



Crystal structures of 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(2,4-dimethylphenyl)acetamide and 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(3-methoxyphenyl)acetamide

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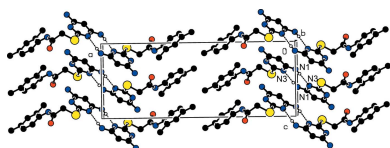
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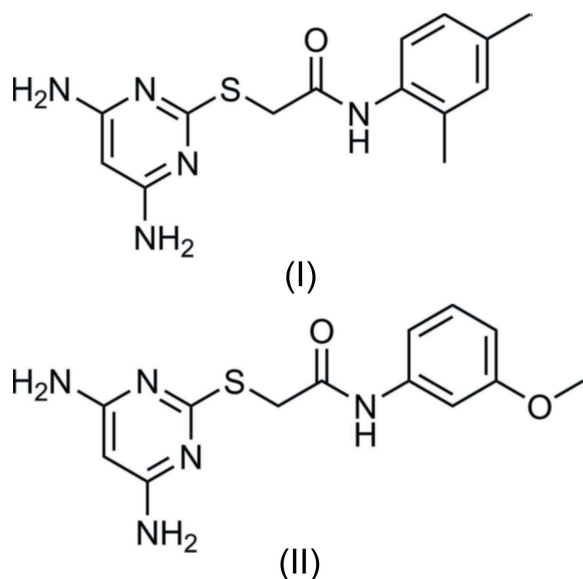
In the title compounds, C₁₄H₁₇N₅OS (I) and C₁₃H₁₅N₅O₂S (II), the dihedral angle between the pyrimidine and benzene rings is 58.64 (8)° in (I) and 78.33 (9)° in (II). In both compounds, there is an intramolecular C—H···O hydrogen bond, and in (II) there is also an intramolecular N—H···N hydrogen bond present. In the crystals of both compounds, a pair of N—H···N hydrogen bonds links the individual molecules to form inversion dimers with *R*₂²(8) ring motifs. In (I), the dimers are linked by N—H···O and C—H···O hydrogen bonds, enclosing *R*₂¹(14), *R*₂¹(11) and *R*₂¹(7) ring motifs, forming layers parallel to the (100) plane. There is also an N—H···π interaction present within the layer. In (II), the inversion dimers are linked by N—H···O hydrogen bonds enclosing an *R*₄¹(18) ring motif. The presence of N—H···O and C—H···O hydrogen bonds generate an *R*₂¹(6) ring motif. The combination of these various hydrogen bonds results in the formation of layers parallel to the (111) plane.

1. Chemical context

Diaminopyrimidine derivatives have been proved to be an important class of compounds because of their therapeutic and pharmacological properties. One such important property is its inhibition potency against cancer targets. As a result of the limited capacity of drugs that can cure or at least prolong the survival of cancer patients, there is always a strong requirement for new chemotherapeutics. It has been reported that diaminopyrimidines show inhibition against cyclin-dependent kinases (cdks), thus arresting cell proliferation in cancer cells (Mesguiche *et al.*, 2003). 2,4-Diaminopyrimidine derivatives have also shown effective suppression of anaplastic lymphoma kinase (ALK), one of the receptor tyrosine kinases that is involved in a variety of tumours (Achary *et al.*, 2017). 2,4-Diaminopyrimidine derivatives have also been reported to exhibit potent inhibitory activity against influenza viruses (Kimura *et al.*, 2006) and have anti-retroviral activity (Hocková *et al.*, 2004), anti-bacterial (Kandeel *et al.*, 1994) and potential anti-microbial properties (Holla *et al.*, 2006). Several diaminopyrimidine derivatives have shown good activity, efficiency against the malarial parasite *Plasmodium falciparum* K1 strain (Phuangasawai *et al.*, 2016; Chiang *et al.*, 2009). Interestingly, they also act as calcium channel blocking agents (Manjula *et al.*, 2004; Singh *et al.*, 2009). As part of our own studies in this area, we report herein on the syntheses and



crystal structure analyses of the title compounds, 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(2,4-dimethylphenyl)acetamide (I) and [2-((4,6-diaminopyrimidin-2-yl)sulfanyl)-*N*-(3-methoxyphenyl)acetamide (II).



2. Structural commentary

The molecular structures of compounds (I) and (II) are shown in Figs. 1 and 2, respectively. Compound (I) crystallizes in the monoclinic space group $P2_1/c$ and compound (II) in the triclinic space group $P\bar{1}$. In compounds (I) and (II), the diaminopyrimidine and benzene rings are inclined to one another by $58.64(8)$ and $78.33(9)^\circ$, respectively. The torsion angle $C4-S1-C5-C6 = 98.12(11)^\circ$ in compound (I) and $-80.14(14)^\circ$ in compound (II), torsion angles $S1-C5-C6-N5 = -101.92(14)^\circ$ in compound (I) and $82.23(16)^\circ$ in compound (II), and $C5-C6-N5-C7 = 178.66(15)^\circ$ in compound (I) and $-172.71(14)^\circ$ in compound (II). The bond lengths $C4-S1 = 1.7650(14)$ Å and $C5-S1 = 1.8053(16)$ Å in compound (I), and $C4-S1 = 1.7721(17)$ Å and $C5-S1 = 1.8126(18)$ Å in compound (II), are comparable with the

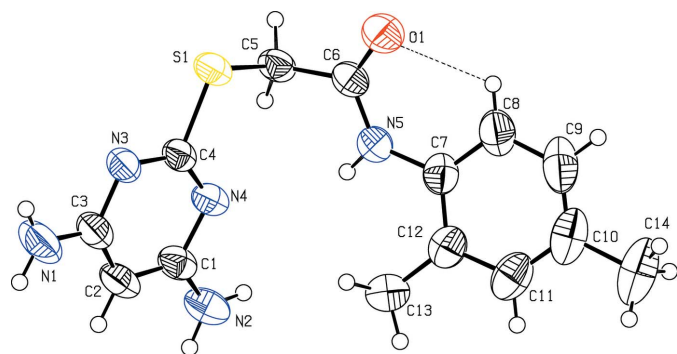


Figure 1

The molecular structure of (I), showing the atom labelling and displacement ellipsoids drawn at 50% probability level. The $C-H \cdots O$ contact is shown as a dashed line (see Table 1).

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

$Cg1$ is the centroid of the $N3/N4/C1-C4$ ring.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C8-H8 \cdots O1$	0.93	2.30	2.8752 (1)	120
$N1-H1A \cdots N3^i$	0.86	2.26	3.1187 (1)	175
$N2-H2A \cdots O1^{ii}$	0.86	2.32	3.1032 (1)	152
$N5-H5 \cdots O1^{ii}$	0.86	2.51	3.2640 (1)	146
$C13-H13C \cdots O1^{ii}$	0.96	2.56	3.3880 (1)	144
$N2-H2B \cdots Cg1^{iii}$	0.86	2.88	3.4851 (1)	130

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

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N5-H5 \cdots N4$	0.86	2.15	2.861 (3)	140
$C8-H8 \cdots O1$	0.93	2.34	2.911 (3)	120
$N1-H1A \cdots N3^i$	0.86	2.21	3.035 (3)	162
$N1-H1B \cdots O1^{ii}$	0.86	2.08	2.891 (3)	157
$N2-H2B \cdots O2^{iii}$	0.86	2.55	3.210 (3)	135
$C2-H2 \cdots O2^{iii}$	0.93	2.59	3.272 (3)	130

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

values reported for a similar structure, 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(2-methylphenyl)acetamide, *viz.* 1.763 and 1.805 Å, respectively (Subasri *et al.*, 2014). In compound (I), atoms C13 and C14 deviate from the benzene ring by 0.010 (3) and 0.012 (3) Å, respectively. Atoms N1 and N2 deviate from the mean plane of the pyrimidine ring by $-0.0819(18)$ and $0.0636(14)$ Å, respectively, in compound (I), and by 0.0360 (3) and 0.0273 (3) Å, respectively, in compound (II). In both compounds, an intramolecular hydrogen bond, $C8-H8 \cdots O1$, forms an $S(6)$ ring motif, and in compound (II) there is also an intramolecular $N-H \cdots N$ hydrogen bond present that forms an $S(7)$ ring motif (see Tables 1 and 2).

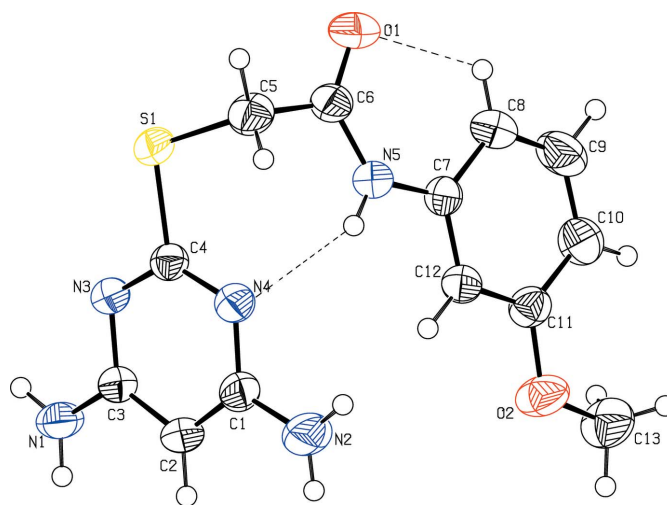


Figure 2

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

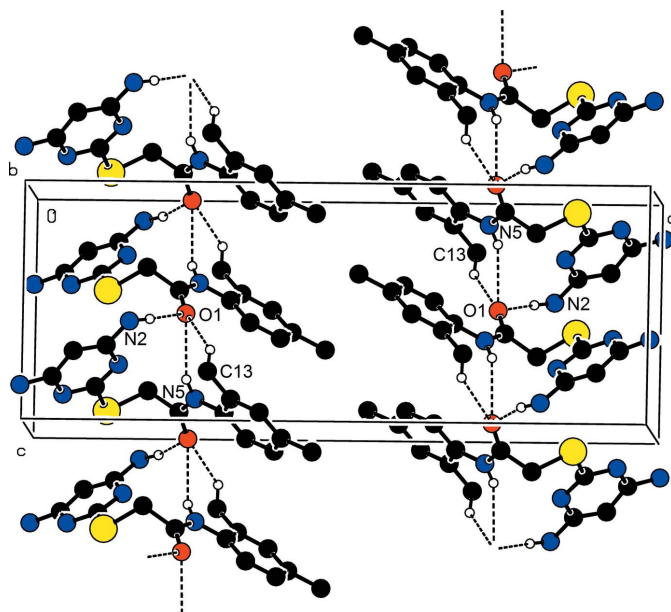


Figure 3
The crystal packing of (I), viewed along the *b* axis, C–H···O and N–H···O hydrogen bonds generate $R_2^2(14)$, $R_2^2(11)$ and $R_2^2(7)$ ring motifs. In this and subsequent figures, the hydrogen bonds are shown as dashed lines and H atoms not involved in hydrogen bonding have been omitted for clarity.

3. Supramolecular features

The hydrogen-bonding geometry of compounds (I) and (II) are given in Tables 1 and 2, respectively. In compound (I), atom O1 is a triple acceptor of hydrogen bonds. The N5–H5···O1ⁱⁱ hydrogen bonds form a chain running along the *c*-axis direction. The N2–H2A···O1ⁱⁱ and C13–H13C···O1ⁱⁱ hydrogen bonds generate an $R_2^2(14)$ ring motif, and the N2–H2A···O1ⁱⁱ and N5–H5···O1ⁱⁱ hydrogen bonds form an $R_2^2(11)$ ring motif, and N5–H5···O1ⁱⁱ and C13–H13···O1ⁱⁱ

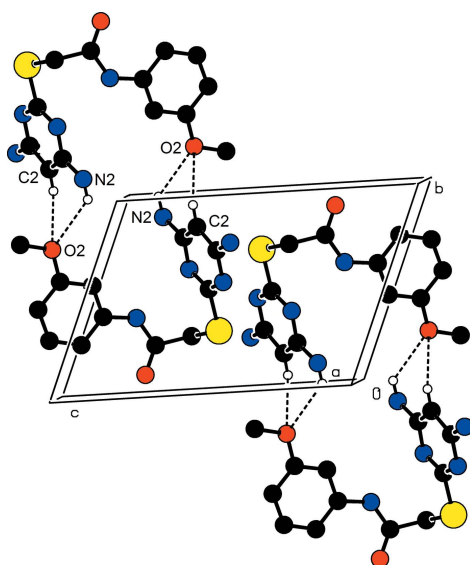


Figure 4
A partial view of the crystal packing of (I), viewed approximately along the *c* axis, showing the N–H··· π interactions.

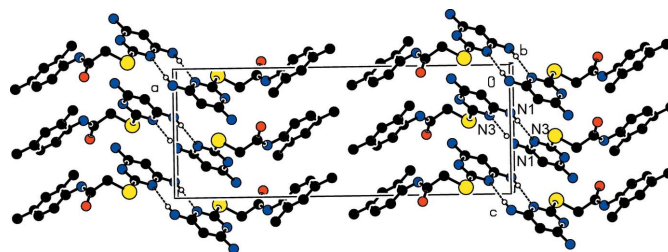


Figure 5
A view along the *b* axis of the crystal packing of (I), showing the N–H···N hydrogen bonds that generate an $R_2^2(8)$ ring motif.

hydrogen bonds generate an $R_2^1(7)$ ring motif (Table 1 and Fig. 3). There is also a N2–H2B··· π interaction present within the layer (Table 1 and Fig. 4), with the separation distance between the donor and acceptor, Cg1, being 3.4851 (1) Å. The N1–H1A···N3ⁱ hydrogen bond generates an inversion dimer with an $R_2^2(8)$ ring motif (Table 1 and Fig. 5). As a result of the hydrogen bonding, layers parallel to the *bc* plane are formed.

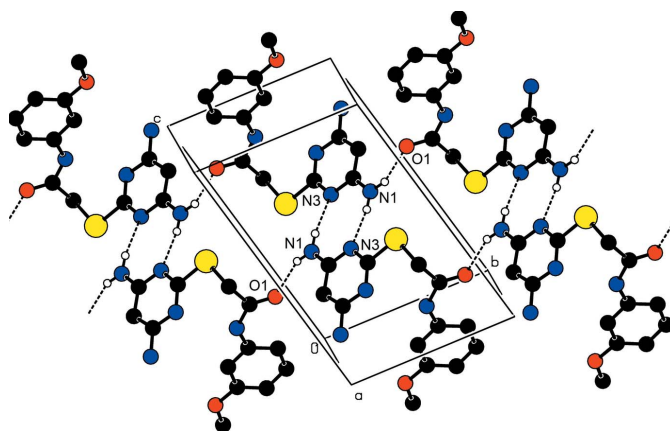


Figure 6
The crystal packing of (II), viewed along the *a* axis, C–H···O and N–H···O hydrogen bonds generate two $R_2^2(26)$ ring motifs and one $R_2^1(6)$ ring motif.

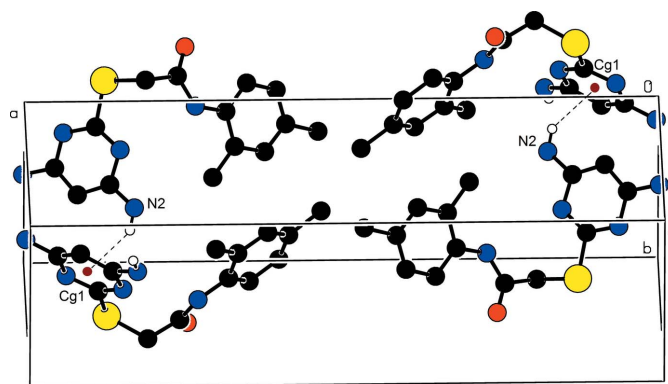


Figure 7
A partial view along the *a* axis of the crystal packing of (II). The N–H···N hydrogen bonds generate an $R_2^2(8)$ ring motif and N–H···O and N–H···N hydrogen bonds an $R_4^1(18)$ ring motif.

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	C ₁₄ H ₁₇ N ₅ OS	C ₁₃ H ₁₅ N ₅ O ₂ S
<i>M_r</i>	303.38	305.36
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	293	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	23.7716 (6), 7.0073 (2), 9.0909 (2)	8.014 (5), 8.724 (5), 12.068 (5)
α , β , γ (°)	90, 90.086 (2), 90	106.561 (5), 97.888 (5), 110.461 (5)
<i>V</i> (Å ³)	1514.31 (7)	730.9 (7)
<i>Z</i>	4	2
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α
μ (mm ⁻¹)	0.22	0.23
Crystal size (mm)	0.24 × 0.18 × 0.12	0.30 × 0.25 × 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)
<i>T_{min}</i> , <i>T_{max}</i>	0.785, 0.854	0.785, 0.843
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	13879, 3705, 2750	10789, 2991, 2616
<i>R_{int}</i>	0.022	0.026
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.666	0.627
Refinement		
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.040, 0.119, 1.06	0.037, 0.110, 0.81
No. of reflections	3705	2991
No. of parameters	192	191
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.22, -0.24	0.17, -0.27

Computer programs: APEX2 and SAINT (Bruker, 2008), SHELXS97 (Sheldrick, 2008), SHELXL2016 (Sheldrick, 2015), ORTEP-3 for Windows (Farrugia, 2012) and PLATON (Spek, 2009).

In compound (II), atom O2 is a double acceptor of hydrogen bonds. The N2—H2B···O2ⁱⁱⁱ hydrogen bond forms an *R*₂²(26) ring motif and hydrogen bond C2—H2···O2ⁱⁱⁱ generates an *R*₂²(26) ring motif (Table 2 and Fig. 6). These two intermolecular hydrogen bonds generate an *R*₂¹(6) ring motif, which is shown in Fig. 6. Molecules are linked by a pair of N1—H1A···N3ⁱ hydrogen bonds, forming an inversion dimer with an *R*₂²(8) ring motif, and hydrogen bonds N1—H1B···O1ⁱⁱ and N1—H1A···N3ⁱ generate an *R*₄⁴(18) ring motif (Table 2 and Fig. 7). The combination of these various hydrogen bonds results in the formation of layers parallel to (1 $\bar{1}$ 1).

4. Database survey

A search of the Cambridge Structure Database (Version 5.37, update May 2016; Groom *et al.*, 2016) for 2-[(pyrimidine-2-yl)sulfanyl]-*N*-phenylacetamide yielded seven hits. Three of these involve (4,6-diaminopyrimidin-2-yl) groups. They include the 2-methylphenyl analogue, 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(2-methylphenyl)acetamide (GOKWIO; Subasri *et al.*, 2014), the 2-chlorophenyl analogue, *N*-(2-chlorophenyl)-2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-acetamide (ARARUI; Subasri *et al.*, 2016) and the 3-nitrophenyl analogue, 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(3-nitrophenyl)acetamide (ARAROC; Subasri *et al.*, 2016). Here the pyrimidine and benzene rings are inclined to one

another by 54.73, 67.11 and 56.19°, respectively, compared to 58.64 (8)° in compound (I), and 78.33 (9)° in compound (II).

5. 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 in a round-bottom flask, potassium hydroxide (0.2 g, 3.52 mmol) was added and the mixture was refluxed for 30 min. 2,4-Dimethylphenyl acetamide (3.52 mmol) was added and the mixture was refluxed for 3 h. At the end of the reaction (observed by TLC), the ethanol was evaporated under vacuum and cold water was added. The precipitate formed was filtered and dried to give compound (I) as a crystalline powder (yield 67%). After purification, the compound was recrystallized from ethanol solution by slow evaporation of the solvent.

Compound (II): To a solution of 4,6-diamino-pyrimidine-2-thiol (0.5 g, 3.52 mmol) in 25 ml of ethanol in a round-bottom flask was added potassium hydroxide (0.2 g, 3.52 mmol) and the mixture was refluxed for 30 min. 3-Methoxyphenyl acetamide (3.52 mmol) was added and the mixture was refluxed for 3 h. At the end of the reaction (observed by TLC), the ethanol was evaporated under vacuum and cold water was added, and the precipitate formed was filtered and dried to give compound (II) as a shiny powder (yield 73%). After purification, the compound was recrystallized from ethanol solution by slow evaporation of the solvent.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. For both compounds the hydrogen atoms were placed in calculated positions and refined using the riding model: C–H = 0.93–0.97 Å and N–H = 0.86 Å, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C-methyl})$ and $1.2U_{\text{eq}}(\text{N,C})$ for other H atoms.

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supporting information

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Crystal structures of 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(2,4-dimethylphenyl)acetamide and 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(3-methoxyphenyl)acetamide

Manisha Choudhury, Vijayan Viswanathan, Ajay Kumar Timiri, Barij Nayan Sinha, Venkatesan Jayaprakash and Devadasan Velmurugan

Computing details

For both compounds, 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: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL2016* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

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

Crystal data

$C_{14}H_{17}N_5OS$

$M_r = 303.38$

Monoclinic, $P2_1/c$

$a = 23.7716$ (6) Å

$b = 7.0073$ (2) Å

$c = 9.0909$ (2) Å

$\beta = 90.086$ (2)°

$V = 1514.31$ (7) Å³

$Z = 4$

$F(000) = 640$

$D_x = 1.331$ Mg m⁻³

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

Cell parameters from 3705 reflections

$\theta = 1.7$ – 28.3 °

$\mu = 0.22$ mm⁻¹

$T = 293$ K

Block, yellow

$0.24 \times 0.18 \times 0.12$ mm

Data collection

Bruker SMART APEXII area-detector diffractometer

ω and ϕ scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2008)

$T_{\min} = 0.785$, $T_{\max} = 0.854$

13879 measured reflections

3705 independent reflections

2750 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$

$\theta_{\max} = 28.3$ °, $\theta_{\min} = 1.7$ °

$h = -31 \rightarrow 31$

$k = -8 \rightarrow 9$

$l = -12 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.119$

$S = 1.06$

3705 reflections

192 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0584P)^2 + 0.2187P]$
 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.22 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.13091 (2)	0.71159 (6)	0.94117 (5)	0.05991 (16)
N4	0.15430 (5)	1.00969 (16)	0.76929 (12)	0.0459 (3)
N3	0.06610 (5)	0.99914 (17)	0.89584 (13)	0.0492 (3)
C4	0.11650 (6)	0.9332 (2)	0.85688 (15)	0.0434 (3)
O1	0.25886 (5)	0.58619 (18)	1.04523 (13)	0.0688 (4)
C6	0.24589 (6)	0.6857 (2)	0.94031 (15)	0.0464 (3)
N2	0.17546 (7)	1.2451 (2)	0.60612 (15)	0.0646 (4)
H2A	0.206833	1.186878	0.592034	0.078*
H2B	0.168182	1.348669	0.559012	0.078*
N5	0.27421 (5)	0.84155 (19)	0.89770 (15)	0.0563 (3)
H5	0.261074	0.898941	0.821415	0.068*
C1	0.13761 (7)	1.1740 (2)	0.70222 (15)	0.0492 (4)
C3	0.05202 (7)	1.1694 (2)	0.83485 (18)	0.0547 (4)
C2	0.08687 (8)	1.2589 (2)	0.73351 (18)	0.0577 (4)
H2	0.076240	1.372376	0.688329	0.069*
C13	0.30123 (8)	1.2195 (2)	0.8120 (2)	0.0647 (5)
H13A	0.314436	1.348741	0.806118	0.097*
H13B	0.262823	1.218807	0.844537	0.097*
H13C	0.303624	1.160894	0.716785	0.097*
C5	0.19468 (6)	0.6392 (2)	0.84913 (17)	0.0503 (4)
H5A	0.193461	0.502920	0.830692	0.060*
H5B	0.197259	0.703824	0.755023	0.060*
C12	0.33675 (7)	1.1105 (3)	0.91894 (17)	0.0562 (4)
C7	0.32294 (7)	0.9247 (3)	0.96134 (18)	0.0565 (4)
N1	0.00214 (7)	1.2404 (2)	0.8769 (2)	0.0826 (5)
H1A	-0.018358	1.178344	0.938385	0.099*
H1B	-0.009323	1.347810	0.842366	0.099*
C11	0.38453 (8)	1.1920 (3)	0.9800 (2)	0.0705 (5)
H11	0.394129	1.315535	0.952417	0.085*
C8	0.35657 (8)	0.8271 (3)	1.0617 (2)	0.0766 (6)
H8	0.347527	0.703240	1.089668	0.092*
C10	0.41862 (8)	1.0979 (4)	1.0800 (2)	0.0808 (6)
C9	0.40379 (8)	0.9168 (4)	1.1195 (3)	0.0893 (7)
H9	0.425969	0.851470	1.187178	0.107*
C14	0.47024 (9)	1.1953 (5)	1.1442 (3)	0.1146 (10)
H14A	0.475144	1.156141	1.244577	0.172*

H14B	0.465342	1.331180	1.140249	0.172*
H14C	0.502847	1.160063	1.088224	0.172*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0529 (3)	0.0458 (2)	0.0810 (3)	0.00850 (17)	0.00160 (19)	0.01998 (19)
N4	0.0599 (8)	0.0368 (6)	0.0410 (6)	0.0054 (5)	-0.0075 (5)	-0.0003 (5)
N3	0.0506 (7)	0.0421 (7)	0.0548 (7)	0.0071 (5)	-0.0109 (5)	0.0004 (5)
C4	0.0536 (8)	0.0356 (7)	0.0410 (7)	0.0034 (6)	-0.0147 (6)	-0.0033 (5)
O1	0.0774 (8)	0.0705 (8)	0.0585 (7)	-0.0070 (6)	-0.0125 (6)	0.0206 (6)
C6	0.0516 (8)	0.0440 (8)	0.0435 (7)	0.0096 (6)	0.0034 (6)	-0.0017 (6)
N2	0.0844 (11)	0.0560 (8)	0.0535 (8)	0.0111 (7)	-0.0005 (7)	0.0154 (6)
N5	0.0545 (8)	0.0549 (8)	0.0594 (8)	-0.0026 (6)	-0.0117 (6)	0.0135 (6)
C1	0.0680 (10)	0.0419 (8)	0.0376 (7)	0.0041 (7)	-0.0122 (6)	-0.0001 (6)
C3	0.0606 (10)	0.0471 (9)	0.0565 (9)	0.0121 (7)	-0.0149 (7)	0.0009 (7)
C2	0.0735 (11)	0.0445 (8)	0.0549 (9)	0.0145 (7)	-0.0132 (8)	0.0076 (7)
C13	0.0729 (12)	0.0532 (10)	0.0679 (11)	-0.0045 (8)	0.0029 (9)	0.0017 (8)
C5	0.0584 (9)	0.0348 (7)	0.0577 (9)	0.0078 (6)	-0.0064 (7)	-0.0034 (6)
C12	0.0504 (9)	0.0651 (11)	0.0530 (9)	-0.0023 (7)	0.0089 (7)	-0.0082 (7)
C7	0.0469 (8)	0.0662 (11)	0.0564 (9)	0.0006 (7)	-0.0009 (7)	0.0014 (8)
N1	0.0686 (10)	0.0731 (11)	0.1062 (13)	0.0325 (8)	0.0045 (9)	0.0260 (9)
C11	0.0574 (10)	0.0841 (14)	0.0700 (11)	-0.0136 (9)	0.0119 (9)	-0.0166 (10)
C8	0.0549 (11)	0.0888 (15)	0.0860 (13)	0.0017 (10)	-0.0144 (9)	0.0159 (11)
C10	0.0484 (10)	0.1182 (19)	0.0758 (13)	-0.0087 (11)	0.0010 (9)	-0.0205 (12)
C9	0.0524 (11)	0.127 (2)	0.0887 (15)	0.0051 (12)	-0.0168 (10)	0.0071 (14)
C14	0.0601 (13)	0.167 (3)	0.117 (2)	-0.0246 (15)	-0.0090 (12)	-0.0338 (19)

Geometric parameters (Å, °)

S1—C4	1.7650 (14)	C13—H13B	0.9600
S1—C5	1.8053 (16)	C13—H13C	0.9600
N4—C4	1.3157 (19)	C5—H5A	0.9700
N4—C1	1.3616 (18)	C5—H5B	0.9700
N3—C4	1.3325 (19)	C12—C11	1.386 (2)
N3—C3	1.3577 (19)	C12—C7	1.397 (3)
O1—C6	1.2209 (17)	C7—C8	1.391 (2)
C6—N5	1.340 (2)	N1—H1A	0.8600
C6—C5	1.507 (2)	N1—H1B	0.8600
N2—C1	1.350 (2)	C11—C10	1.384 (3)
N2—H2A	0.8600	C11—H11	0.9300
N2—H2B	0.8600	C8—C9	1.389 (3)
N5—C7	1.419 (2)	C8—H8	0.9300
N5—H5	0.8600	C10—C9	1.365 (3)
C1—C2	1.375 (2)	C10—C14	1.520 (3)
C3—N1	1.342 (2)	C9—H9	0.9300
C3—C2	1.389 (2)	C14—H14A	0.9600
C2—H2	0.9300	C14—H14B	0.9600

C13—C12	1.496 (2)	C14—H14C	0.9600
C13—H13A	0.9600		
C4—S1—C5	102.04 (7)	S1—C5—H5A	109.4
C4—N4—C1	114.62 (13)	C6—C5—H5B	109.4
C4—N3—C3	114.68 (14)	S1—C5—H5B	109.4
N4—C4—N3	129.41 (13)	H5A—C5—H5B	108.0
N4—C4—S1	119.27 (11)	C11—C12—C7	117.76 (17)
N3—C4—S1	111.33 (11)	C11—C12—C13	120.75 (17)
O1—C6—N5	124.39 (14)	C7—C12—C13	121.48 (15)
O1—C6—C5	120.58 (14)	C8—C7—C12	120.26 (16)
N5—C6—C5	115.02 (13)	C8—C7—N5	122.22 (17)
C1—N2—H2A	120.0	C12—C7—N5	117.53 (14)
C1—N2—H2B	120.0	C3—N1—H1A	120.0
H2A—N2—H2B	120.0	C3—N1—H1B	120.0
C6—N5—C7	128.82 (13)	H1A—N1—H1B	120.0
C6—N5—H5	115.6	C10—C11—C12	123.1 (2)
C7—N5—H5	115.6	C10—C11—H11	118.5
N2—C1—N4	114.07 (14)	C12—C11—H11	118.5
N2—C1—C2	124.03 (14)	C9—C8—C7	119.3 (2)
N4—C1—C2	121.90 (15)	C9—C8—H8	120.4
N1—C3—N3	115.25 (16)	C7—C8—H8	120.4
N1—C3—C2	123.37 (15)	C9—C10—C11	117.66 (18)
N3—C3—C2	121.35 (15)	C9—C10—C14	121.7 (2)
C1—C2—C3	117.79 (14)	C11—C10—C14	120.7 (2)
C1—C2—H2	121.1	C10—C9—C8	122.0 (2)
C3—C2—H2	121.1	C10—C9—H9	119.0
C12—C13—H13A	109.5	C8—C9—H9	119.0
C12—C13—H13B	109.5	C10—C14—H14A	109.5
H13A—C13—H13B	109.5	C10—C14—H14B	109.5
C12—C13—H13C	109.5	H14A—C14—H14B	109.5
H13A—C13—H13C	109.5	C10—C14—H14C	109.5
H13B—C13—H13C	109.5	H14A—C14—H14C	109.5
C6—C5—S1	111.24 (10)	H14B—C14—H14C	109.5
C6—C5—H5A	109.4		
C1—N4—C4—N3	-4.6 (2)	N5—C6—C5—S1	-101.92 (14)
C1—N4—C4—S1	175.79 (10)	C4—S1—C5—C6	98.12 (11)
C3—N3—C4—N4	0.5 (2)	C11—C12—C7—C8	0.0 (3)
C3—N3—C4—S1	-179.87 (10)	C13—C12—C7—C8	-179.62 (17)
C5—S1—C4—N4	-8.96 (12)	C11—C12—C7—N5	-179.55 (15)
C5—S1—C4—N3	171.36 (10)	C13—C12—C7—N5	0.8 (2)
O1—C6—N5—C7	-0.7 (3)	C6—N5—C7—C8	15.4 (3)
C5—C6—N5—C7	178.66 (15)	C6—N5—C7—C12	-165.04 (15)
C4—N4—C1—N2	-176.34 (12)	C7—C12—C11—C10	-0.1 (3)
C4—N4—C1—C2	4.7 (2)	C13—C12—C11—C10	179.58 (17)
C4—N3—C3—N1	-177.94 (14)	C12—C7—C8—C9	0.3 (3)
C4—N3—C3—C2	3.6 (2)	N5—C7—C8—C9	179.83 (18)

N2—C1—C2—C3	179.97 (15)	C12—C11—C10—C9	-0.2 (3)
N4—C1—C2—C3	-1.2 (2)	C12—C11—C10—C14	-179.48 (19)
N1—C3—C2—C1	178.45 (16)	C11—C10—C9—C8	0.5 (3)
N3—C3—C2—C1	-3.2 (2)	C14—C10—C9—C8	179.8 (2)
O1—C6—C5—S1	77.43 (16)	C7—C8—C9—C10	-0.6 (4)

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the N3/N4/C1—C4 ring.

<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>
C8—H8...O1	0.93	2.30	2.8752 (1)	120
N1—H1 <i>A</i> ...N3 ⁱ	0.86	2.26	3.1187 (1)	175
N2—H2 <i>A</i> ...O1 ⁱⁱ	0.86	2.32	3.1032 (1)	152
N5—H5...O1 ⁱⁱ	0.86	2.51	3.2640 (1)	146
C13—H13 <i>C</i> ...O1 ⁱⁱ	0.96	2.56	3.3880 (1)	144
N2—H2 <i>B</i> ...Cg1 ⁱⁱⁱ	0.86	2.88	3.4851 (1)	130

Symmetry codes: (i) $-x, -y+2, -z+2$; (ii) $x, -y+3/2, z-1/2$; (iii) $x, -y+3/2, z-3/2$.**(II) 2-[(4,6-Diaminopyrimidin-2-yl)sulfanyl]-*N*-(3-methoxyphenyl)acetamide***Crystal data*C₁₃H₁₅N₅O₂S $M_r = 305.36$ Triclinic, $P\bar{1}$ $a = 8.014$ (5) Å $b = 8.724$ (5) Å $c = 12.068$ (5) Å $\alpha = 106.561$ (5)° $\beta = 97.888$ (5)° $\gamma = 110.461$ (5)° $V = 730.9$ (7) Å³ $Z = 2$ $F(000) = 320$ $D_x = 1.388$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2991 reflections

 $\theta = 1.8$ – 26.5° $\mu = 0.23$ mm⁻¹ $T = 293$ K

Block, yellow

 $0.30 \times 0.25 \times 0.20$ mm*Data collection*Bruker SMART APEXII area-detector
diffractometer ω and φ scansAbsorption correction: multi-scan
(*SADABS*; Bruker, 2008) $T_{\min} = 0.785$, $T_{\max} = 0.843$

10789 measured reflections

2991 independent reflections

2616 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.026$ $\theta_{\max} = 26.5^\circ$, $\theta_{\min} = 1.8^\circ$ $h = -10 \rightarrow 9$ $k = -10 \rightarrow 10$ $l = -15 \rightarrow 15$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.037$ $wR(F^2) = 0.110$ $S = 0.81$

2991 reflections

191 parameters

0 restraints

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

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.082P)^2 + 0.3261P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.17$ e Å⁻³ $\Delta\rho_{\min} = -0.27$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2721 (2)	0.7765 (2)	0.75950 (14)	0.0415 (4)
C2	0.4285 (2)	0.8303 (2)	0.72068 (14)	0.0416 (4)
H2	0.517868	0.944735	0.755617	0.050*
C3	0.4481 (2)	0.70658 (19)	0.62691 (13)	0.0371 (3)
C4	0.1714 (2)	0.50538 (19)	0.61966 (13)	0.0345 (3)
C5	-0.1544 (2)	0.2625 (2)	0.63675 (15)	0.0478 (4)
H5A	-0.175956	0.368379	0.661775	0.057*
H5B	-0.271283	0.165803	0.589640	0.057*
C6	-0.0831 (2)	0.2295 (2)	0.74625 (15)	0.0451 (4)
C7	0.1429 (2)	0.3944 (2)	0.94683 (13)	0.0388 (3)
C8	0.1195 (3)	0.2573 (2)	0.98958 (17)	0.0524 (4)
H8	0.029765	0.145119	0.945410	0.063*
C9	0.2324 (3)	0.2922 (3)	1.09848 (19)	0.0610 (5)
H9	0.217277	0.201394	1.127299	0.073*
C10	0.3670 (3)	0.4566 (2)	1.16652 (17)	0.0519 (4)
H10	0.441229	0.476596	1.239984	0.062*
C11	0.3892 (2)	0.5915 (2)	1.12302 (14)	0.0414 (4)
C12	0.2776 (2)	0.5599 (2)	1.01376 (14)	0.0397 (3)
H12	0.293260	0.650900	0.985061	0.048*
C13	0.6424 (3)	0.7978 (3)	1.29014 (18)	0.0632 (5)
H13A	0.576735	0.780929	1.349543	0.095*
H13B	0.731248	0.917131	1.317583	0.095*
H13C	0.704699	0.720780	1.276837	0.095*
N4	0.13965 (18)	0.61019 (17)	0.70978 (11)	0.0396 (3)
N3	0.31604 (17)	0.54040 (16)	0.57426 (11)	0.0368 (3)
N2	0.2417 (3)	0.8847 (2)	0.85299 (15)	0.0634 (5)
H2A	0.143870	0.846000	0.876513	0.076*
H2B	0.320263	0.991812	0.888534	0.076*
N1	0.5973 (2)	0.74522 (19)	0.58440 (14)	0.0527 (4)
H1A	0.606000	0.666365	0.526465	0.063*
H1B	0.684496	0.848902	0.615032	0.063*
N5	0.03559 (19)	0.37602 (17)	0.83726 (12)	0.0425 (3)
H5	0.047786	0.472628	0.827087	0.051*
O1	-0.1275 (2)	0.08145 (17)	0.74876 (13)	0.0675 (4)
O2	0.51589 (19)	0.76002 (16)	1.18149 (11)	0.0584 (4)
S1	0.00691 (5)	0.28602 (5)	0.54469 (3)	0.04131 (14)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0530 (9)	0.0339 (8)	0.0391 (8)	0.0203 (7)	0.0146 (7)	0.0113 (6)
C2	0.0476 (9)	0.0276 (7)	0.0427 (8)	0.0118 (6)	0.0105 (7)	0.0081 (6)
C3	0.0413 (8)	0.0308 (7)	0.0357 (7)	0.0122 (6)	0.0090 (6)	0.0106 (6)
C4	0.0364 (7)	0.0323 (7)	0.0323 (7)	0.0130 (6)	0.0046 (6)	0.0113 (6)
C5	0.0302 (7)	0.0491 (10)	0.0466 (9)	0.0049 (7)	0.0058 (6)	0.0087 (7)
C6	0.0359 (8)	0.0407 (9)	0.0453 (9)	0.0031 (7)	0.0145 (7)	0.0103 (7)
C7	0.0421 (8)	0.0363 (8)	0.0376 (8)	0.0151 (6)	0.0163 (6)	0.0115 (6)
C8	0.0598 (10)	0.0365 (9)	0.0551 (10)	0.0112 (8)	0.0152 (8)	0.0187 (8)
C9	0.0724 (13)	0.0485 (10)	0.0673 (12)	0.0203 (9)	0.0154 (10)	0.0348 (9)
C10	0.0593 (10)	0.0522 (10)	0.0500 (10)	0.0255 (9)	0.0104 (8)	0.0248 (8)
C11	0.0459 (8)	0.0374 (8)	0.0417 (8)	0.0201 (7)	0.0111 (7)	0.0119 (7)
C12	0.0472 (8)	0.0330 (8)	0.0397 (8)	0.0163 (7)	0.0127 (7)	0.0139 (6)
C13	0.0604 (11)	0.0612 (12)	0.0535 (11)	0.0200 (10)	-0.0085 (9)	0.0171 (9)
N4	0.0433 (7)	0.0355 (7)	0.0396 (7)	0.0161 (6)	0.0133 (5)	0.0117 (5)
N3	0.0382 (6)	0.0315 (6)	0.0349 (6)	0.0108 (5)	0.0090 (5)	0.0082 (5)
N2	0.0777 (11)	0.0396 (8)	0.0652 (10)	0.0191 (8)	0.0375 (9)	0.0052 (7)
N1	0.0504 (8)	0.0339 (7)	0.0568 (9)	0.0046 (6)	0.0241 (7)	0.0037 (6)
N5	0.0473 (7)	0.0336 (7)	0.0391 (7)	0.0098 (6)	0.0117 (6)	0.0108 (5)
O1	0.0721 (9)	0.0383 (7)	0.0593 (8)	-0.0068 (6)	0.0068 (7)	0.0129 (6)
O2	0.0670 (8)	0.0390 (7)	0.0513 (7)	0.0153 (6)	-0.0123 (6)	0.0118 (5)
S1	0.0384 (2)	0.0372 (2)	0.0341 (2)	0.00654 (16)	0.00462 (15)	0.00617 (16)

Geometric parameters (\AA , $^\circ$)

C1—N4	1.358 (2)	C8—C9	1.375 (3)
C1—C2	1.374 (2)	C8—H8	0.9300
C1—N2	1.361 (2)	C9—C10	1.378 (3)
C2—C3	1.393 (2)	C9—H9	0.9300
C2—H2	0.9300	C10—C11	1.387 (3)
C3—N1	1.339 (2)	C10—H10	0.9300
C3—N3	1.357 (2)	C11—O2	1.363 (2)
C4—N4	1.325 (2)	C11—C12	1.383 (2)
C4—N3	1.327 (2)	C12—H12	0.9300
C4—S1	1.7721 (17)	C13—O2	1.418 (2)
C5—C6	1.510 (3)	C13—H13A	0.9600
C5—S1	1.8126 (18)	C13—H13B	0.9600
C5—H5A	0.9700	C13—H13C	0.9600
C5—H5B	0.9700	N2—H2A	0.8600
C6—O1	1.224 (2)	N2—H2B	0.8600
C6—N5	1.345 (2)	N1—H1A	0.8600
C7—C12	1.381 (2)	N1—H1B	0.8600
C7—C8	1.397 (2)	N5—H5	0.8600
C7—N5	1.409 (2)		
N4—C1—C2	122.38 (14)	C8—C9—H9	118.7

N4—C1—N2	115.28 (15)	C9—C10—C11	118.53 (17)
C2—C1—N2	122.31 (16)	C9—C10—H10	120.7
C1—C2—C3	117.36 (14)	C11—C10—H10	120.7
C1—C2—H2	121.3	O2—C11—C12	115.38 (14)
C3—C2—H2	121.3	O2—C11—C10	124.50 (15)
N1—C3—N3	116.77 (14)	C12—C11—C10	120.12 (16)
N1—C3—C2	121.86 (14)	C7—C12—C11	120.61 (15)
N3—C3—C2	121.37 (14)	C7—C12—H12	119.7
N4—C4—N3	128.70 (14)	C11—C12—H12	119.7
N4—C4—S1	119.42 (12)	O2—C13—H13A	109.5
N3—C4—S1	111.88 (11)	O2—C13—H13B	109.5
C6—C5—S1	111.79 (12)	H13A—C13—H13B	109.5
C6—C5—H5A	109.3	O2—C13—H13C	109.5
S1—C5—H5A	109.3	H13A—C13—H13C	109.5
C6—C5—H5B	109.3	H13B—C13—H13C	109.5
S1—C5—H5B	109.3	C4—N4—C1	114.83 (14)
H5A—C5—H5B	107.9	C4—N3—C3	115.33 (13)
O1—C6—N5	124.17 (17)	C1—N2—H2A	120.0
O1—C6—C5	122.10 (15)	C1—N2—H2B	120.0
N5—C6—C5	113.70 (15)	H2A—N2—H2B	120.0
C12—C7—C8	119.78 (15)	C3—N1—H1A	120.0
C12—C7—N5	116.25 (14)	C3—N1—H1B	120.0
C8—C7—N5	123.97 (15)	H1A—N1—H1B	120.0
C9—C8—C7	118.46 (17)	C6—N5—C7	129.44 (15)
C9—C8—H8	120.8	C6—N5—H5	115.3
C7—C8—H8	120.8	C7—N5—H5	115.3
C10—C9—C8	122.51 (17)	C11—O2—C13	117.88 (14)
C10—C9—H9	118.7	C4—S1—C5	103.05 (8)
N4—C1—C2—C3	-0.1 (2)	S1—C4—N4—C1	-178.68 (11)
N2—C1—C2—C3	177.81 (16)	C2—C1—N4—C4	-1.3 (2)
C1—C2—C3—N1	-178.60 (15)	N2—C1—N4—C4	-179.36 (14)
C1—C2—C3—N3	1.3 (2)	N4—C4—N3—C3	-0.6 (2)
S1—C5—C6—O1	-95.98 (18)	S1—C4—N3—C3	179.78 (10)
S1—C5—C6—N5	82.23 (16)	N1—C3—N3—C4	178.93 (14)
C12—C7—C8—C9	0.2 (3)	C2—C3—N3—C4	-1.0 (2)
N5—C7—C8—C9	-179.56 (17)	O1—C6—N5—C7	5.5 (3)
C7—C8—C9—C10	0.0 (3)	C5—C6—N5—C7	-172.71 (14)
C8—C9—C10—C11	-0.1 (3)	C12—C7—N5—C6	168.50 (15)
C9—C10—C11—O2	179.53 (18)	C8—C7—N5—C6	-11.7 (3)
C9—C10—C11—C12	0.1 (3)	C12—C11—O2—C13	-175.89 (16)
C8—C7—C12—C11	-0.2 (2)	C10—C11—O2—C13	4.7 (3)
N5—C7—C12—C11	179.57 (14)	N4—C4—S1—C5	-8.27 (14)
O2—C11—C12—C7	-179.39 (14)	N3—C4—S1—C5	171.36 (11)
C10—C11—C12—C7	0.1 (2)	C6—C5—S1—C4	-80.14 (14)
N3—C4—N4—C1	1.8 (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>
N5—H5 \cdots N4	0.86	2.15	2.861 (3)	140
C8—H8 \cdots O1	0.93	2.34	2.911 (3)	120
N1—H1 <i>A</i> \cdots N3 ⁱ	0.86	2.21	3.035 (3)	162
N1—H1 <i>B</i> \cdots O1 ⁱⁱ	0.86	2.08	2.891 (3)	157
N2—H2 <i>B</i> \cdots O2 ⁱⁱⁱ	0.86	2.55	3.210 (3)	135
C2—H2 \cdots O2 ⁱⁱⁱ	0.93	2.59	3.272 (3)	130

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