and a dihedral angle of 62.93 (15)° with the pyrazine ring in compound (II). In (I) the ethanamine group (N5/O1/C6/C5) and the pyridine ring are coplanar, as evidenced by torsion angle C7—N5—C6—C5 = 179.1 (2)°. In (II) the ethanamine group (N5/O1/C6/C5) and pyrazine ring also lie in a plane [C7—N5—C6—C5 = 177.6 (3)°]. Bond lengths C4—S1 [1.768 (2) Å] and C5—S1 [1.802 (2) Å] for compound (I), and C4—S1 [1.768 (3) Å] and C5—S1 [1.795 (3) Å] for compound (II), are comparable with values reported for similar compounds (see Section 4. *Database survey*).

3. Supramolecular features

The crystal packing in compound (I) is illustrated in Fig. 3, and that for compound (II) in Fig. 4. Details of the hydrogen-bonding geometry in compound (I) are given in Table 1 and in
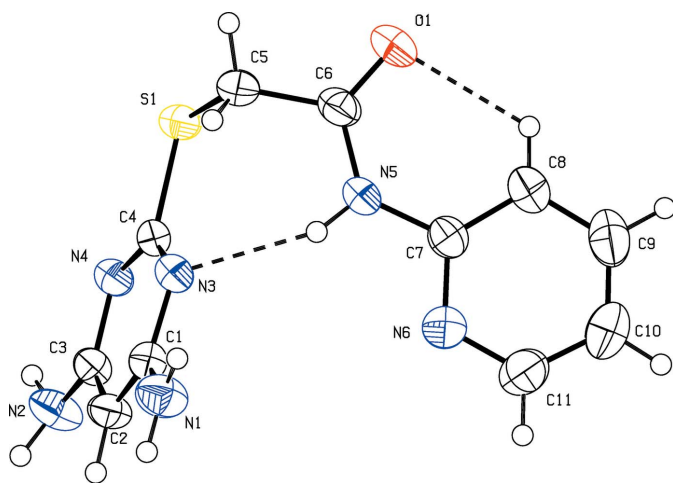

Figure 1
The molecular structure of the compound (I), showing the atom labelling and displacement ellipsoids drawn at the 50% probability level. The intramolecular N—H$\cdots$N and C—H$\cdots$O hydrogen bonds (see Table 1) are shown as dashed lines.
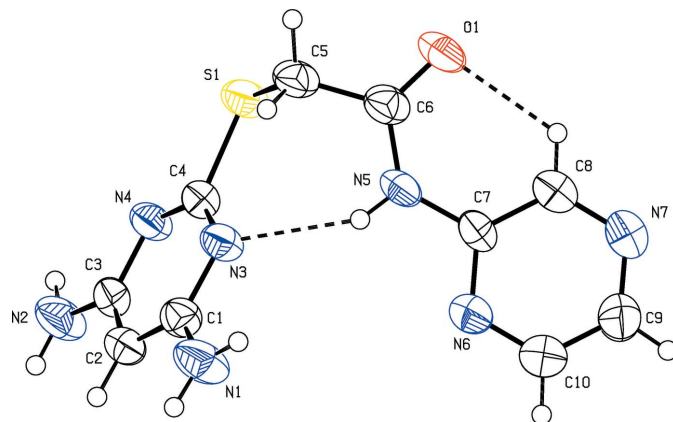

Figure 2
The molecular structure of the compound (II), showing the atom labelling and displacement ellipsoids drawn at the 50% probability level. The intramolecular N—H$\cdots$N and C—H$\cdots$O hydrogen bonds (see Table 2) are shown as dashed lines.

Table 2 for (II). In the crystals of both compounds, molecules are linked by pairs of N2—H2B$\cdots$N4^i hydrogen bonds, forming inversion dimers with $R_2^2(8)$ ring motifs (Figs. 3 and 4, respectively).

In the crystal of (I), the dimers are linked by N2—H2A$\cdots$O1^{iii} hydrogen bonds, forming ribbons along [010], enclosing $R_4^4(18)$ ring motifs. Adjacent ribbons are linked by N1—H1A$\cdots$N6^{ii} hydrogen bonds, forming sheets lying parallel to the (1$\overline{1}\overline{1}$) plane, see Fig. 3. The layers are linked by offset π–π interactions, forming a three-dimensional supramolecular structure [$Cg\cdots Cg^v$ = 3.777 (1) Å, interplanar distance = 3.483 (1) Å, slippage = 1.459 Å, Cg is the centroid of the pyridine ring (N6/C7–C11); symmetry code: (v) $-x + 1$, $-y$, $-z + 1$)].

In the crystal of (II), the dimers are linked by N1—H1A$\cdots$O^{ii}, N2—H2A$\cdots$N7^{iii} and C9—H9$\cdots$O1^{iv} hydrogen bonds (Table 2), forming a three-dimensional supramolecular structure (Fig. 4). In contrast, in the crystal of (II) there are no π–π interactions present.

4. Database survey

A search of the Cambridge Structure Database (Version 5.39, last update February 2018; Groom *et al.*, 2016) for [(4,6-di-aminopyrmidin-2-yl)sulfanyl]acetamide yielded nine hits,
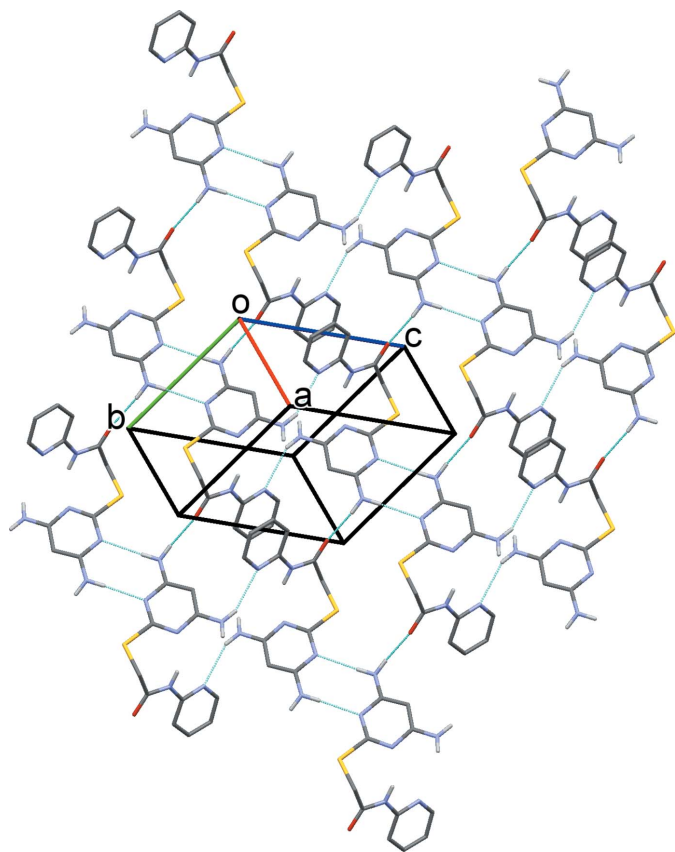

Figure 3
A view normal to the (1$\overline{1}\overline{1}$) plane of the crystal packing of compound (I). The hydrogen bonds (see Table 1) are shown as dashed lines and C-bound H atoms have been omitted for clarity.

Figure 4
A view along the *a* axis of the crystal packing of compound (II). The hydrogen bonds (see Table 2) are shown as dashed lines, and C-bound H atoms have been omitted for clarity.

eight of which have a substituted phenyl substituent in place of the pyridine ring in (I) and the pyrazine ring in (II), and one a naphthalene group (JARPOK; Subasri *et al.*, 2017a). They include the following analogues: 3-nitrophenyl (ARAROC; Subasri *et al.*, 2016), 2-chlorophenyl (ARARUI; Subasri *et al.*, 2016), 2-methylphenyl (GOKWIO; Subasri *et al.*, 2014), 4-fluorophenyl (JARPUQ; Subasri *et al.*, 2017a), 2,4-di-methylphenyl (JAXFIA; Choudhury *et al.*, 2017), 3-methoxy-phenyl (JAXFOG; Choudhury *et al.*, 2017), 4-chlorophenyl (KAPQIE; Subasri *et al.*, 2017b), and 3-chlorophenyl (KAPQOK; Subasri *et al.*, 2017b).

In these eight compounds, the diaminopyrimidine and benzene rings are inclined to one another by dihedral angles varying from *ca* 42.25 to 78.33°. The dihedral angle between the diaminopyrimidine and the pyridine ring in (I) is 71.10 (9)° and with the pyrazine ring in (II) is 62.93 (15)°, well within these limits. As in the title compounds, there is also an intra-molecular N—H$\cdots$N hydrogen bond present in all eight compounds, stabilizing the folded conformation of each mol-ecule. In the crystals of all but two compounds (ARAROC and JARPUQ), molecules are linked by pairs of N—H$\cdots$N

Figure 5
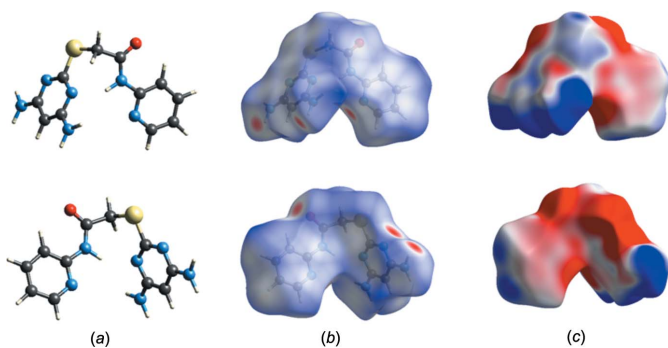Ball and stick, Hirshfeld surface and electrostatic potential surface diagrams for compound (I).

5. Hirshfeld surface analysis

In Figs. 5 and 6, the ball and stick model of the front and back views of the compounds (I) and (II), respectively, and the intermolecular contacts are shown by conventional mapping of d_{norm} on the molecular Hirshfeld surfaces, where the red-spot areas denote intermolecular contacts involved in the hydrogen-bonding interactions (McKinnon *et al.*, 2007). The electrostatic potential is mapped on the Hirshfeld surface using the STO-3G basis set at the Hartree–Fock theory over the range of ±0.025 a.u. The positive electrostatic potential (blue region) over the surface shows hydrogen-donor potential, and the hydrogen-bond acceptors are shown by negative electrostatic potential (red regions); see Figs. 5 and 6. The two-dimensional fingerprint plots [Fig. 7 for (I) and Fig. 8 for (II)] are deconvoluted to highlight atom-pair close contacts by which different atomic types, overlapping the full fingerprint can be separated based on different interaction types. For compound (I), intermolecular H⋯H contacts of 39.1% are the most significant, followed by 17.7% for N⋯H/H⋯N, 12% for C⋯H/H⋯C, 9.3% for O⋯H/H⋯O, 8.4% for S⋯H/H⋯S and 4.1% for C⋯C contacts. In contrast, for compound

Figure 6
Ball and stick, Hirshfeld surface and electrostatic potential surface diagrams for compound (II).

Figure 7
The 2D fingerprint plot for all the intermolecular contacts for compound (I).

(II) the H⋯H contacts at 28.2% are significantly lower than in (I), while the N⋯H/H⋯N contacts at 27% are significantly higher than in (I). The C⋯C contacts at only 1.9% are much lower than in (I) where offset π–π interactions are observed in the crystal structure.

6. Synthesis and crystallization

Compound (I): To a solution of 4, 6-diamino-pyrimidine-2-thiol (0.5 g; 3.52 mmol) in 25 ml of ethanol, (0.2g; 3.52 mmol) potassium hydroxide was added and refluxed for about 30 min. Then an equimolar quantity of 2-chloro-*N*-(pyridin-2-yl)acetamide (3.52 mmol) was added to the above reaction mixture and it was refluxed for 5 h. Evaporation of the organic layer under vacuum provided compound (I). After purification, the compound was crystallized from ethanol solution by slow evaporation of the solvent giving yellow block-like crystals.

Compound (II): To a solution of 4, 6-diamino-pyrimidine-2-thiol (0.5 g; 3.52 mmol) in 25 ml of ethanol, (0.2g; 3.52 mmol) potassium hydroxide was added and refluxed for about

Figure 8
The 2D fingerprint plot for all the intermolecular contacts for compound (II).

Table 3
Experimental details.

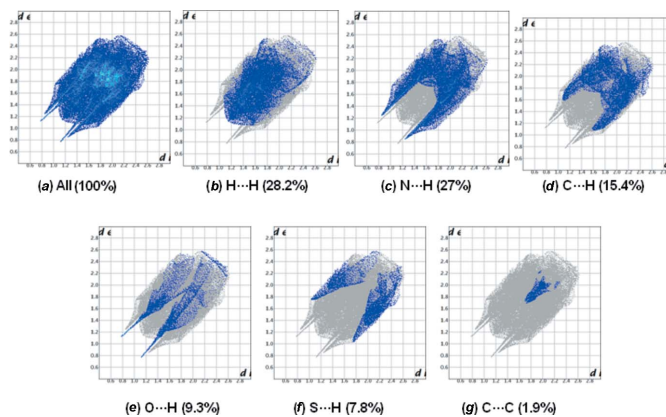|	(I)	(II)
Crystal data		
Chemical formula	$C_{11}H_{12}N_6OS$	$C_{10}H_{11}N_7OS$
M_r	276.33	277.32
Crystal system, space group	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/n$
Temperature (K)	293	293
a, b, c (Å)	7.2341 (2), 9.3852 (2), 9.7971 (2)	12.1333 (5), 8.1561 (3), 12.8442 (5)
α, β, γ (°)	95.820 (1), 91.116 (1), 105.682 (1)	90, 94.307 (3), 90
V (Å^3)	636.33 (3)	1267.48 (9)
Z	2	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.26	0.26
Crystal size (mm)	$0.30 \times 0.25 \times 0.20$	$0.28 \times 0.25 \times 0.20$
Data collection		
Diffractometer	Bruker SMART APEXII area-detector	Bruker SMART APEXII area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.742, 0.841	0.723, 0.863
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9447, 2605, 2160	11968, 3124, 1320
R_{int}	0.020	0.084
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.626	0.667
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.094, 1.05	0.054, 0.126, 0.94
No. of reflections	2605	3124
No. of parameters	192	192
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.23, −0.20	0.20, −0.23

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

30 min. Then an equimolar quantity of 2-chloro-*N*-(pyrazin-2-yl)acetamide (3.52 mmol) was added to the above reaction mixture and it was refluxed for 5.5 h. Evaporation of the organic layer under vacuum resulted in compound (II). After purification, the compound was crystallized from ethanol solution by slow evaporation of the solvent giving yellow block-like crystals.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. For both compounds, the NH$_2$ and NH H atoms were located in difference-Fourier maps and freely refined, and the C-bound H atoms were placed in calculated positions and refined in the riding model: C—H = 0.93–0.97 Å with U_{iso}(H) = 1.2U_{eq}(C).

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supporting information

Crystal structures and Hirshfeld surface analyses of 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(pyridin-2-yl)acetamide and 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(pyrazin-2-yl)acetamide

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Computing details

For both structures, data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2016* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

2-[(4,6-Diaminopyrimidin-2-yl)sulfanyl]-*N*-(pyridin-2-yl)acetamide (I)

Crystal data

$C_{11}H_{12}N_6OS$	$Z = 2$
$M_r = 276.33$	$F(000) = 288$
Triclinic, $P\overline{1}$	$D_x = 1.442$ Mg m^{-3}
$a = 7.2341$ (2) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 9.3852$ (2) Å	Cell parameters from 2605 reflections
$c = 9.7971$ (2) Å	$\theta = 2.1$–26.4°
$\alpha = 95.820$ (1)°	$\mu = 0.26$ mm^{-1}
$\beta = 91.116$ (1)°	$T = 293$ K
$\gamma = 105.682$ (1)°	Block, yellow
$V = 636.33$ (3) Å^3	0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEXII area-detector diffractometer	2605 independent reflections
Radiation source: X-ray	2160 reflections with $I > 2\sigma(I)$
ω and φ scans	$R_{int} = 0.020$
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)	$\theta_{max} = 26.4°$, $\theta_{min} = 2.1°$
	$h = -9 \rightarrow 9$
	$k = -11 \rightarrow 11$
$T_{min} = 0.742$, $T_{max} = 0.841$	$l = -10 \rightarrow 12$
9447 measured reflections	

Refinement

Refinement on F^2	2605 reflections
Least-squares matrix: full	192 parameters
$R[F^2 > 2\sigma(F^2)] = 0.034$	0 restraints
$wR(F^2) = 0.094$	Primary atom site location: structure-invariant
$S = 1.05$	direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 0.1669P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	0.47564 (6)	0.24187 (5)	0.97878 (4)	0.04443 (15)
O1	0.1201 (2)	−0.07191 (14)	0.81504 (14)	0.0637 (4)
N1	0.4212 (3)	0.58093 (19)	0.63223 (17)	0.0509 (4)
H1A	0.470 (3)	0.652 (2)	0.584 (2)	0.059 (6)*
H1B	0.299 (3)	0.546 (2)	0.641 (2)	0.066 (7)*
N2	1.0373 (2)	0.60541 (19)	0.83751 (19)	0.0500 (4)
H2A	1.087 (3)	0.696 (2)	0.820 (2)	0.059 (6)*
H2B	1.092 (3)	0.590 (2)	0.914 (2)	0.071 (7)*
N3	0.45530 (19)	0.42030 (14)	0.78589 (14)	0.0378 (3)
N4	0.75997 (18)	0.44133 (14)	0.89781 (13)	0.0374 (3)
N5	0.2555 (2)	0.10689 (16)	0.67916 (14)	0.0395 (3)
H5	0.304 (3)	0.201 (2)	0.6830 (18)	0.046 (5)*
N6	0.3287 (2)	0.11118 (16)	0.45436 (15)	0.0458 (4)
C1	0.5404 (2)	0.53494 (17)	0.71413 (16)	0.0373 (4)
C2	0.7366 (2)	0.59919 (18)	0.72509 (17)	0.0398 (4)
H2	0.795008	0.672763	0.670694	0.048*
C3	0.8435 (2)	0.55043 (16)	0.81970 (16)	0.0367 (4)
C4	0.5717 (2)	0.38421 (16)	0.87394 (15)	0.0351 (4)
C5	0.2265 (2)	0.17793 (19)	0.91965 (17)	0.0452 (4)
H5A	0.149123	0.139634	0.994486	0.054*
H5B	0.185101	0.261192	0.891905	0.054*
C6	0.1943 (2)	0.05740 (18)	0.80001 (18)	0.0415 (4)
C7	0.2500 (2)	0.02603 (17)	0.55029 (17)	0.0369 (4)
C8	0.1697 (3)	−0.12615 (19)	0.5237 (2)	0.0506 (4)
H8	0.118824	−0.182978	0.593511	0.061*
C9	0.1674 (3)	−0.1909 (2)	0.3911 (2)	0.0603 (5)
H9	0.113148	−0.292746	0.369861	0.072*
C10	0.2447 (3)	−0.1056 (2)	0.2905 (2)	0.0574 (5)
H10	0.243138	−0.147400	0.200125	0.069*
C11	0.3246 (3)	0.0435 (2)	0.32694 (19)	0.0551 (5)
H11	0.379420	0.101358	0.258857	0.066*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0510 (3)	0.0393 (2)	0.0344 (2)	−0.00414 (19)	0.00358 (18)	0.00918 (17)
O1	0.0848 (10)	0.0348 (7)	0.0585 (8)	−0.0084 (6)	0.0102 (7)	0.0109 (6)
N1	0.0466 (10)	0.0522 (10)	0.0532 (10)	0.0079 (8)	−0.0012 (8)	0.0183 (8)
N2	0.0377 (8)	0.0444 (9)	0.0648 (11)	0.0003 (7)	0.0006 (7)	0.0222 (8)
N3	0.0399 (7)	0.0308 (7)	0.0382 (7)	0.0019 (6)	0.0022 (6)	0.0041 (5)
N4	0.0404 (8)	0.0310 (7)	0.0369 (7)	0.0020 (6)	0.0018 (6)	0.0064 (5)
N5	0.0438 (8)	0.0288 (7)	0.0397 (8)	−0.0008 (6)	0.0032 (6)	0.0044 (6)
N6	0.0523 (9)	0.0425 (8)	0.0418 (8)	0.0106 (7)	0.0039 (7)	0.0070 (6)
C1	0.0443 (9)	0.0331 (8)	0.0332 (8)	0.0084 (7)	0.0034 (7)	0.0030 (6)
C2	0.0427 (9)	0.0349 (8)	0.0411 (9)	0.0058 (7)	0.0085 (7)	0.0127 (7)
C3	0.0395 (9)	0.0281 (8)	0.0397 (9)	0.0042 (6)	0.0063 (7)	0.0040 (6)
C4	0.0427 (9)	0.0266 (7)	0.0311 (8)	0.0022 (6)	0.0056 (7)	−0.0004 (6)
C5	0.0451 (10)	0.0417 (9)	0.0412 (9)	−0.0018 (7)	0.0134 (8)	0.0050 (7)
C6	0.0385 (9)	0.0354 (9)	0.0458 (10)	0.0003 (7)	0.0037 (7)	0.0087 (7)
C7	0.0319 (8)	0.0358 (8)	0.0419 (9)	0.0079 (6)	−0.0010 (7)	0.0038 (7)
C8	0.0531 (11)	0.0375 (9)	0.0546 (11)	0.0026 (8)	0.0031 (9)	0.0009 (8)
C9	0.0629 (13)	0.0441 (11)	0.0672 (13)	0.0099 (9)	−0.0011 (10)	−0.0111 (9)
C10	0.0611 (12)	0.0643 (13)	0.0488 (11)	0.0266 (10)	−0.0007 (9)	−0.0100 (10)
C11	0.0636 (12)	0.0607 (12)	0.0436 (10)	0.0204 (10)	0.0081 (9)	0.0073 (9)

Geometric parameters (Å, º)

S1—C4	1.7682 (15)	N6—C7	1.332 (2)
S1—C5	1.8021 (18)	N6—C11	1.338 (2)
O1—C6	1.2124 (19)	C1—C2	1.381 (2)
N1—C1	1.348 (2)	C2—C3	1.384 (2)
N1—H1A	0.86 (2)	C2—H2	0.9300
N1—H1B	0.86 (2)	C5—C6	1.512 (2)
N2—C3	1.358 (2)	C5—H5A	0.9700
N2—H2A	0.86 (2)	C5—H5B	0.9700
N2—H2B	0.88 (2)	C7—C8	1.384 (2)
N3—C4	1.324 (2)	C8—C9	1.376 (3)
N3—C1	1.358 (2)	C8—H8	0.9300
N4—C4	1.328 (2)	C9—C10	1.365 (3)
N4—C3	1.3570 (19)	C9—H9	0.9300
N5—C6	1.354 (2)	C10—C11	1.368 (3)
N5—C7	1.400 (2)	C10—H10	0.9300
N5—H5	0.856 (19)	C11—H11	0.9300
C4—S1—C5	102.83 (8)	C6—C5—S1	111.72 (12)
C1—N1—H1A	118.3 (14)	C6—C5—H5A	109.3
C1—N1—H1B	117.3 (15)	S1—C5—H5A	109.3
H1A—N1—H1B	124 (2)	C6—C5—H5B	109.3
C3—N2—H2A	117.2 (13)	S1—C5—H5B	109.3
C3—N2—H2B	117.6 (15)	H5A—C5—H5B	107.9

H2A—N2—H2B	110 (2)	O1—C6—N5	124.47 (16)
C4—N3—C1	114.94 (13)	O1—C6—C5	121.07 (15)
C4—N4—C3	115.04 (13)	N5—C6—C5	114.46 (14)
C6—N5—C7	129.23 (14)	N6—C7—C8	123.05 (16)
C6—N5—H5	114.6 (12)	N6—C7—N5	112.92 (13)
C7—N5—H5	116.2 (12)	C8—C7—N5	124.02 (15)
C7—N6—C11	116.91 (15)	C9—C8—C7	118.03 (18)
N1—C1—N3	115.65 (15)	C9—C8—H8	121.0
N1—C1—C2	122.72 (15)	C7—C8—H8	121.0
N3—C1—C2	121.63 (15)	C10—C9—C8	120.00 (18)
C1—C2—C3	117.79 (14)	C10—C9—H9	120.0
C1—C2—H2	121.1	C8—C9—H9	120.0
C3—C2—H2	121.1	C9—C10—C11	117.86 (18)
N4—C3—N2	116.08 (15)	C9—C10—H10	121.1
N4—C3—C2	121.51 (14)	C11—C10—H10	121.1
N2—C3—C2	122.39 (15)	N6—C11—C10	124.13 (18)
N3—C4—N4	128.88 (14)	N6—C11—H11	117.9
N3—C4—S1	119.16 (12)	C10—C11—H11	117.9
N4—C4—S1	111.95 (12)		
C4—N3—C1—N1	−174.86 (14)	C7—N5—C6—O1	−0.5 (3)
C4—N3—C1—C2	5.2 (2)	C7—N5—C6—C5	179.12 (15)
N1—C1—C2—C3	175.39 (15)	S1—C5—C6—O1	105.06 (17)
N3—C1—C2—C3	−4.7 (2)	S1—C5—C6—N5	−74.58 (17)
C4—N4—C3—N2	−176.87 (14)	C11—N6—C7—C8	1.2 (2)
C4—N4—C3—C2	1.5 (2)	C11—N6—C7—N5	−178.11 (15)
C1—C2—C3—N4	1.2 (2)	C6—N5—C7—N6	−178.11 (16)
C1—C2—C3—N2	179.38 (15)	C6—N5—C7—C8	2.5 (3)
C1—N3—C4—N4	−2.5 (2)	N6—C7—C8—C9	−1.7 (3)
C1—N3—C4—S1	177.30 (10)	N5—C7—C8—C9	177.57 (17)
C3—N4—C4—N3	−0.8 (2)	C7—C8—C9—C10	0.7 (3)
C3—N4—C4—S1	179.39 (10)	C8—C9—C10—C11	0.7 (3)
C5—S1—C4—N3	3.32 (14)	C7—N6—C11—C10	0.2 (3)
C5—S1—C4—N4	−176.85 (11)	C9—C10—C11—N6	−1.2 (3)
C4—S1—C5—C6	87.65 (13)		

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N5—H5⋯N3	0.86 (2)	2.18 (2)	2.975 (2)	154 (2)
C8—H8⋯O1	0.93	2.31	2.894 (2)	121
N2—H2B⋯N4[i]	0.88 (2)	2.20 (2)	3.082 (2)	178 (2)
N1—H1A⋯N6[ii]	0.86 (2)	2.38 (2)	3.174 (2)	155 (2)
N2—H2A⋯O1[iii]	0.86 (2)	2.13 (2)	2.956 (2)	159 (2)

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

2-[(4,6-Diaminopyrimidin-2-yl)sulfanyl]-*N*-(pyrazin-2-yl)acetamide (II)

Crystal data

$C_{10}H_{11}N_7OS$	$F(000) = 576$
$M_r = 277.32$	$D_x = 1.453$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 12.1333$ (5) Å	Cell parameters from 3124 reflections
$b = 8.1561$ (3) Å	$\theta = 2.2–28.3°$
$c = 12.8442$ (5) Å	$\mu = 0.26$ mm^{-1}
$\beta = 94.307$ (3)°	$T = 293$ K
$V = 1267.48$ (9) Å^3	Block, yellow
$Z = 4$	$0.28 \times 0.25 \times 0.20$ mm

Data collection

Bruker SMART APEXII area-detector diffractometer	3124 independent reflections
Radiation source: X-ray	1320 reflections with $I > 2\sigma(I)$
ω and φ scans	$R_{int} = 0.084$
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)	$\theta_{max} = 28.3°$, $\theta_{min} = 2.2°$
$T_{min} = 0.723$, $T_{max} = 0.863$	$h = -16 \rightarrow 12$
11968 measured reflections	$k = -10 \rightarrow 9$
	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)] = 0.054$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.126$	$w = 1/[\sigma^2(F_o^2) + (0.0452P)^2]$
$S = 0.94$	where $P = (F_o^2 + 2F_c^2)/3$
3124 reflections	$(\Delta/\sigma)_{max} = 0.001$
192 parameters	$\Delta\rho_{max} = 0.20$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.23$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	0.77107 (6)	0.20394 (11)	0.50448 (6)	0.0525 (3)
O1	1.06221 (18)	0.2503 (3)	0.55054 (17)	0.0779 (8)
N1	0.6951 (3)	0.2961 (4)	0.8740 (2)	0.0651 (9)
H1A	0.651 (3)	0.297 (4)	0.923 (3)	0.084 (13)*
H1B	0.760 (3)	0.342 (4)	0.881 (3)	0.079 (13)*
N2	0.4369 (2)	0.0046 (4)	0.6423 (3)	0.0635 (9)
H2A	0.391 (2)	−0.015 (4)	0.687 (2)	0.060 (11)*
H2B	0.423 (2)	−0.044 (4)	0.571 (3)	0.080 (11)*
N3	0.72886 (19)	0.2473 (3)	0.70403 (17)	0.0452 (7)

N4	0.59901 (19)	0.1011 (3)	0.58901 (17)	0.0463 (7)
N5	0.9712 (2)	0.1889 (3)	0.69294 (19)	0.0494 (7)
H5	0.912 (2)	0.197 (4)	0.719 (2)	0.057 (11)*
N6	1.0164 (2)	0.0445 (3)	0.84291 (19)	0.0545 (7)
N7	1.2266 (2)	−0.0273 (4)	0.7815 (2)	0.0659 (8)
C1	0.6580 (3)	0.2321 (4)	0.7813 (2)	0.0450 (8)
C2	0.5579 (2)	0.1540 (4)	0.7649 (2)	0.0466 (8)
H2	0.509877	0.146453	0.817830	0.056*
C3	0.5306 (2)	0.0872 (4)	0.6680 (2)	0.0438 (8)
C4	0.6909 (2)	0.1845 (4)	0.6132 (2)	0.0421 (7)
C5	0.8779 (2)	0.3427 (4)	0.5525 (2)	0.0497 (9)
H5A	0.897729	0.412594	0.495784	0.060*
H5B	0.849528	0.412281	0.605640	0.060*
C6	0.9796 (3)	0.2561 (4)	0.5981 (2)	0.0499 (9)
C7	1.0498 (2)	0.0968 (4)	0.7528 (2)	0.0440 (8)
C8	1.1544 (3)	0.0605 (4)	0.7222 (3)	0.0613 (10)
H8	1.174535	0.098921	0.658172	0.074*
C9	1.1922 (3)	−0.0808 (4)	0.8710 (3)	0.0610 (10)
H9	1.239366	−0.144894	0.914481	0.073*
C10	1.0895 (3)	−0.0446 (4)	0.9011 (2)	0.0598 (9)
H10	1.069630	−0.083866	0.965011	0.072*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0478 (5)	0.0731 (6)	0.0376 (4)	−0.0116 (5)	0.0092 (3)	−0.0006 (4)
O1	0.0459 (15)	0.134 (3)	0.0572 (14)	0.0005 (14)	0.0236 (12)	0.0208 (14)
N1	0.062 (2)	0.091 (2)	0.0445 (17)	−0.021 (2)	0.0163 (16)	−0.0161 (17)
N2	0.0446 (19)	0.090 (3)	0.0569 (19)	−0.0240 (17)	0.0124 (16)	−0.0020 (18)
N3	0.0437 (16)	0.0552 (19)	0.0379 (13)	−0.0049 (12)	0.0104 (12)	−0.0024 (12)
N4	0.0372 (15)	0.0617 (18)	0.0408 (14)	−0.0088 (14)	0.0095 (12)	−0.0002 (13)
N5	0.0379 (18)	0.069 (2)	0.0428 (15)	−0.0018 (16)	0.0162 (13)	0.0043 (14)
N6	0.0478 (17)	0.072 (2)	0.0447 (15)	0.0030 (15)	0.0119 (13)	0.0055 (14)
N7	0.0512 (19)	0.079 (2)	0.0690 (19)	0.0126 (17)	0.0169 (15)	0.0064 (17)
C1	0.049 (2)	0.046 (2)	0.0402 (16)	0.0041 (16)	0.0087 (15)	−0.0021 (15)
C2	0.042 (2)	0.058 (2)	0.0416 (17)	−0.0005 (17)	0.0110 (14)	0.0027 (15)
C3	0.0338 (19)	0.049 (2)	0.0493 (18)	0.0015 (16)	0.0076 (15)	0.0061 (16)
C4	0.0395 (19)	0.047 (2)	0.0410 (16)	0.0036 (16)	0.0083 (14)	0.0024 (15)
C5	0.047 (2)	0.055 (2)	0.0479 (18)	−0.0136 (16)	0.0103 (15)	0.0067 (15)
C6	0.044 (2)	0.061 (2)	0.0449 (18)	−0.0142 (17)	0.0067 (16)	0.0004 (16)
C7	0.0338 (19)	0.053 (2)	0.0463 (18)	−0.0016 (16)	0.0105 (15)	−0.0048 (16)
C8	0.053 (2)	0.076 (3)	0.057 (2)	0.007 (2)	0.0187 (18)	0.0088 (19)
C9	0.054 (2)	0.073 (3)	0.057 (2)	0.012 (2)	0.0051 (17)	0.0020 (19)
C10	0.061 (3)	0.069 (3)	0.0508 (19)	0.002 (2)	0.0107 (18)	0.0063 (19)

Geometric parameters (Å, º)

S1—C4	1.768 (3)	N6—C7	1.325 (3)
S1—C5	1.795 (3)	N6—C10	1.331 (4)
O1—C6	1.213 (3)	N7—C8	1.326 (4)
N1—C1	1.346 (4)	N7—C9	1.326 (4)
N1—H1A	0.86 (3)	C1—C2	1.374 (4)
N1—H1B	0.88 (3)	C2—C3	1.375 (4)
N2—C3	1.341 (4)	C2—H2	0.9300
N2—H2A	0.85 (3)	C5—C6	1.502 (4)
N2—H2B	1.00 (3)	C5—H5A	0.9700
N3—C4	1.325 (3)	C5—H5B	0.9700
N3—C1	1.367 (3)	C7—C8	1.389 (4)
N4—C4	1.323 (3)	C8—H8	0.9300
N4—C3	1.364 (3)	C9—C10	1.364 (4)
N5—C6	1.347 (4)	C9—H9	0.9300
N5—C7	1.398 (4)	C10—H10	0.9300
N5—H5	0.82 (3)		
C4—S1—C5	102.17 (14)	N4—C4—S1	111.4 (2)
C1—N1—H1A	118 (2)	N3—C4—S1	119.0 (2)
C1—N1—H1B	120 (2)	C6—C5—S1	112.8 (2)
H1A—N1—H1B	122 (3)	C6—C5—H5A	109.0
C3—N2—H2A	121 (2)	S1—C5—H5A	109.0
C3—N2—H2B	120.4 (17)	C6—C5—H5B	109.0
H2A—N2—H2B	118 (3)	S1—C5—H5B	109.0
C4—N3—C1	114.1 (2)	H5A—C5—H5B	107.8
C4—N4—C3	114.7 (3)	O1—C6—N5	124.1 (3)
C6—N5—C7	128.4 (3)	O1—C6—C5	120.5 (3)
C6—N5—H5	118 (2)	N5—C6—C5	115.4 (3)
C7—N5—H5	114 (2)	N6—C7—C8	121.7 (3)
C7—N6—C10	115.5 (3)	N6—C7—N5	114.4 (3)
C8—N7—C9	116.0 (3)	C8—C7—N5	124.0 (3)
N1—C1—N3	114.9 (3)	N7—C8—C7	122.1 (3)
N1—C1—C2	123.3 (3)	N7—C8—H8	119.0
N3—C1—C2	121.9 (3)	C7—C8—H8	119.0
C1—C2—C3	118.2 (3)	N7—C9—C10	121.9 (3)
C1—C2—H2	120.9	N7—C9—H9	119.1
C3—C2—H2	120.9	C10—C9—H9	119.1
N2—C3—N4	114.2 (3)	N6—C10—C9	122.9 (3)
N2—C3—C2	124.3 (3)	N6—C10—H10	118.5
N4—C3—C2	121.4 (3)	C9—C10—H10	118.5
N4—C4—N3	129.6 (3)		
C4—N3—C1—N1	−179.7 (3)	C7—N5—C6—O1	−2.8 (5)
C4—N3—C1—C2	1.7 (4)	C7—N5—C6—C5	177.6 (3)
N1—C1—C2—C3	−177.3 (3)	S1—C5—C6—O1	105.2 (3)
N3—C1—C2—C3	1.3 (5)	S1—C5—C6—N5	−75.2 (3)

C4—N4—C3—N2	179.0 (3)	C10—N6—C7—C8	−0.1 (5)
C4—N4—C3—C2	−0.9 (4)	C10—N6—C7—N5	179.5 (3)
C1—C2—C3—N2	178.4 (3)	C6—N5—C7—N6	−178.8 (3)
C1—C2—C3—N4	−1.7 (5)	C6—N5—C7—C8	0.8 (5)
C3—N4—C4—N3	4.6 (5)	C9—N7—C8—C7	1.1 (5)
C3—N4—C4—S1	−177.3 (2)	N6—C7—C8—N7	−0.4 (5)
C1—N3—C4—N4	−5.0 (5)	N5—C7—C8—N7	180.0 (3)
C1—N3—C4—S1	177.1 (2)	C8—N7—C9—C10	−1.3 (5)
C5—S1—C4—N4	172.4 (2)	C7—N6—C10—C9	−0.1 (5)
C5—S1—C4—N3	−9.3 (3)	N7—C9—C10—N6	0.9 (5)
C4—S1—C5—C6	93.4 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5···N3	0.82 (3)	2.25 (3)	2.993 (4)	151 (3)
C8—H8···O1	0.93	2.24	2.854 (4)	123
N2—H2*B*···N4[i]	1.00 (3)	2.11 (3)	3.092 (4)	169 (3)
N1—H1*A*···O1[ii]	0.86 (3)	2.06 (4)	2.904 (4)	167 (3)
N2—H2*A*···N7[iii]	0.85 (3)	2.41 (3)	3.235 (4)	164 (3)
C9—H9···O1[iv]	0.93	2.56	3.368 (4)	145

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) *x*−1/2, −*y*+1/2, *z*+1/2; (iii) *x*−1, *y*, *z*; (iv) −*x*+5/2, *y*−1/2, −*z*+3/2.