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

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CCDC references: 1534990; 1534989

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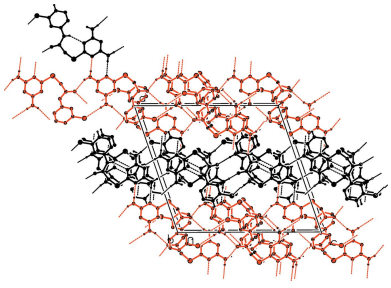
The title compounds, $C_{12}H_{12}ClN_5OS$, (I), and $C_{12}H_{12}ClN_5OS$, (II), are 2-[(diaminopyrimidin-2-yl)sulfanyl]acetamides. Compound (II), crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. In each of the molecules, in both (I) and (II), an intramolecular N—H···N hydrogen bond forms an *S*(7) ring motif. The pyrimidine ring is inclined to the benzene ring by 42.25 (14)° in (I), and by 59.70 (16) and 62.18 (15)° in molecules *A* and *B*, respectively, of compound (II). In the crystal of (I), molecules are linked by pairs of N—H···N hydrogen bonds, forming inversion dimers with an $R_2^2(8)$ ring motif. The dimers are linked *via* bifurcated N—H···O and C—H···O hydrogen bonds, forming corrugated layers parallel to the *ac* plane. In the crystal of (II), the *A* molecules are linked through N—H···O and N—H···Cl hydrogen bonds, forming layers parallel to (100). The *B* molecules are also linked by N—H···O and N—H···Cl hydrogen bonds, also forming layers parallel to (100). The parallel layers of *A* and *B* molecules are linked *via* N—H···N hydrogen bonds, forming a three-dimensional structure.

1. Chemical context

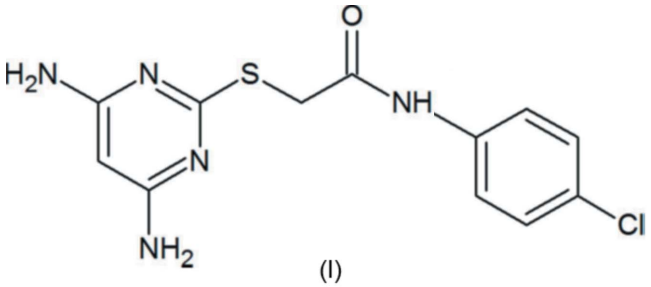
Diaminopyrimidine derivatives are reported to be therapeutic agents towards anti-cancer activity, selectively inhibiting c-Fms kinase of M-CSF-dependent myeloid leukemia cells (Xu *et al.*, 2010). They have also shown antibacterial activity (Kandeel *et al.*, 1994), are potential antimicrobial (Holla *et al.*, 2006) and anti-AIDS agents (Nogueras *et al.*, 1993) and anti-viral agents (Hocková *et al.*, 2003, 2004) and have shown promise as immunosuppressants (Blumenkopf *et al.*, 2002). In this connection, the title 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl] based analogues have been synthesized as anti-viral agents against NS2B/NS3 Dengue protease. We report herein on the syntheses and crystal structures of the title compounds, (I) and (II).



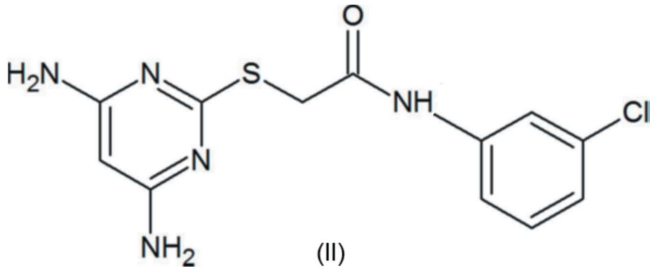
2. Structural commentary

The molecular structures of compounds (I) and (II) are shown in Figs. 1 and 2, respectively. Compound (II) crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit, which have similar conformations (Fig. 3). The molecules of both compounds are folded with the pyrimidine ring being inclined to the benzene ring by 42.25 (14)° in (I), and by

59.70 (16) and 62.18 (15)° in molecules *A* and *B*, respectively, of compound (II). In compound (I), the N1—C7—C8—S1 torsion angle is 77.2 (3)°, while in molecule *A* of compound (II), N5—C6—C5—S1 is 85.2 (3)°, and in molecule *B* N10—C18—C17—S2 is 68.4 (3)°.



(I)



(II)

In compound (I), the intramolecular N1—H1*A*···N2 hydrogen bond (Table 1) generates an *S*(7) ring motif, as shown in Fig. 1. Amine atoms N4 and N5 attached to the pyrimidine ring deviate by 0.018 (3) and 0.060 (3) Å, respectively. The chlorine atom Cl1 attached to the benzene ring deviates by 0.058 (1) Å.

In compound (II), intramolecular N5—H5···N4 and N10—H10···N9 hydrogen bonds (Table 2 and Fig. 2) in molecules *A* and *B*, respectively, also generate *S*(7) ring motifs. In molecule *A*, the amine group atoms N1 and N2 attached to the pyrimidine ring deviate by 0.006 (3) and 0.004 (3) Å, respectively. The chlorine atom Cl1 attached to the benzene ring deviates by 0.013 (1) Å. In molecule *B*, the amine group atoms N6 and N7 attached to the pyrimidine ring deviate by −0.003 (3) and 0.050 (3) Å, respectively. Atom Cl2 attached to the benzene ring deviates by 0.074 (1) Å.

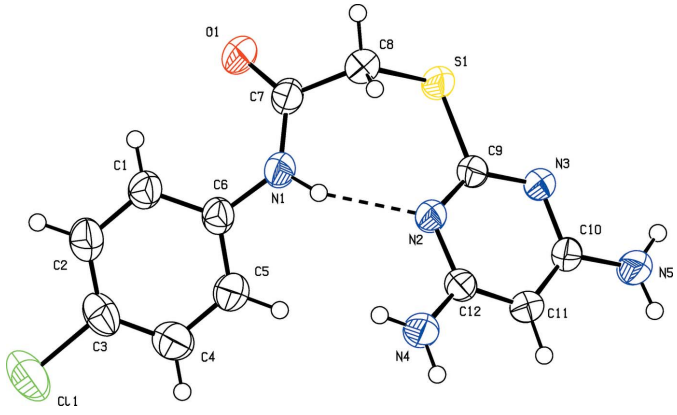


Figure 1
The molecular structure of compound (I), with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular N—H···N hydrogen bond is shown as a dashed lines (see Table 1).

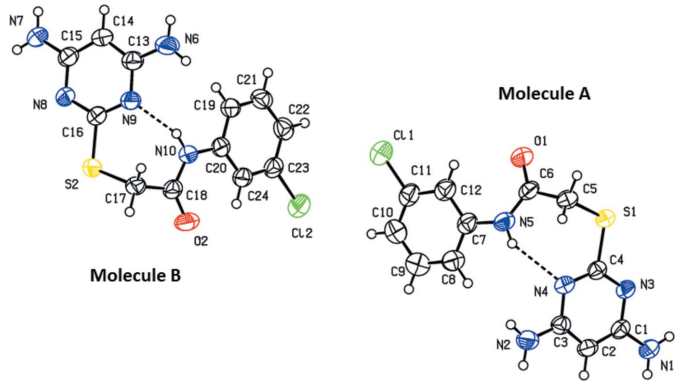


Figure 2
The molecular structure of the two independent molecules (*A* and *B*) of compound (II), with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular N—H···N hydrogen bonds are shown as dashed lines (see Table 2).

3. Supramolecular features

In the crystal of (I), molecules are linked by pairs of N—H···N hydrogen bonds, forming inversion dimers with an $R_2^2(8)$ ring motif (Table 1 and Fig. 4). The dimers are linked by *via* bifurcated N—H···O and C—H···O hydrogen bonds, forming corrugated layers parallel to the *ac* plane (Table 1 and Fig. 5).

In the crystal of (II), the *A* molecules are linked through N—H···O and N—H···Cl hydrogen bonds, forming layers parallel to (100). Likewise the *B* molecules are also linked by N—H···O and N—H···Cl hydrogen bonds, forming layers parallel to (100). The parallel layers of *A* and layers of *B* molecules are linked *via* N—H···N hydrogen bonds, forming a three-dimensional structure (Table 2 and Fig. 6).

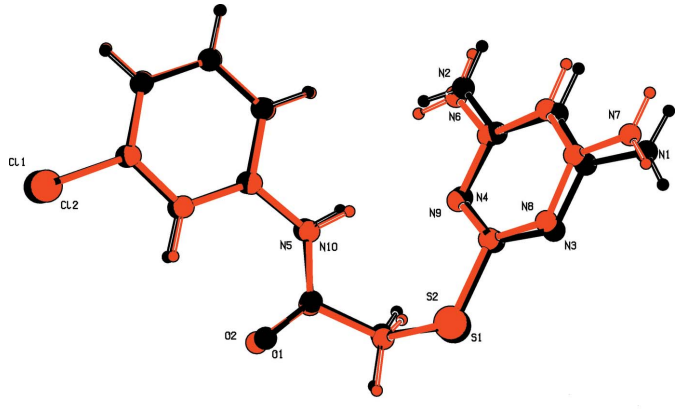


Figure 3
An AutoMolFit (*PLATON*; Spek, 2009) view of molecule *B* (red) on molecule *A* (back) of (II).

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N2	0.86	2.06	2.856 (3)	154
N5—H5A···N3^{i}	0.86	2.16	2.990 (3)	162
N4—H4B···O1^{ii}	0.86	2.22	2.969 (3)	146
C11—H11···O1^{ii}	0.93	2.45	3.144 (3)	132

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

4. Database survey

A search of the Cambridge Structural Database (Version 5.37, update May 2016; Groom *et al.*, 2016) for 2-[(pyrimidine-2-yl)sulfanyl]-*N*-phenylacetamide yielded five hits. Three of these involve (4,6-diaminopyrmidin-2-yl) groups. They include the 2-chlorophenyl analogue, *N*-(2-chlorophenyl)-2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]acetamide (ARARUI; Subasri *et al.*, 2016). Here the pyrimidine and benzene rings are inclined to one another by 67.84 (6)°, compared to 42.25 (14)° in (I), and 59.70 (16) and 62.18 (15)° in molecules *A* and *B*, respectively, of compound (II). As in the title compounds, there is also an intramolecular N—H···N hydrogen bond present, stabilizing the folded conformation of the molecule.

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···N4	0.86	2.25	2.962 (3)	140
N10—H10A···N9	0.86	2.02	2.826 (3)	157
N1—H1B···O1^{i}	0.86	2.19	2.931 (4)	145
N2—H2B···Cl1^{i}	0.86	2.76	3.405 (3)	133
N6—H6A···O2^{ii}	0.86	2.51	3.340 (4)	162
N6—H6B···Cl2^{iii}	0.86	2.70	3.556 (3)	176
N7—H7B···O2^{iii}	0.86	2.24	3.002 (4)	148
N1—H1A···N8^{iv}	0.86	2.21	3.070 (4)	174
N7—H7A···N3^{v}	0.86	2.19	3.046 (4)	178

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

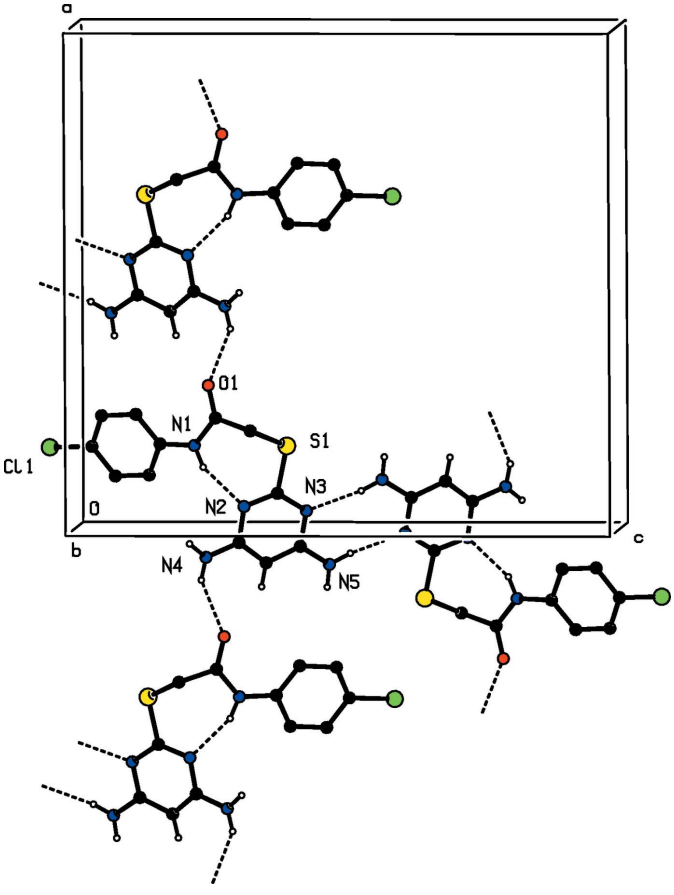


Figure 4
The crystal packing of compound (I) viewed along the *b* axis. H atoms not involved in hydrogen bonding (see Table 1), have been excluded for clarity.

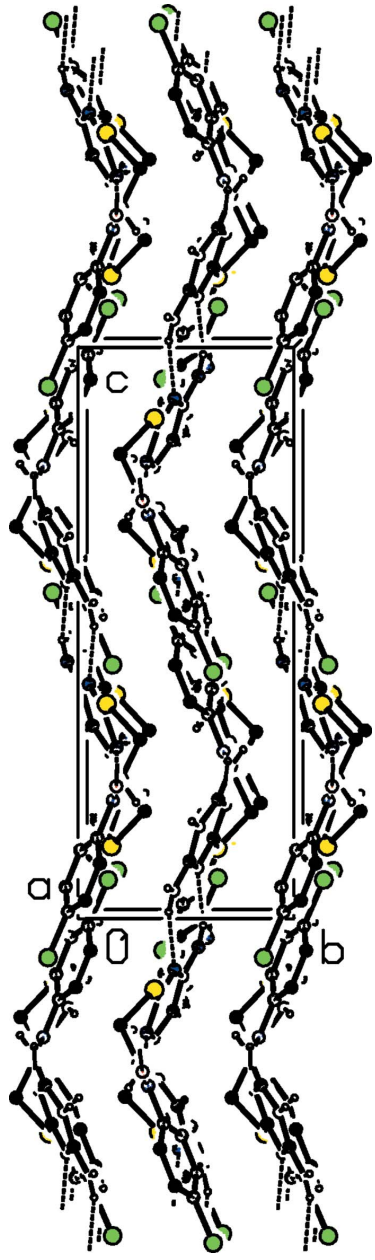


Figure 5
The crystal packing of compound (I) viewed along the *a* axis. H atoms not involved in hydrogen bonding (see Table 1), have been excluded for clarity.

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{12}H_{12}ClN_5OS$	$C_{12}H_{12}ClN_5OS$
M_r	309.78	309.78
Crystal system, space group	Orthorhombic, *Pbca*	Monoclinic, $P2_1/c$
Temperature (K)	293	293
a, b, c (Å)	18.2743 (12), 7.4835 (5), 19.8021 (12)	18.220 (2), 8.1180 (12), 19.628 (2)
α, β, γ (°)	90, 90, 90	90, 108.761 (8), 90
V (Å^3)	2708.1 (3)	2748.9 (6)
Z	8	8
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.44	0.43
Crystal size (mm)	0.28 × 0.25 × 0.18	0.31 × 0.22 × 0.16
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}	0.741, 0.863	0.742, 0.892
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22685, 3372, 2007	25810, 6858, 3462
R_{int}	0.060	0.075
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.669	0.668
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.161, 1.08	0.050, 0.155, 0.96
No. of reflections	3372	6858
No. of parameters	181	361
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.69	0.42, −0.42

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

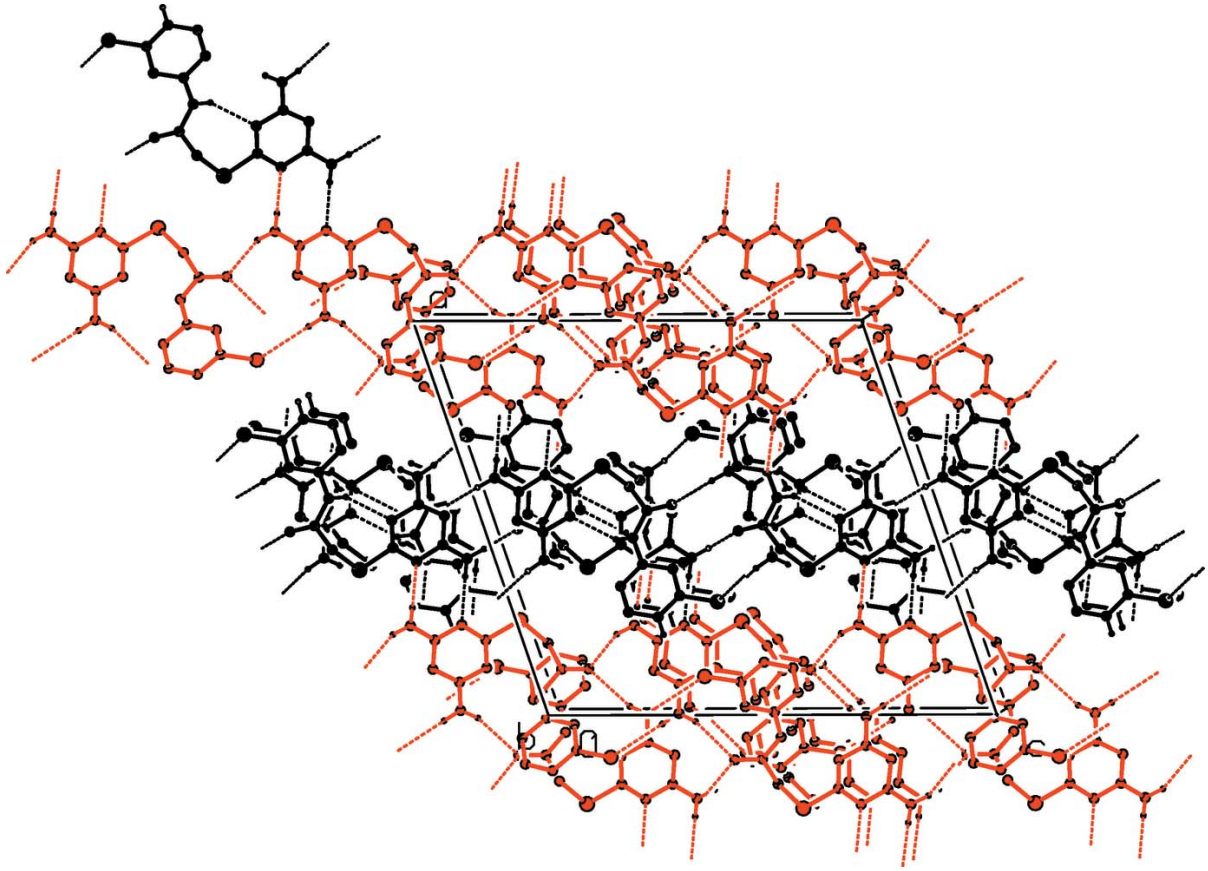


Figure 6
The crystal packing of compound (II) viewed along the *b* axis (colour code: *A* molecules black, *B* molecules red). H atoms not involved in hydrogen bonding (see Table 2), have been excluded for clarity.

5. Synthesis and crystallization

Compound (I):

To a solution of 4,6-diamino-pyrimidine-2-sulfanyl (0.5 g; 3.52 mmol) in 25 ml of ethanol, was added potassium hydroxide (0.2g; 3.52 mmol) and the mixture was refluxed for 30 min, after which 3.52 mmol of 2-chloro-*N*-(4-chlorophenyl)acetamide derivative was added and refluxed for 4 h. At the end of the reaction (monitored by TLC), the ethanol was evaporated *in vacuo* and cold water was added; the precipitate formed was filtered and dried to give compound (I) as a crystalline powder (yield 97%). Colourless block-like crystals were obtained from a solution in methanol and ethyl acetate (1:1) by slow evaporation of the solvents at room temperature.

Compound (II):

To a solution of 4,6-diamino-pyrimidine-2-thiol (0.5 g; 3.52 mmol) in 25 ml of ethanol was added potassium hydroxide (0.2g; 3.52 mmol) and the mixture was refluxed for 30 min. Then 3.52 mmol of 2-chloro-*N*-(3-chlorophenyl)acetamide was added and refluxed for 3 h. At the end of the reaction (monitored by TLC), the ethanol was evaporated *in vacuo* and cold water was added and the precipitate formed was filtered and dried to give compound (II) as a crystalline powder (yield 92%). Colourless block-like crystals were obtained from a solution in methanol and ethyl acetate (2:1) by slow evaporation of the solvents at room temperature.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. For both (I) and (II), hydrogen atoms were placed in calculated positions and refined as riding: C—H = 0.93–0.97 Å and N—H = 0.86 Å, with U_{iso}(H) = 1.2U_{eq}(N,C).

Acknowledgements

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supporting information

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

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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: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL2016* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

(I) *N*-(4-Chlorophenyl)-2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]acetamide

Crystal data

$C_{12}H_{12}ClN_5OS$
$M_r = 309.78$
Orthorhombic, *Pbca*
$a = 18.2743$ (12) Å
$b = 7.4835$ (5) Å
$c = 19.8021$ (12) Å
$V = 2708.1$ (3) Å^3
$Z = 8$
$F(000) = 1280$
$D_x = 1.520$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3372 reflections
$\theta = 2.1$–$28.4°$
$\mu = 0.44$ mm^{-1}
$T = 293$ K
Block, colourless
0.28 × 0.25 × 0.18 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.741$, $T_{max} = 0.863$
22685 measured reflections
3372 independent reflections
2007 reflections with $I > 2\sigma(I)$
$R_{int} = 0.060$
$\theta_{max} = 28.4°$, $\theta_{min} = 2.1°$
$h = -23 \rightarrow 24$
$k = -9 \rightarrow 9$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.161$
$S = 1.08$
3372 reflections
181 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
$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2 + 0.3384P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.69$ 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_{iso}*/U_{eq}
C1	0.21682 (15)	0.1105 (4)	0.10059 (13)	0.0467 (7)
H1	0.259655	0.165974	0.114873	0.056*
C2	0.21206 (16)	0.0419 (4)	0.03543 (13)	0.0524 (7)
H2	0.251506	0.052014	0.006002	0.063*
C3	0.14875 (17)	−0.0409 (4)	0.01479 (13)	0.0523 (7)
C4	0.08942 (17)	−0.0537 (4)	0.05714 (15)	0.0563 (8)
H4	0.046632	−0.108550	0.042405	0.068*
C5	0.09364 (15)	0.0152 (4)	0.12158 (14)	0.0505 (7)
H5	0.053355	0.007491	0.150122	0.061*
C6	0.15764 (13)	0.0963 (4)	0.14435 (12)	0.0411 (6)
C7	0.21262 (13)	0.2114 (4)	0.25020 (12)	0.0417 (6)
C8	0.18937 (14)	0.2955 (4)	0.31653 (13)	0.0466 (7)
H8A	0.151615	0.383361	0.307401	0.056*
H8B	0.230953	0.358263	0.335629	0.056*
C9	0.06049 (13)	0.1256 (4)	0.36033 (12)	0.0370 (6)
C10	−0.04825 (13)	0.0187 (4)	0.39846 (12)	0.0388 (6)
C11	−0.07960 (13)	0.0629 (4)	0.33698 (12)	0.0423 (6)
H11	−0.127989	0.033707	0.327503	0.051*
C12	−0.03712 (13)	0.1511 (4)	0.29042 (12)	0.0384 (6)
N1	0.15680 (11)	0.1680 (3)	0.20979 (10)	0.0439 (6)
H1A	0.113996	0.186830	0.226380	0.053*
N2	0.03568 (10)	0.1801 (3)	0.30081 (10)	0.0393 (5)
N3	0.02360 (10)	0.0518 (3)	0.41104 (10)	0.0396 (5)
N4	−0.06459 (12)	0.2133 (4)	0.23153 (10)	0.0513 (6)
H4A	−0.036471	0.267317	0.203330	0.062*
H4B	−0.110188	0.198752	0.222276	0.062*
N5	−0.08599 (12)	−0.0543 (4)	0.44936 (11)	0.0533 (7)
H5A	−0.064552	−0.077179	0.487041	0.064*
H5B	−0.131697	−0.078337	0.444396	0.064*
O1	0.27697 (10)	0.1893 (4)	0.23652 (10)	0.0662 (7)
S1	0.15519 (3)	0.13935 (11)	0.37853 (3)	0.0458 (2)
CL1	0.14411 (6)	−0.13289 (15)	−0.06572 (4)	0.0831 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0401 (14)	0.061 (2)	0.0392 (13)	0.0034 (13)	0.0018 (11)	0.0079 (13)
C2	0.0559 (17)	0.060 (2)	0.0414 (14)	0.0041 (15)	0.0078 (13)	0.0057 (14)
C3	0.076 (2)	0.0448 (17)	0.0356 (13)	−0.0015 (15)	0.0010 (13)	0.0034 (12)
C4	0.0668 (19)	0.054 (2)	0.0478 (15)	−0.0159 (15)	−0.0061 (14)	0.0062 (15)
C5	0.0508 (16)	0.056 (2)	0.0446 (15)	−0.0121 (14)	0.0037 (12)	0.0070 (14)
C6	0.0404 (14)	0.0481 (17)	0.0349 (12)	0.0039 (12)	0.0025 (10)	0.0061 (12)
C7	0.0361 (13)	0.0500 (17)	0.0390 (13)	0.0010 (12)	0.0049 (11)	0.0045 (12)
C8	0.0396 (14)	0.0560 (18)	0.0441 (14)	−0.0070 (12)	0.0021 (11)	−0.0017 (13)
C9	0.0320 (12)	0.0451 (16)	0.0338 (11)	0.0015 (11)	0.0008 (9)	−0.0041 (11)
C10	0.0361 (13)	0.0442 (16)	0.0362 (12)	−0.0026 (11)	0.0054 (10)	−0.0040 (11)
C11	0.0329 (13)	0.0544 (18)	0.0396 (13)	−0.0040 (11)	−0.0016 (11)	−0.0011 (12)
C12	0.0347 (13)	0.0466 (17)	0.0339 (12)	0.0035 (11)	−0.0013 (10)	−0.0046 (11)
N1	0.0330 (11)	0.0617 (16)	0.0370 (11)	0.0029 (10)	0.0041 (9)	0.0006 (10)
N2	0.0307 (10)	0.0526 (14)	0.0344 (10)	0.0011 (9)	0.0008 (9)	0.0016 (10)
N3	0.0328 (11)	0.0517 (15)	0.0344 (10)	−0.0028 (9)	0.0001 (8)	0.0007 (10)
N4	0.0372 (12)	0.0783 (19)	0.0385 (11)	−0.0016 (12)	−0.0058 (10)	0.0095 (12)
N5	0.0426 (13)	0.0767 (19)	0.0405 (11)	−0.0161 (12)	−0.0008 (10)	0.0088 (12)
O1	0.0304 (10)	0.114 (2)	0.0538 (12)	0.0020 (11)	0.0062 (8)	−0.0101 (12)
S1	0.0312 (3)	0.0698 (5)	0.0363 (3)	−0.0015 (3)	−0.0016 (3)	0.0060 (3)
CL1	0.1216 (9)	0.0854 (7)	0.0422 (4)	−0.0171 (6)	0.0013 (4)	−0.0090 (4)

Geometric parameters (Å, º)

C1—C6	1.390 (3)	C8—H8B	0.9700
C1—C2	1.391 (4)	C9—N2	1.327 (3)
C1—H1	0.9300	C9—N3	1.329 (3)
C2—C3	1.375 (4)	C9—S1	1.771 (2)
C2—H2	0.9300	C10—N5	1.338 (3)
C3—C4	1.374 (4)	C10—N3	1.359 (3)
C3—CL1	1.739 (3)	C10—C11	1.386 (3)
C4—C5	1.378 (4)	C11—C12	1.374 (4)
C4—H4	0.9300	C11—H11	0.9300
C5—C6	1.393 (4)	C12—N4	1.352 (3)
C5—H5	0.9300	C12—N2	1.364 (3)
C6—N1	1.403 (3)	N1—H1A	0.8600
C7—O1	1.218 (3)	N4—H4A	0.8600
C7—N1	1.337 (3)	N4—H4B	0.8600
C7—C8	1.517 (4)	N5—H5A	0.8600
C8—S1	1.807 (3)	N5—H5B	0.8600
C8—H8A	0.9700		
C6—C1—C2	120.1 (3)	H8A—C8—H8B	107.6
C6—C1—H1	120.0	N2—C9—N3	128.7 (2)
C2—C1—H1	120.0	N2—C9—S1	119.79 (18)
C3—C2—C1	119.7 (3)	N3—C9—S1	111.47 (17)

C3—C2—H2	120.2	N5—C10—N3	115.8 (2)
C1—C2—H2	120.2	N5—C10—C11	123.1 (2)
C4—C3—C2	120.9 (3)	N3—C10—C11	121.1 (2)
C4—C3—CL1	119.6 (2)	C12—C11—C10	118.1 (2)
C2—C3—CL1	119.5 (2)	C12—C11—H11	121.0
C3—C4—C5	119.7 (3)	C10—C11—H11	121.0
C3—C4—H4	120.2	N4—C12—N2	116.0 (2)
C5—C4—H4	120.2	N4—C12—C11	122.3 (2)
C4—C5—C6	120.7 (3)	N2—C12—C11	121.7 (2)
C4—C5—H5	119.7	C7—N1—C6	129.6 (2)
C6—C5—H5	119.7	C7—N1—H1A	115.2
C1—C6—C5	119.0 (2)	C6—N1—H1A	115.2
C1—C6—N1	123.7 (2)	C9—N2—C12	114.7 (2)
C5—C6—N1	117.2 (2)	C9—N3—C10	115.3 (2)
O1—C7—N1	124.8 (3)	C12—N4—H4A	120.0
O1—C7—C8	121.3 (2)	C12—N4—H4B	120.0
N1—C7—C8	113.9 (2)	H4A—N4—H4B	120.0
C7—C8—S1	114.6 (2)	C10—N5—H5A	120.0
C7—C8—H8A	108.6	C10—N5—H5B	120.0
S1—C8—H8A	108.6	H5A—N5—H5B	120.0
C7—C8—H8B	108.6	C9—S1—C8	103.73 (12)
S1—C8—H8B	108.6		

C6—C1—C2—C3	−0.4 (4)	O1—C7—N1—C6	−2.5 (5)
C1—C2—C3—C4	1.4 (5)	C8—C7—N1—C6	176.8 (3)
C1—C2—C3—CL1	−177.9 (2)	C1—C6—N1—C7	−22.2 (5)
C2—C3—C4—C5	−0.9 (5)	C5—C6—N1—C7	161.4 (3)
CL1—C3—C4—C5	178.4 (2)	N3—C9—N2—C12	−2.0 (4)
C3—C4—C5—C6	−0.5 (5)	S1—C9—N2—C12	175.36 (19)
C2—C1—C6—C5	−1.0 (4)	N4—C12—N2—C9	176.9 (2)
C2—C1—C6—N1	−177.3 (3)	C11—C12—N2—C9	−3.5 (4)
C4—C5—C6—C1	1.5 (4)	N2—C9—N3—C10	4.2 (4)
C4—C5—C6—N1	178.1 (3)	S1—C9—N3—C10	−173.28 (19)
O1—C7—C8—S1	−103.4 (3)	N5—C10—N3—C9	−179.5 (2)
N1—C7—C8—S1	77.2 (3)	C11—C10—N3—C9	−1.0 (4)
N5—C10—C11—C12	174.5 (3)	N2—C9—S1—C8	17.9 (2)
N3—C10—C11—C12	−3.8 (4)	N3—C9—S1—C8	−164.3 (2)
C10—C11—C12—N4	−174.2 (3)	C7—C8—S1—C9	−88.3 (2)
C10—C11—C12—N2	6.3 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N2	0.86	2.06	2.856 (3)	154
N5—H5*A*···N3^{i}	0.86	2.16	2.990 (3)	162

N4—H4*B*···O1^{ii}	0.86	2.22	2.969 (3)	146
C11—H11···O1^{ii}	0.93	2.45	3.144 (3)	132

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

(II) *N*-(3-Chlorophenyl)-2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]acetamide

Crystal data

$C_{12}H_{12}ClN_5OS$
M_r = 309.78
Monoclinic, $P2_1/c$
a = 18.220 (2) Å
b = 8.1180 (12) Å
c = 19.628 (2) Å
β = 108.761 (8)°
V = 2748.9 (6) Å^3
Z = 8
$F(000)$ = 1280
D_x = 1.497 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6858 reflections
θ = 1.2–28.4°
μ = 0.43 mm^{-1}
T = 293 K
Block, colourless
0.31 × 0.22 × 0.16 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.742, T_{max} = 0.892
25810 measured reflections
6858 independent reflections
3462 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 28.4°, θ_{min} = 1.2°
h = −24→24
k = −10→10
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.155
S = 0.96
6858 reflections
361 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
$w = 1/[\sigma^2(F_o^2) + (0.0646P)^2 + 0.6656P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 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}
C1	0.43039 (17)	0.6518 (4)	0.39062 (15)	0.0438 (7)
C2	0.50489 (17)	0.5880 (4)	0.41809 (15)	0.0461 (8)
H2	0.533524	0.599968	0.466472	0.055*
C3	0.53498 (16)	0.5069 (4)	0.37174 (15)	0.0424 (7)
C4	0.42495 (16)	0.5606 (4)	0.27980 (15)	0.0400 (7)

C5	0.42189 (17)	0.4300 (4)	0.14672 (16)	0.0485 (8)
H5A	0.448033	0.345147	0.180668	0.058*
H5B	0.385949	0.375940	0.105242	0.058*
C6	0.48119 (18)	0.5233 (4)	0.12307 (16)	0.0473 (8)
C7	0.61562 (17)	0.6320 (4)	0.17094 (16)	0.0476 (8)
C8	0.67034 (19)	0.6788 (5)	0.23523 (18)	0.0592 (9)
H8	0.663419	0.650619	0.278689	0.071*
C9	0.7347 (2)	0.7666 (5)	0.2351 (2)	0.0737 (11)
H9	0.770444	0.800365	0.278367	0.088*
C10	0.7465 (2)	0.8045 (5)	0.1718 (2)	0.0663 (10)
H10	0.790323	0.863055	0.171667	0.080*
C11	0.69326 (19)	0.7553 (4)	0.10864 (18)	0.0554 (9)
C12	0.62693 (19)	0.6684 (4)	0.10619 (18)	0.0538 (8)
H12	0.591368	0.635782	0.062620	0.065*
C13	1.07720 (18)	0.5427 (4)	−0.18594 (16)	0.0518 (8)
C14	1.11114 (17)	0.6066 (4)	−0.23360 (16)	0.0545 (9)
H14	1.085128	0.607744	−0.282867	0.065*
C15	1.18621 (18)	0.6699 (4)	−0.20499 (16)	0.0504 (8)
C16	1.18492 (16)	0.6063 (4)	−0.09333 (15)	0.0422 (7)
C17	1.17491 (16)	0.5113 (4)	0.04034 (15)	0.0474 (8)
H17A	1.152219	0.418732	0.009504	0.057*
H17B	1.207528	0.467064	0.085940	0.057*
C18	1.11047 (17)	0.6094 (4)	0.05351 (16)	0.0457 (7)
C19	0.98833 (16)	0.7549 (4)	−0.01350 (15)	0.0428 (7)
C20	0.93861 (17)	0.7880 (4)	−0.08218 (16)	0.0488 (8)
H20	0.948465	0.742561	−0.121865	0.059*
C21	0.87475 (18)	0.8876 (4)	−0.09216 (17)	0.0554 (9)
H21	0.841809	0.907855	−0.138552	0.066*
C22	0.85896 (18)	0.9577 (4)	−0.03444 (17)	0.0533 (8)
H22	0.815921	1.024970	−0.041084	0.064*
C23	0.90908 (17)	0.9246 (4)	0.03344 (16)	0.0477 (8)
C24	0.97354 (17)	0.8249 (4)	0.04526 (16)	0.0460 (8)
H24	1.006364	0.805075	0.091743	0.055*
N1	0.39450 (15)	0.7294 (4)	0.43183 (13)	0.0584 (8)
H1A	0.347948	0.765256	0.412896	0.070*
H1B	0.418159	0.742920	0.477051	0.070*
N2	0.60725 (15)	0.4414 (4)	0.39269 (13)	0.0573 (7)
H2A	0.624904	0.396367	0.361454	0.069*
H2B	0.635444	0.444816	0.437208	0.069*
N3	0.38865 (13)	0.6359 (3)	0.31978 (12)	0.0436 (6)
N4	0.49560 (13)	0.4945 (3)	0.30007 (12)	0.0412 (6)
N5	0.55000 (14)	0.5449 (3)	0.17471 (13)	0.0501 (7)
H5	0.554587	0.499513	0.215468	0.060*
N6	1.00456 (16)	0.4803 (4)	−0.20701 (15)	0.0811 (11)
H6A	0.984742	0.445292	−0.175429	0.097*
H6B	0.978147	0.475742	−0.252009	0.097*
N7	1.22370 (15)	0.7369 (4)	−0.24649 (14)	0.0698 (9)
H7A	1.269792	0.775136	−0.227375	0.084*

H7B	1.201739	0.741880	−0.292327	0.084*
N8	1.22428 (13)	0.6664 (3)	−0.13364 (12)	0.0461 (6)
N9	1.11350 (14)	0.5443 (3)	−0.11441 (12)	0.0479 (6)
N10	1.05376 (13)	0.6562 (3)	−0.00640 (12)	0.0448 (6)
H10A	1.058236	0.620508	−0.046127	0.054*
O1	0.46540 (13)	0.5750 (4)	0.06196 (11)	0.0714 (7)
O2	1.11150 (13)	0.6397 (3)	0.11485 (11)	0.0643 (7)
S1	0.36824 (4)	0.56020 (11)	0.18798 (4)	0.0463 (2)
S2	1.23535 (4)	0.62488 (11)	−0.00038 (4)	0.0492 (2)
CL1	0.70803 (5)	0.80248 (14)	0.02776 (5)	0.0738 (3)
CL2	0.89352 (5)	1.01784 (12)	0.10723 (5)	0.0649 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0507 (17)	0.045 (2)	0.0406 (16)	−0.0074 (15)	0.0221 (14)	−0.0013 (14)
C2	0.0525 (17)	0.053 (2)	0.0330 (15)	−0.0094 (16)	0.0143 (13)	−0.0020 (15)
C3	0.0464 (16)	0.0413 (19)	0.0398 (16)	−0.0036 (14)	0.0143 (13)	0.0040 (14)
C4	0.0466 (16)	0.0371 (18)	0.0393 (15)	−0.0063 (14)	0.0178 (13)	−0.0023 (13)
C5	0.0539 (17)	0.052 (2)	0.0403 (16)	−0.0006 (16)	0.0166 (14)	−0.0116 (15)
C6	0.0552 (18)	0.055 (2)	0.0380 (16)	0.0100 (16)	0.0232 (15)	0.0024 (15)
C7	0.0521 (17)	0.046 (2)	0.0499 (18)	0.0132 (16)	0.0232 (15)	0.0032 (16)
C8	0.061 (2)	0.069 (3)	0.0482 (19)	0.0039 (19)	0.0180 (17)	0.0030 (18)
C9	0.066 (2)	0.089 (3)	0.062 (2)	−0.001 (2)	0.0159 (19)	−0.002 (2)
C10	0.054 (2)	0.073 (3)	0.069 (2)	−0.0075 (19)	0.0165 (19)	−0.003 (2)
C11	0.059 (2)	0.056 (2)	0.058 (2)	0.0111 (18)	0.0301 (17)	0.0080 (18)
C12	0.0582 (19)	0.055 (2)	0.0527 (19)	0.0064 (17)	0.0240 (16)	0.0013 (17)
C13	0.0544 (18)	0.059 (2)	0.0405 (17)	−0.0068 (17)	0.0129 (15)	−0.0037 (16)
C14	0.0539 (18)	0.075 (3)	0.0339 (16)	−0.0053 (18)	0.0128 (14)	−0.0001 (16)
C15	0.0532 (18)	0.059 (2)	0.0424 (17)	0.0088 (16)	0.0201 (15)	0.0042 (16)
C16	0.0478 (16)	0.0424 (19)	0.0394 (15)	0.0039 (15)	0.0182 (13)	0.0018 (14)
C17	0.0470 (16)	0.055 (2)	0.0384 (16)	−0.0037 (15)	0.0117 (13)	0.0106 (15)
C18	0.0487 (17)	0.050 (2)	0.0405 (17)	−0.0135 (15)	0.0176 (14)	−0.0007 (15)
C19	0.0411 (15)	0.0448 (19)	0.0436 (17)	−0.0150 (14)	0.0151 (13)	−0.0049 (15)
C20	0.0448 (17)	0.060 (2)	0.0409 (17)	−0.0111 (16)	0.0123 (14)	0.0017 (16)
C21	0.0499 (18)	0.064 (2)	0.0470 (18)	−0.0147 (17)	0.0079 (15)	0.0024 (17)
C22	0.0452 (17)	0.053 (2)	0.060 (2)	−0.0072 (16)	0.0147 (16)	0.0037 (17)
C23	0.0510 (17)	0.050 (2)	0.0471 (18)	−0.0123 (16)	0.0227 (15)	−0.0012 (15)
C24	0.0470 (17)	0.050 (2)	0.0417 (17)	−0.0109 (15)	0.0149 (14)	0.0024 (15)
N1	0.0530 (15)	0.086 (2)	0.0404 (14)	0.0043 (15)	0.0203 (12)	−0.0148 (14)
N2	0.0543 (15)	0.071 (2)	0.0427 (15)	0.0115 (15)	0.0108 (12)	0.0000 (14)
N3	0.0461 (13)	0.0513 (17)	0.0367 (13)	−0.0030 (12)	0.0180 (11)	−0.0083 (12)
N4	0.0487 (14)	0.0416 (15)	0.0345 (13)	0.0011 (12)	0.0153 (11)	−0.0003 (11)
N5	0.0552 (15)	0.0582 (19)	0.0387 (14)	0.0041 (14)	0.0178 (12)	0.0082 (13)
N6	0.0650 (18)	0.131 (3)	0.0406 (16)	−0.044 (2)	0.0086 (14)	−0.0034 (18)
N7	0.0558 (16)	0.114 (3)	0.0421 (15)	−0.0083 (17)	0.0198 (13)	0.0182 (16)
N8	0.0448 (13)	0.0557 (18)	0.0399 (14)	0.0009 (12)	0.0167 (11)	0.0077 (12)
N9	0.0468 (14)	0.0583 (18)	0.0372 (14)	−0.0109 (13)	0.0115 (11)	−0.0003 (13)

N10	0.0414 (13)	0.0570 (18)	0.0359 (13)	−0.0045 (12)	0.0126 (11)	−0.0002 (12)
O1	0.0594 (14)	0.113 (2)	0.0437 (13)	0.0075 (14)	0.0188 (11)	0.0222 (14)
O2	0.0714 (15)	0.0839 (18)	0.0362 (12)	0.0075 (14)	0.0152 (11)	−0.0032 (12)
S1	0.0464 (4)	0.0585 (6)	0.0351 (4)	0.0021 (4)	0.0146 (3)	−0.0024 (4)
S2	0.0415 (4)	0.0653 (6)	0.0391 (4)	−0.0092 (4)	0.0107 (3)	0.0047 (4)
CL1	0.0698 (6)	0.0948 (8)	0.0647 (6)	−0.0090 (5)	0.0327 (5)	0.0072 (5)
CL2	0.0665 (5)	0.0756 (7)	0.0602 (5)	0.0000 (5)	0.0308 (4)	−0.0049 (5)

Geometric parameters (Å, º)

C1—N1	1.348 (4)	C15—N7	1.336 (4)
C1—N3	1.360 (3)	C15—N8	1.348 (4)
C1—C2	1.389 (4)	C16—N8	1.320 (3)
C2—C3	1.372 (4)	C16—N9	1.331 (4)
C2—H2	0.9300	C16—S2	1.766 (3)
C3—N2	1.355 (4)	C17—C18	1.508 (4)
C3—N4	1.362 (3)	C17—S2	1.808 (3)
C4—N3	1.327 (3)	C17—H17A	0.9700
C4—N4	1.332 (4)	C17—H17B	0.9700
C4—S1	1.766 (3)	C18—O2	1.223 (3)
C5—C6	1.510 (4)	C18—N10	1.346 (4)
C5—S1	1.800 (3)	C19—C24	1.388 (4)
C5—H5A	0.9700	C19—C20	1.387 (4)
C5—H5B	0.9700	C19—N10	1.405 (4)
C6—O1	1.215 (3)	C20—C21	1.378 (4)
C6—N5	1.346 (4)	C20—H20	0.9300
C7—C12	1.383 (4)	C21—C22	1.378 (4)
C7—C8	1.386 (4)	C21—H21	0.9300
C7—N5	1.411 (4)	C22—C23	1.378 (4)
C8—C9	1.374 (5)	C22—H22	0.9300
C8—H8	0.9300	C23—C24	1.383 (4)
C9—C10	1.361 (5)	C23—CL2	1.736 (3)
C9—H9	0.9300	C24—H24	0.9300
C10—C11	1.366 (5)	N1—H1A	0.8600
C10—H10	0.9300	N1—H1B	0.8600
C11—C12	1.387 (4)	N2—H2A	0.8600
C11—CL1	1.736 (3)	N2—H2B	0.8600
C12—H12	0.9300	N5—H5	0.8600
C13—N9	1.346 (4)	N6—H6A	0.8600
C13—N6	1.352 (4)	N6—H6B	0.8600
C13—C14	1.378 (4)	N7—H7A	0.8600
C14—C15	1.398 (4)	N7—H7B	0.8600
C14—H14	0.9300	N10—H10A	0.8600
N1—C1—N3	116.0 (3)	C18—C17—S2	115.1 (2)
N1—C1—C2	122.9 (3)	C18—C17—H17A	108.5
N3—C1—C2	121.1 (3)	S2—C17—H17A	108.5
C3—C2—C1	118.1 (3)	C18—C17—H17B	108.5

C3—C2—H2	121.0	S2—C17—H17B	108.5
C1—C2—H2	121.0	H17A—C17—H17B	107.5
N2—C3—N4	115.0 (3)	O2—C18—N10	124.6 (3)
N2—C3—C2	122.9 (3)	O2—C18—C17	120.6 (3)
N4—C3—C2	122.0 (3)	N10—C18—C17	114.9 (2)
N3—C4—N4	128.8 (3)	C24—C19—C20	119.2 (3)
N3—C4—S1	111.4 (2)	C24—C19—N10	122.4 (3)
N4—C4—S1	119.8 (2)	C20—C19—N10	118.3 (3)
C6—C5—S1	112.9 (2)	C21—C20—C19	120.6 (3)
C6—C5—H5A	109.0	C21—C20—H20	119.7
S1—C5—H5A	109.0	C19—C20—H20	119.7
C6—C5—H5B	109.0	C22—C21—C20	121.0 (3)
S1—C5—H5B	109.0	C22—C21—H21	119.5
H5A—C5—H5B	107.8	C20—C21—H21	119.5
O1—C6—N5	124.5 (3)	C23—C22—C21	117.8 (3)
O1—C6—C5	120.8 (3)	C23—C22—H22	121.1
N5—C6—C5	114.8 (3)	C21—C22—H22	121.1
C12—C7—C8	120.1 (3)	C22—C23—C24	122.6 (3)
C12—C7—N5	122.3 (3)	C22—C23—CL2	119.1 (3)
C8—C7—N5	117.6 (3)	C24—C23—CL2	118.2 (2)
C9—C8—C7	120.3 (3)	C23—C24—C19	118.8 (3)
C9—C8—H8	119.8	C23—C24—H24	120.6
C7—C8—H8	119.8	C19—C24—H24	120.6
C10—C9—C8	120.3 (4)	C1—N1—H1A	120.0
C10—C9—H9	119.8	C1—N1—H1B	120.0
C8—C9—H9	119.8	H1A—N1—H1B	120.0
C9—C10—C11	119.2 (3)	C3—N2—H2A	120.0
C9—C10—H10	120.4	C3—N2—H2B	120.0
C11—C10—H10	120.4	H2A—N2—H2B	120.0
C10—C11—C12	122.5 (3)	C4—N3—C1	115.3 (2)
C10—C11—CL1	119.5 (3)	C4—N4—C3	114.6 (2)
C12—C11—CL1	118.0 (3)	C6—N5—C7	128.7 (3)
C7—C12—C11	117.5 (3)	C6—N5—H5	115.6
C7—C12—H12	121.2	C7—N5—H5	115.6
C11—C12—H12	121.2	C13—N6—H6A	120.0
N9—C13—N6	115.3 (3)	C13—N6—H6B	120.0
N9—C13—C14	121.8 (3)	H6A—N6—H6B	120.0
N6—C13—C14	122.8 (3)	C15—N7—H7A	120.0
C13—C14—C15	117.4 (3)	C15—N7—H7B	120.0
C13—C14—H14	121.3	H7A—N7—H7B	120.0
C15—C14—H14	121.3	C16—N8—C15	115.7 (3)
N7—C15—N8	116.7 (3)	C16—N9—C13	115.5 (2)
N7—C15—C14	122.0 (3)	C18—N10—C19	129.5 (3)
N8—C15—C14	121.3 (3)	C18—N10—H10A	115.3
N8—C16—N9	128.2 (3)	C19—N10—H10A	115.3
N8—C16—S2	112.7 (2)	C4—S1—C5	103.66 (14)
N9—C16—S2	119.0 (2)	C16—S2—C17	102.99 (14)

N1—C1—C2—C3	178.0 (3)	N10—C19—C24—C23	178.0 (3)
N3—C1—C2—C3	−0.6 (4)	N4—C4—N3—C1	2.2 (5)
C1—C2—C3—N2	179.3 (3)	S1—C4—N3—C1	−175.7 (2)
C1—C2—C3—N4	3.1 (4)	N1—C1—N3—C4	179.5 (3)
S1—C5—C6—O1	−93.7 (3)	C2—C1—N3—C4	−1.9 (4)
S1—C5—C6—N5	85.2 (3)	N3—C4—N4—C3	0.1 (4)
C12—C7—C8—C9	2.3 (5)	S1—C4—N4—C3	177.8 (2)
N5—C7—C8—C9	−178.8 (3)	N2—C3—N4—C4	−179.4 (3)
C7—C8—C9—C10	−1.9 (6)	C2—C3—N4—C4	−2.9 (4)
C8—C9—C10—C11	0.6 (6)	O1—C6—N5—C7	2.0 (5)
C9—C10—C11—C12	0.3 (6)	C5—C6—N5—C7	−176.9 (3)
C9—C10—C11—CL1	−179.8 (3)	C12—C7—N5—C6	−20.0 (5)
C8—C7—C12—C11	−1.4 (5)	C8—C7—N5—C6	161.1 (3)
N5—C7—C12—C11	179.7 (3)	N9—C16—N8—C15	2.3 (5)
C10—C11—C12—C7	0.1 (5)	S2—C16—N8—C15	−174.2 (2)
CL1—C11—C12—C7	−179.8 (2)	N7—C15—N8—C16	177.1 (3)
N9—C13—C14—C15	1.8 (5)	C14—C15—N8—C16	−2.7 (5)
N6—C13—C14—C15	179.0 (3)	N8—C16—N9—C13	0.1 (5)
C13—C14—C15—N7	−178.9 (3)	S2—C16—N9—C13	176.4 (2)
C13—C14—C15—N8	0.8 (5)	N6—C13—N9—C16	−179.7 (3)
S2—C17—C18—O2	−112.5 (3)	C14—C13—N9—C16	−2.2 (5)
S2—C17—C18—N10	68.4 (3)	O2—C18—N10—C19	4.6 (5)
C24—C19—C20—C21	−0.7 (4)	C17—C18—N10—C19	−176.3 (3)
N10—C19—C20—C21	−178.3 (3)	C24—C19—N10—C18	1.4 (5)
C19—C20—C21—C22	0.5 (5)	C20—C19—N10—C18	178.8 (3)
C20—C21—C22—C23	−0.1 (5)	N3—C4—S1—C5	−172.4 (2)
C21—C22—C23—C24	−0.1 (5)	N4—C4—S1—C5	9.5 (3)
C21—C22—C23—CL2	177.2 (2)	C6—C5—S1—C4	−88.7 (2)
C22—C23—C24—C19	−0.1 (4)	N8—C16—S2—C17	−172.9 (2)
CL2—C23—C24—C19	−177.5 (2)	N9—C16—S2—C17	10.3 (3)
C20—C19—C24—C23	0.6 (4)	C18—C17—S2—C16	−86.9 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5···N4	0.86	2.25	2.962 (3)	140
N10—H10*A*···N9	0.86	2.02	2.826 (3)	157
N1—H1*B*···O1^{i}	0.86	2.19	2.931 (4)	145
N2—H2*B*···Cl1^{i}	0.86	2.76	3.405 (3)	133
N6—H6*A*···O2^{ii}	0.86	2.51	3.340 (4)	162
N6—H6*B*···Cl2^{iii}	0.86	2.70	3.556 (3)	176
N7—H7*B*···O2^{iii}	0.86	2.24	3.002 (4)	148
N1—H1*A*···N8^{iv}	0.86	2.21	3.070 (4)	174
N7—H7*A*···N3^{v}	0.86	2.19	3.046 (4)	178

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