



Crystal structures of 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(naphthalen-1-yl)acetamide and 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(4-fluorophenyl)acetamide

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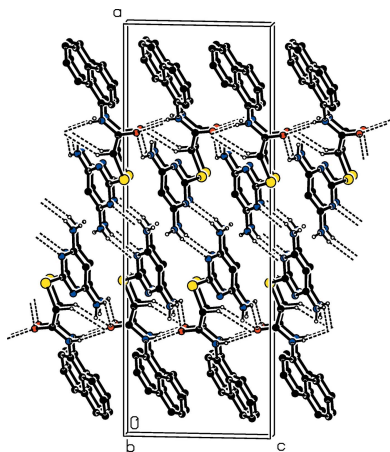
The title compounds, C₁₆H₁₅N₅OS, (I), and C₁₂H₁₂FN₅OS, (II), are [(diaminopyrimidine)sulfanyl]acetamide derivatives. In (I), the pyrimidine ring is inclined to the naphthalene ring system by 55.5 (1)°, while in (II), the pyrimidine ring is inclined to the benzene ring by 58.93 (8)°. In (II), there is an intramolecular N—H···N hydrogen bond and a short C—H···O contact. In the crystals of (I) and (II), molecules are linked by pairs of N—H···N hydrogen bonds, forming inversion dimers with R₂²(8) ring motifs. In the crystal of (I), the dimers are linked by bifurcated N—H···(O,O) and C—H···O hydrogen bonds, forming layers parallel to (100). In the crystal of (II), the dimers are linked by N—H···O hydrogen bonds, also forming layers parallel to (100). The layers are linked by C—H···F hydrogen bonds, forming a three-dimensional architecture.

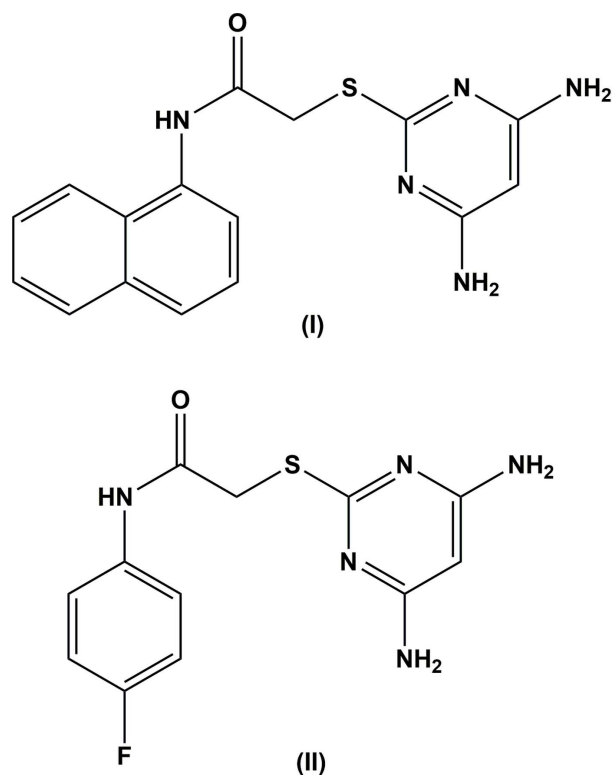
1. Chemical context

As a result of the innate ability of bacteria to develop resistance to available antibiotics, there is a critical need to develop new agents to treat more strains that are resilient. Several classes of diaminopyrimidines have been reported as new therapeutic agents. Derivatives of diaminopyrimidines also exhibit anti-cancer activity (Xu *et al.*, 2010), immune suppressant activity (Blumenkopf *et al.*, 2002), hair-growth-stimulant properties, anti-bacterial (Kandeel *et al.*, 1994) and potential anti-microbial properties (Holla *et al.*, 2006). They are also used as potential anti-AIDS agents (Nogueras *et al.*, 1993) and anti-viral agents (Hocková *et al.*, 2004). In this connection, the title 4,6-diaminopyrimidine-based analogues have been synthesized as potential antiviral agents against dengue for targeting NS2B/NS3 protease.

2. Structural commentary

The molecular structure of compound (I) is shown in Fig. 1. The pyrimidine ring is twisted with respect to the thioacetamide unit with the N1—C11—C12—S1 torsion angle being 140.88 (18)°. The pyrimidine ring (C13—C16/N2/N3) makes a dihedral angle of 55.5 (1)° with the naphthalene ring system (C1—C10). The amine nitrogen atoms, N4 and N5, deviate by 0.0235 and 0.0291 Å, respectively, from the plane of the pyrimidine ring.





The molecular structure of compound (II) is shown in Fig. 2. Here, the pyrimidine ring is twisted with respect to the thioacetamide unit with the N1–C7–C8–S1 torsion angle being $-82.44(14)^\circ$. The pyrimidine ring (C9–C12/N2/N3) makes a dihedral angle of $58.93(8)^\circ$ with the benzene ring (C1–C6). The amine nitrogen atoms, N4 and N5, deviate by 0.0247 and 0.0564 Å, respectively, from the pyrimidine ring. In compound (II), there is an intramolecular N–H···N hydrogen bond and a short C–H···O interaction present (Table 2 and Fig. 2).

3. Supramolecular features

In the crystal of compound (I), molecules are linked by pairs of N5–H5A···N3ⁱ hydrogen bonds, forming inversion dimers with an $R_2^2(8)$ ring motif (Table 1 and Fig. 3). The dimers are

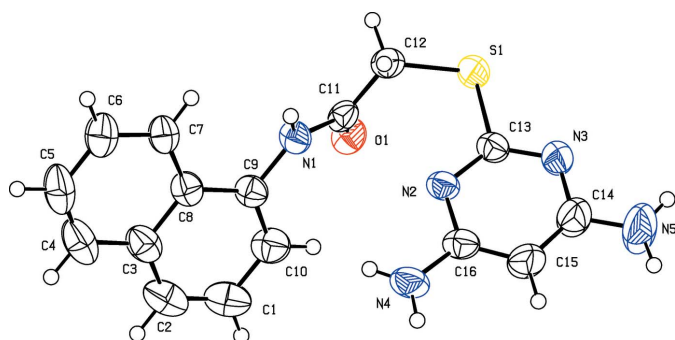


Figure 1
The molecular structure of compound (I), showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

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

| <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> |
|-----------------------------|-------------|---------------|-----------------------|-------------------------|
| N5–H5A···N3 ⁱ | 0.86 | 2.27 | 3.110 (4) | 167 |
| N1–H1A···O1 ⁱⁱ | 0.86 | 2.05 | 2.890 (3) | 165 |
| N4–H4B···O1 ⁱⁱⁱ | 0.86 | 2.36 | 2.964 (3) | 127 |
| C12–H12A···O1 ⁱⁱ | 0.97 | 2.58 | 3.408 (3) | 143 |

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

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

| <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> |
|---------------------------|-------------|---------------|-----------------------|-------------------------|
| N1–H1···N3 | 0.86 | 2.25 | 2.990 (2) | 145 |
| C3–H3···O1 | 0.93 | 2.31 | 2.903 (2) | 121 |
| N5–H5A···N2 ⁱ | 0.86 | 2.29 | 3.139 (2) | 169 |
| N4–H4A···O1 ⁱⁱ | 0.86 | 2.23 | 2.9852 (18) | 146 |
| C2–H2···F1 ⁱⁱⁱ | 0.93 | 2.48 | 3.404 (3) | 172 |

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

linked by bifurcated N–H···(O,O) and C–H···O hydrogen bonds, forming layers parallel to the *bc* plane (Table 1 and Fig. 3).

In the crystal of compound (II), inversion dimers, with an $R_2^2(8)$, ring motif, are also formed *via* pairs of N5–H5A···N2ⁱ hydrogen bonds (Table 2 and Fig. 4). This time the dimers are linked by N–H···O hydrogen bonds and also form layers parallel to the *bc* plane (Table 2 and Fig. 4). The layers are linked by C–H···F hydrogen bonds, forming a three-dimensional architecture (Table 2 and Fig. 4).

4. Database survey

A search of the Cambridge Structural Database (Version 5.37, update May 2016; Groom *et al.*, 2016) for 2-(pyrimidin-2-yl)-*N*-phenylacetamide yielded only five hits. They include two 4,6-dimethylpyrimidine analogues *viz.* 2-(4,6-dimethylpyrimidin-2-ylsulfanyl)-*N*-phenyl acetamide (DIWXAJ; Gao

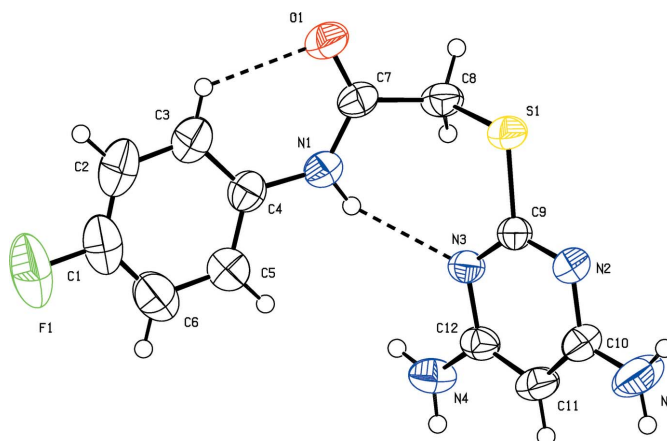


Figure 2
The molecular structure of compound (II), showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

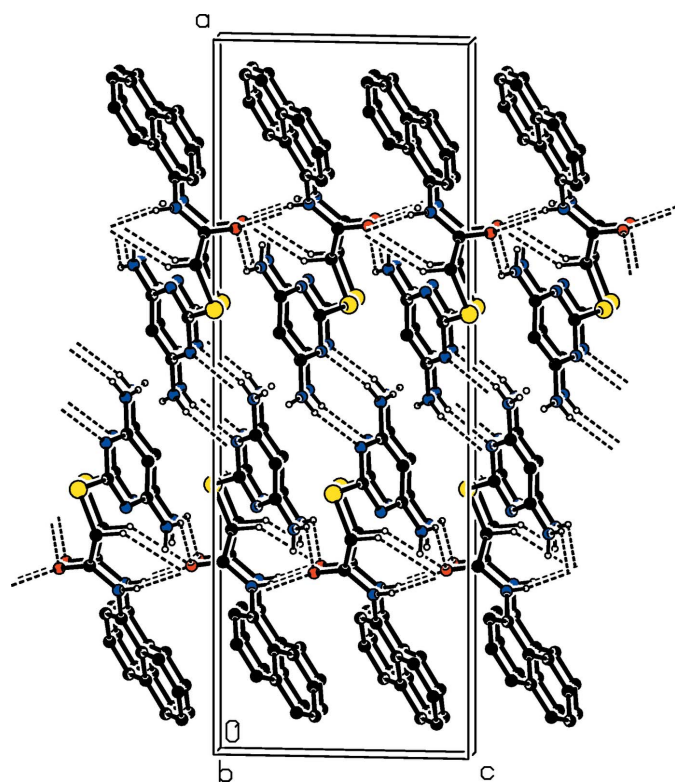


Figure 3
A view along the *b* axis, of the crystal packing of compound (I). Hydrogen bonds are shown as dashed lines (see Table 1). For clarity, only the NH and NH₂ hydrogens and the C-bound H atoms involved in hydrogen bonding have been included.

et al., 2008) and *N*-(2-chlorophenyl)-2-(4,6-dimethylpyrimidin-2-ylsulfanyl)acetamide (QOTQEW; Li *et al.*, 2009), and three 4,6-diaminopyrimidine compounds *viz.* 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-2-methylphenylacetamide (GOKWIO; Subasri *et al.*, 2014), 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(3-nitrophenyl)acetamide (Subasri *et al.*, 2014) and 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(2-chlorophenyl)acetamide (Subasri *et al.*, 2014).

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, potassium hydroxide (0.2 g, 3.52 mmol) was added and the mixture refluxed for 30 min. Then 3.52 mmol of 2-chloro-*N*-(naphthalen-1-yl)acetamide was added and the mixture refluxed for 2.5 h. On completion of the reaction (monitored by TLC), the ethanol was evaporated *in vacuo* and cold water was added. The precipitate that formed was filtered and dried to give compound (I) as a crystalline powder (yield 92%).

Compound (II): To a solution of 4,6-diamino-pyrimidine-2-thiol (0.5 g, 3.52 mmol) in 25 ml of ethanol, potassium hydroxide (0.2 g, 3.52 mmol) was added and the mixture refluxed for 30 min. Then 3.52 mmol of 2-chloro-*N*-(4-fluorophenyl)acetamide was added and the mixture refluxed for 4 h. On completion of the reaction (monitored by TLC), 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 88%).

Colourless block-like crystals were obtained by slow evaporation of a solution in CH₃OH for compound (I) and C₄H₈O₂ for compound (II).

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 as

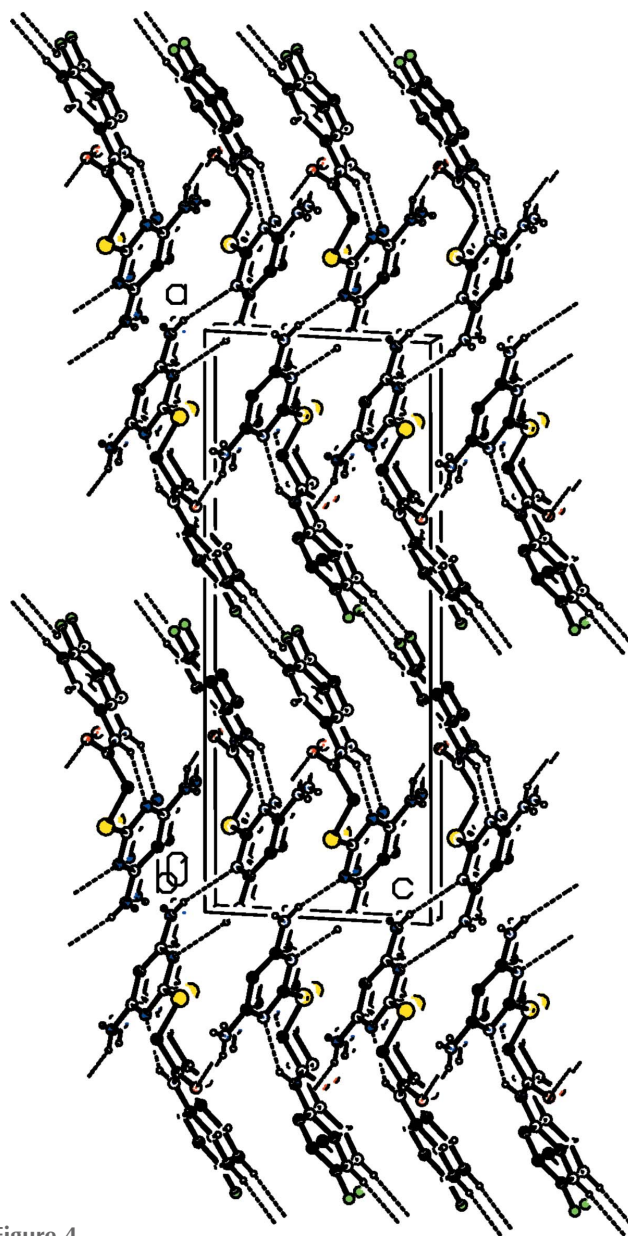


Figure 4
The crystal packing of compound (II) viewed along the *b* axis. Hydrogen bonds are shown as dashed lines (see Table 2). For clarity, only the NH and NH₂ hydrogens and the C-bound H atoms involved in hydrogen bonding have been included.

Table 3
Experimental details.

| | (I) | (II) |
|---|---|--|
| Crystal data | | |
| Chemical formula | C ₁₆ H ₁₅ N ₅ OS | C ₁₂ H ₁₂ FN ₅ OS |
| <i>M_r</i> | 325.39 | 293.33 |
| Crystal system, space group | Monoclinic, <i>P</i> 2 ₁ / <i>c</i> | Monoclinic, <i>P</i> 2 ₁ / <i>c</i> |
| Temperature (K) | 293 | 293 |
| <i>a</i> , <i>b</i> , <i>c</i> (Å) | 25.1895 (16), 6.9411 (4), 8.9697 (6) | 21.7358 (7), 7.3726 (3), 8.4487 (3) |
| β (°) | 90.943 (4) | 93.092 (1) |
| <i>V</i> (Å ³) | 1568.08 (17) | 1351.93 (9) |
| <i>Z</i> | 4 | 4 |
| Radiation type | Mo <i>K</i> α | Mo <i>K</i> α |
| μ (mm ⁻¹) | 0.22 | 0.25 |
| Crystal size (mm) | 0.30 × 0.25 × 0.20 | 0.31 × 0.25 × 0.20 |
| Data collection | | |
| Diffractometer | Bruker SMART APEXII area-detector | Bruker SMART APEXII area-detector |
| Absorption correction | Multi-scan (<i>SADABS</i> ; Bruker, 2008) | Multi-scan (<i>SADABS</i> ; Bruker, 2008) |
| <i>T</i> _{min} – <i>T</i> _{max} | 0.752, 0.831 | 0.652, 0.753 |
| No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections | 14522, 3849, 2095 | 12316, 3312, 2829 |
| <i>R</i> _{int} | 0.063 | 0.025 |
| (<i>sin</i> θ / λ) _{max} (Å ⁻¹) | 0.669 | 0.667 |
| Refinement | | |
| <i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i> | 0.052, 0.153, 0.98 | 0.037, 0.109, 1.05 |
| No. of reflections | 3849 | 3312 |
| No. of parameters | 208 | 181 |
| H-atom treatment | H-atom parameters constrained | H-atom parameters constrained |
| $\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³) | 0.38, -0.23 | 0.22, -0.22 |

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

riding: C–H = 0.93–0.97 Å, N–H = 0.86 Å with *U*_{iso}(H) = 1.2*U*_{eq}(N,C).

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supporting information

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Crystal structures of 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(naphthalen-1-yl)acetamide and 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(4-fluorophenyl)-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) for (I); *SHELXL2016/4* (Sheldrick, 2015) and *PLATON* (Spek, 2009) for (II).

(I) 2-[(4,6-Diaminopyrimidin-2-yl)sulfanyl]-*N*-(naphthalen-1-yl)acetamide

Crystal data

$C_{16}H_{15}N_5OS$

$M_r = 325.39$

Monoclinic, $P2_1/c$

$a = 25.1895$ (16) Å

$b = 6.9411$ (4) Å

$c = 8.9697$ (6) Å

$\beta = 90.943$ (4)°

$V = 1568.08$ (17) Å³

$Z = 4$

$F(000) = 680$

$D_x = 1.378$ Mg m⁻³

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

Cell parameters from 3849 reflections

$\theta = 1.6$ – 28.4 °

$\mu = 0.22$ mm⁻¹

$T = 293$ K

Block, colourless

$0.30 \times 0.25 \times 0.20$ mm

Data collection

Bruker SMART APEXII area-detector diffractometer

ω and φ scans

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

$T_{\min} = 0.752$, $T_{\max} = 0.831$

14522 measured reflections

3849 independent reflections

2095 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.063$

$\theta_{\max} = 28.4$ °, $\theta_{\min} = 1.6$ °

$h = -33 \rightarrow 33$

$k = -7 \rightarrow 9$

$l = -11 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.052$

$wR(F^2) = 0.153$

$S = 0.98$

3849 reflections

208 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

$$w = 1/[\sigma^2(F_o^2) + (0.0671P)^2 + 0.3358P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.38 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|-------------|------------|----------------------------------|
| N5 | 0.49526 (12) | -0.2169 (5) | 0.6491 (4) | 0.1242 (15) |
| H5A | 0.517831 | -0.151383 | 0.599131 | 0.149* |
| H5B | 0.505205 | -0.319772 | 0.695198 | 0.149* |
| C1 | 0.15258 (14) | -0.2816 (4) | 0.5842 (3) | 0.0706 (9) |
| H1 | 0.156295 | -0.401205 | 0.538876 | 0.085* |
| C2 | 0.10801 (13) | -0.2407 (5) | 0.6613 (3) | 0.0696 (9) |
| H2 | 0.081326 | -0.332820 | 0.667315 | 0.084* |
| C3 | 0.10145 (10) | -0.0625 (4) | 0.7317 (3) | 0.0562 (7) |
| C4 | 0.05553 (12) | -0.0167 (6) | 0.8124 (3) | 0.0725 (9) |
| H4 | 0.028614 | -0.107749 | 0.819483 | 0.087* |
| C5 | 0.04960 (12) | 0.1557 (6) | 0.8794 (3) | 0.0740 (9) |
| H5 | 0.019065 | 0.181697 | 0.932778 | 0.089* |
| C6 | 0.08929 (11) | 0.2952 (5) | 0.8688 (3) | 0.0634 (8) |
| H6 | 0.085036 | 0.413896 | 0.915302 | 0.076* |
| C7 | 0.13418 (10) | 0.2591 (4) | 0.7911 (3) | 0.0501 (6) |
| H7 | 0.160100 | 0.354018 | 0.784284 | 0.060* |
| C8 | 0.14195 (9) | 0.0796 (4) | 0.7205 (2) | 0.0452 (6) |
| C9 | 0.18804 (10) | 0.0334 (4) | 0.6386 (2) | 0.0432 (6) |
| C10 | 0.19288 (11) | -0.1441 (4) | 0.5729 (3) | 0.0576 (7) |
| H10 | 0.223334 | -0.173379 | 0.520215 | 0.069* |
| C11 | 0.26297 (9) | 0.1951 (3) | 0.5182 (2) | 0.0413 (6) |
| C12 | 0.30711 (10) | 0.3383 (4) | 0.5478 (3) | 0.0483 (6) |
| H12A | 0.310700 | 0.357511 | 0.654569 | 0.058* |
| H12B | 0.297111 | 0.460871 | 0.503592 | 0.058* |
| C13 | 0.38351 (10) | 0.0615 (3) | 0.5853 (2) | 0.0422 (6) |
| C14 | 0.44443 (12) | -0.1587 (5) | 0.6552 (3) | 0.0688 (8) |
| C15 | 0.40599 (12) | -0.2535 (4) | 0.7352 (3) | 0.0668 (8) |
| H15 | 0.414154 | -0.364339 | 0.789169 | 0.080* |
| C16 | 0.35572 (11) | -0.1801 (4) | 0.7331 (3) | 0.0481 (6) |
| N1 | 0.22916 (8) | 0.1726 (3) | 0.6311 (2) | 0.0438 (5) |
| H1A | 0.232751 | 0.249634 | 0.705663 | 0.053* |
| N2 | 0.34334 (7) | -0.0183 (3) | 0.6559 (2) | 0.0427 (5) |
| N3 | 0.43337 (8) | 0.0052 (3) | 0.5783 (2) | 0.0540 (6) |
| N4 | 0.31453 (10) | -0.2587 (3) | 0.8082 (2) | 0.0607 (6) |

| | | | | |
|-----|-------------|--------------|--------------|------------|
| H4A | 0.283743 | -0.205232 | 0.803960 | 0.073* |
| H4B | 0.319286 | -0.361782 | 0.859841 | 0.073* |
| O1 | 0.25760 (7) | 0.1132 (3) | 0.39688 (16) | 0.0502 (5) |
| S1 | 0.37019 (3) | 0.26816 (10) | 0.47685 (8) | 0.0554 (2) |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| N5 | 0.0625 (18) | 0.132 (3) | 0.179 (3) | 0.0403 (19) | 0.033 (2) | 0.099 (3) |
| C1 | 0.092 (2) | 0.0530 (19) | 0.0668 (19) | -0.0148 (18) | 0.0000 (17) | -0.0022 (14) |
| C2 | 0.077 (2) | 0.064 (2) | 0.0671 (19) | -0.0257 (17) | -0.0050 (16) | 0.0057 (15) |
| C3 | 0.0522 (17) | 0.065 (2) | 0.0511 (14) | -0.0107 (14) | 0.0013 (12) | 0.0105 (13) |
| C4 | 0.0508 (18) | 0.102 (3) | 0.0654 (18) | -0.0192 (18) | 0.0071 (14) | 0.0168 (18) |
| C5 | 0.0437 (17) | 0.113 (3) | 0.0657 (18) | 0.0019 (19) | 0.0160 (13) | 0.008 (2) |
| C6 | 0.0519 (17) | 0.082 (2) | 0.0570 (16) | 0.0086 (16) | 0.0112 (13) | -0.0039 (15) |
| C7 | 0.0420 (14) | 0.0617 (18) | 0.0467 (14) | 0.0001 (13) | 0.0078 (11) | -0.0006 (12) |
| C8 | 0.0440 (14) | 0.0538 (16) | 0.0380 (12) | -0.0021 (12) | 0.0010 (10) | 0.0044 (11) |
| C9 | 0.0475 (14) | 0.0455 (15) | 0.0370 (11) | -0.0025 (12) | 0.0051 (10) | 0.0015 (10) |
| C10 | 0.0686 (19) | 0.0518 (17) | 0.0526 (15) | -0.0014 (15) | 0.0095 (13) | -0.0034 (13) |
| C11 | 0.0460 (14) | 0.0401 (14) | 0.0383 (12) | 0.0119 (11) | 0.0109 (10) | 0.0039 (10) |
| C12 | 0.0532 (16) | 0.0384 (14) | 0.0538 (14) | 0.0032 (12) | 0.0137 (12) | 0.0049 (11) |
| C13 | 0.0452 (14) | 0.0398 (14) | 0.0417 (12) | -0.0040 (12) | 0.0053 (10) | 0.0008 (10) |
| C14 | 0.0571 (19) | 0.070 (2) | 0.080 (2) | 0.0153 (16) | 0.0118 (15) | 0.0257 (17) |
| C15 | 0.069 (2) | 0.0556 (19) | 0.0763 (19) | 0.0123 (16) | 0.0136 (16) | 0.0266 (15) |
| C16 | 0.0615 (17) | 0.0387 (15) | 0.0444 (13) | -0.0024 (13) | 0.0094 (12) | 0.0017 (11) |
| N1 | 0.0465 (12) | 0.0458 (12) | 0.0395 (10) | -0.0020 (10) | 0.0129 (8) | -0.0056 (9) |
| N2 | 0.0477 (12) | 0.0369 (12) | 0.0437 (10) | -0.0037 (9) | 0.0069 (9) | 0.0039 (9) |
| N3 | 0.0437 (13) | 0.0538 (14) | 0.0646 (13) | 0.0023 (11) | 0.0074 (10) | 0.0137 (11) |
| N4 | 0.0713 (16) | 0.0460 (14) | 0.0656 (14) | -0.0062 (12) | 0.0217 (12) | 0.0134 (11) |
| O1 | 0.0575 (11) | 0.0562 (11) | 0.0373 (9) | 0.0086 (9) | 0.0110 (7) | -0.0004 (8) |
| S1 | 0.0494 (4) | 0.0524 (5) | 0.0651 (4) | 0.0038 (3) | 0.0200 (3) | 0.0208 (3) |

Geometric parameters (Å, °)

| | | | |
|--------|-----------|----------|-----------|
| N5—C14 | 1.345 (4) | C9—N1 | 1.419 (3) |
| N5—H5A | 0.8600 | C10—H10 | 0.9300 |
| N5—H5B | 0.8600 | C11—O1 | 1.234 (3) |
| C1—C2 | 1.358 (4) | C11—N1 | 1.343 (3) |
| C1—C10 | 1.398 (4) | C11—C12 | 1.512 (4) |
| C1—H1 | 0.9300 | C12—S1 | 1.789 (2) |
| C2—C3 | 1.400 (4) | C12—H12A | 0.9700 |
| C2—H2 | 0.9300 | C12—H12B | 0.9700 |
| C3—C4 | 1.411 (4) | C13—N3 | 1.318 (3) |
| C3—C8 | 1.424 (4) | C13—N2 | 1.324 (3) |
| C4—C5 | 1.349 (5) | C13—S1 | 1.762 (2) |
| C4—H4 | 0.9300 | C14—N3 | 1.357 (3) |
| C5—C6 | 1.396 (4) | C14—C15 | 1.382 (4) |
| C5—H5 | 0.9300 | C15—C16 | 1.365 (4) |

| | | | |
|--------------|------------|----------------|-------------|
| C6—C7 | 1.362 (3) | C15—H15 | 0.9300 |
| C6—H6 | 0.9300 | C16—N2 | 1.353 (3) |
| C7—C8 | 1.413 (3) | C16—N4 | 1.360 (3) |
| C7—H7 | 0.9300 | N1—H1A | 0.8600 |
| C8—C9 | 1.421 (3) | N4—H4A | 0.8600 |
| C9—C10 | 1.372 (3) | N4—H4B | 0.8600 |
| C14—N5—H5A | 120.0 | C1—C10—H10 | 119.6 |
| C14—N5—H5B | 120.0 | O1—C11—N1 | 123.4 (2) |
| H5A—N5—H5B | 120.0 | O1—C11—C12 | 121.8 (2) |
| C2—C1—C10 | 120.1 (3) | N1—C11—C12 | 114.7 (2) |
| C2—C1—H1 | 119.9 | C11—C12—S1 | 114.45 (17) |
| C10—C1—H1 | 119.9 | C11—C12—H12A | 108.6 |
| C1—C2—C3 | 121.3 (3) | S1—C12—H12A | 108.6 |
| C1—C2—H2 | 119.4 | C11—C12—H12B | 108.6 |
| C3—C2—H2 | 119.4 | S1—C12—H12B | 108.6 |
| C2—C3—C4 | 122.3 (3) | H12A—C12—H12B | 107.6 |
| C2—C3—C8 | 119.4 (3) | N3—C13—N2 | 129.4 (2) |
| C4—C3—C8 | 118.3 (3) | N3—C13—S1 | 112.83 (17) |
| C5—C4—C3 | 121.8 (3) | N2—C13—S1 | 117.67 (18) |
| C5—C4—H4 | 119.1 | N5—C14—N3 | 114.8 (3) |
| C3—C4—H4 | 119.1 | N5—C14—C15 | 123.6 (3) |
| C4—C5—C6 | 120.0 (3) | N3—C14—C15 | 121.6 (3) |
| C4—C5—H5 | 120.0 | C16—C15—C14 | 118.2 (3) |
| C6—C5—H5 | 120.0 | C16—C15—H15 | 120.9 |
| C7—C6—C5 | 120.6 (3) | C14—C15—H15 | 120.9 |
| C7—C6—H6 | 119.7 | N2—C16—N4 | 114.5 (2) |
| C5—C6—H6 | 119.7 | N2—C16—C15 | 121.5 (2) |
| C6—C7—C8 | 120.9 (3) | N4—C16—C15 | 123.9 (2) |
| C6—C7—H7 | 119.5 | C11—N1—C9 | 126.0 (2) |
| C8—C7—H7 | 119.5 | C11—N1—H1A | 117.0 |
| C7—C8—C9 | 123.4 (2) | C9—N1—H1A | 117.0 |
| C7—C8—C3 | 118.4 (2) | C13—N2—C16 | 114.9 (2) |
| C9—C8—C3 | 118.2 (2) | C13—N3—C14 | 114.3 (2) |
| C10—C9—N1 | 121.4 (2) | C16—N4—H4A | 120.0 |
| C10—C9—C8 | 120.2 (2) | C16—N4—H4B | 120.0 |
| N1—C9—C8 | 118.3 (2) | H4A—N4—H4B | 120.0 |
| C9—C10—C1 | 120.8 (3) | C13—S1—C12 | 100.80 (11) |
| C9—C10—H10 | 119.6 | | |
| C10—C1—C2—C3 | -0.5 (5) | O1—C11—C12—S1 | -42.3 (3) |
| C1—C2—C3—C4 | 180.0 (3) | N1—C11—C12—S1 | 140.88 (18) |
| C1—C2—C3—C8 | 1.0 (4) | N5—C14—C15—C16 | 179.9 (3) |
| C2—C3—C4—C5 | -179.8 (3) | N3—C14—C15—C16 | 1.3 (5) |
| C8—C3—C4—C5 | -0.8 (4) | C14—C15—C16—N2 | -0.4 (4) |
| C3—C4—C5—C6 | 0.7 (5) | C14—C15—C16—N4 | -179.3 (3) |
| C4—C5—C6—C7 | 0.0 (5) | O1—C11—N1—C9 | 10.4 (4) |
| C5—C6—C7—C8 | -0.6 (4) | C12—C11—N1—C9 | -172.8 (2) |

| | | | |
|--------------|------------|----------------|--------------|
| C6—C7—C8—C9 | -179.7 (2) | C10—C9—N1—C11 | 31.7 (4) |
| C6—C7—C8—C3 | 0.5 (4) | C8—C9—N1—C11 | -150.3 (2) |
| C2—C3—C8—C7 | 179.3 (2) | N3—C13—N2—C16 | 0.8 (4) |
| C4—C3—C8—C7 | 0.2 (4) | S1—C13—N2—C16 | 177.84 (17) |
| C2—C3—C8—C9 | -0.6 (4) | N4—C16—N2—C13 | 178.5 (2) |
| C4—C3—C8—C9 | -179.7 (2) | C15—C16—N2—C13 | -0.5 (3) |
| C7—C8—C9—C10 | -180.0 (2) | N2—C13—N3—C14 | 0.0 (4) |
| C3—C8—C9—C10 | -0.1 (3) | S1—C13—N3—C14 | -177.2 (2) |
| C7—C8—C9—N1 | 2.1 (3) | N5—C14—N3—C13 | -179.8 (3) |
| C3—C8—C9—N1 | -178.1 (2) | C15—C14—N3—C13 | -1.1 (4) |
| N1—C9—C10—C1 | 178.4 (2) | N3—C13—S1—C12 | -165.84 (19) |
| C8—C9—C10—C1 | 0.6 (4) | N2—C13—S1—C12 | 16.6 (2) |
| C2—C1—C10—C9 | -0.2 (4) | C11—C12—S1—C13 | -64.63 (19) |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|--------------------------------------|-------------|---------------|-----------------------|-------------------------|
| N5—H5 <i>A</i> ...N3 ⁱ | 0.86 | 2.27 | 3.110 (4) | 167 |
| N1—H1 <i>A</i> ...O1 ⁱⁱ | 0.86 | 2.05 | 2.890 (3) | 165 |
| N4—H4 <i>B</i> ...O1 ⁱⁱⁱ | 0.86 | 2.36 | 2.964 (3) | 127 |
| C12—H12 <i>A</i> ...O1 ⁱⁱ | 0.97 | 2.58 | 3.408 (3) | 143 |

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

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

C₁₂H₁₂FN₅OS

M_r = 293.33

Monoclinic, *P*2₁/*c*

a = 21.7358 (7) Å

b = 7.3726 (3) Å

c = 8.4487 (3) Å

β = 93.092 (1)°

V = 1351.93 (9) Å³

Z = 4

F(000) = 608

D_x = 1.441 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 3312 reflections

θ = 1.9–28.3°

μ = 0.25 mm⁻¹

T = 293 K

Block, colourless

0.31 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEXII area-detector
diffractometer

ω and φ scans

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

T_{min} = 0.652, *T_{max}* = 0.753

12316 measured reflections

3312 independent reflections

2829 reflections with *I* > 2σ(*I*)

R_{int} = 0.025

θ_{max} = 28.3°, θ_{min} = 1.9°

h = -28→28

k = -5→9

l = -7→11

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.037

wR(*F*²) = 0.109

S = 1.05

3312 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

$$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.3099P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.22 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|---------------|--------------|----------------------------------|
| C1 | 0.43036 (9) | -0.1374 (4) | 0.4152 (3) | 0.0777 (6) |
| C2 | 0.42379 (9) | 0.0399 (4) | 0.3738 (3) | 0.0824 (6) |
| H2 | 0.450358 | 0.092466 | 0.304272 | 0.099* |
| C3 | 0.37714 (8) | 0.1422 (3) | 0.4359 (2) | 0.0658 (4) |
| H3 | 0.372002 | 0.263568 | 0.408377 | 0.079* |
| C4 | 0.33831 (6) | 0.0600 (2) | 0.53966 (17) | 0.0480 (3) |
| C5 | 0.34659 (8) | -0.1211 (2) | 0.5791 (2) | 0.0605 (4) |
| H5 | 0.320667 | -0.175666 | 0.649109 | 0.073* |
| C6 | 0.39282 (10) | -0.2211 (3) | 0.5158 (3) | 0.0746 (5) |
| H6 | 0.398185 | -0.342957 | 0.541273 | 0.089* |
| C7 | 0.26854 (6) | 0.32063 (19) | 0.58470 (16) | 0.0432 (3) |
| C8 | 0.21206 (7) | 0.36589 (19) | 0.67409 (17) | 0.0482 (3) |
| H8A | 0.210250 | 0.496199 | 0.688963 | 0.058* |
| H8B | 0.216105 | 0.310216 | 0.778152 | 0.058* |
| C9 | 0.13013 (6) | 0.07360 (17) | 0.65615 (14) | 0.0378 (3) |
| C10 | 0.06207 (7) | -0.1564 (2) | 0.67975 (18) | 0.0501 (3) |
| C11 | 0.10494 (7) | -0.2466 (2) | 0.77884 (18) | 0.0505 (3) |
| H11 | 0.095821 | -0.358065 | 0.823502 | 0.061* |
| C12 | 0.16170 (7) | -0.16497 (18) | 0.80890 (15) | 0.0415 (3) |
| F1 | 0.47632 (7) | -0.2347 (3) | 0.3527 (2) | 0.1187 (6) |
| N1 | 0.28896 (5) | 0.15094 (17) | 0.60807 (15) | 0.0480 (3) |
| H1 | 0.269193 | 0.087989 | 0.674351 | 0.058* |
| N2 | 0.07407 (5) | 0.00964 (16) | 0.61864 (14) | 0.0452 (3) |
| N3 | 0.17559 (5) | -0.00336 (14) | 0.74173 (12) | 0.0390 (2) |
| N4 | 0.20765 (7) | -0.23810 (17) | 0.90067 (16) | 0.0546 (3) |
| H4A | 0.242409 | -0.182765 | 0.912926 | 0.066* |
| H4B | 0.202291 | -0.340228 | 0.947136 | 0.066* |
| N5 | 0.00588 (8) | -0.2236 (2) | 0.6394 (2) | 0.0815 (5) |
| H5A | -0.019470 | -0.162080 | 0.579047 | 0.098* |
| H5B | -0.004701 | -0.328149 | 0.674068 | 0.098* |
| O1 | 0.29125 (5) | 0.43187 (15) | 0.49776 (14) | 0.0597 (3) |
| S1 | 0.14082 (2) | 0.29101 (5) | 0.57535 (5) | 0.05097 (13) |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|---------------|--------------|--------------|
| C1 | 0.0526 (10) | 0.0988 (16) | 0.0819 (13) | 0.0139 (10) | 0.0035 (9) | -0.0235 (12) |
| C2 | 0.0581 (11) | 0.1083 (18) | 0.0830 (13) | -0.0068 (11) | 0.0248 (10) | -0.0037 (13) |
| C3 | 0.0548 (9) | 0.0710 (11) | 0.0728 (11) | -0.0055 (8) | 0.0142 (8) | 0.0061 (9) |
| C4 | 0.0429 (7) | 0.0532 (8) | 0.0478 (7) | -0.0038 (6) | -0.0002 (6) | -0.0007 (6) |
| C5 | 0.0577 (9) | 0.0563 (10) | 0.0677 (10) | 0.0023 (7) | 0.0049 (7) | 0.0015 (8) |
| C6 | 0.0682 (11) | 0.0665 (12) | 0.0885 (14) | 0.0138 (9) | -0.0011 (10) | -0.0103 (10) |
| C7 | 0.0453 (7) | 0.0420 (7) | 0.0418 (6) | -0.0102 (5) | -0.0029 (5) | 0.0014 (5) |
| C8 | 0.0597 (8) | 0.0347 (7) | 0.0508 (7) | -0.0064 (6) | 0.0081 (6) | -0.0023 (6) |
| C9 | 0.0447 (6) | 0.0333 (6) | 0.0366 (6) | 0.0004 (5) | 0.0123 (5) | -0.0009 (5) |
| C10 | 0.0498 (8) | 0.0469 (8) | 0.0543 (8) | -0.0080 (6) | 0.0102 (6) | 0.0061 (6) |
| C11 | 0.0604 (9) | 0.0395 (7) | 0.0521 (8) | -0.0086 (6) | 0.0088 (7) | 0.0089 (6) |
| C12 | 0.0551 (7) | 0.0340 (6) | 0.0361 (6) | 0.0012 (5) | 0.0082 (5) | -0.0014 (5) |
| F1 | 0.0774 (9) | 0.1484 (14) | 0.1323 (13) | 0.0357 (9) | 0.0230 (8) | -0.0415 (11) |
| N1 | 0.0499 (6) | 0.0442 (6) | 0.0508 (6) | -0.0030 (5) | 0.0106 (5) | 0.0070 (5) |
| N2 | 0.0442 (6) | 0.0422 (6) | 0.0499 (6) | -0.0029 (5) | 0.0079 (5) | 0.0056 (5) |
| N3 | 0.0467 (6) | 0.0320 (5) | 0.0390 (5) | -0.0001 (4) | 0.0081 (4) | 0.0003 (4) |
| N4 | 0.0677 (8) | 0.0397 (6) | 0.0557 (7) | -0.0015 (6) | -0.0045 (6) | 0.0089 (5) |
| N5 | 0.0586 (9) | 0.0747 (11) | 0.1098 (14) | -0.0267 (8) | -0.0091 (8) | 0.0363 (10) |
| O1 | 0.0564 (6) | 0.0514 (6) | 0.0719 (7) | -0.0071 (5) | 0.0085 (5) | 0.0188 (5) |
| S1 | 0.0472 (2) | 0.0404 (2) | 0.0655 (2) | -0.00120 (14) | 0.00437 (16) | 0.01690 (16) |

Geometric parameters (Å, °)

| | | | |
|----------|-------------|------------|-------------|
| C1—C6 | 1.358 (3) | C8—H8B | 0.9700 |
| C1—C2 | 1.359 (3) | C9—N3 | 1.3207 (17) |
| C1—F1 | 1.359 (2) | C9—N2 | 1.3288 (17) |
| C2—C3 | 1.389 (3) | C9—S1 | 1.7625 (13) |
| C2—H2 | 0.9300 | C10—N5 | 1.345 (2) |
| C3—C4 | 1.388 (2) | C10—N2 | 1.3594 (18) |
| C3—H3 | 0.9300 | C10—C11 | 1.388 (2) |
| C4—C5 | 1.386 (2) | C11—C12 | 1.384 (2) |
| C4—N1 | 1.4144 (19) | C11—H11 | 0.9300 |
| C5—C6 | 1.378 (3) | C12—N4 | 1.3438 (19) |
| C5—H5 | 0.9300 | C12—N3 | 1.3606 (17) |
| C6—H6 | 0.9300 | N1—H1 | 0.8600 |
| C7—O1 | 1.2227 (16) | N4—H4A | 0.8600 |
| C7—N1 | 1.3386 (19) | N4—H4B | 0.8600 |
| C7—C8 | 1.513 (2) | N5—H5A | 0.8600 |
| C8—S1 | 1.8054 (15) | N5—H5B | 0.8600 |
| C8—H8A | 0.9700 | | |
| C6—C1—C2 | 122.69 (18) | H8A—C8—H8B | 107.7 |
| C6—C1—F1 | 118.8 (2) | N3—C9—N2 | 128.87 (12) |
| C2—C1—F1 | 118.5 (2) | N3—C9—S1 | 119.50 (10) |
| C1—C2—C3 | 119.57 (19) | N2—C9—S1 | 111.64 (10) |

| | | | |
|----------------|--------------|---------------|--------------|
| C1—C2—H2 | 120.2 | N5—C10—N2 | 115.21 (15) |
| C3—C2—H2 | 120.2 | N5—C10—C11 | 123.17 (14) |
| C4—C3—C2 | 118.9 (2) | N2—C10—C11 | 121.61 (14) |
| C4—C3—H3 | 120.6 | C12—C11—C10 | 117.71 (13) |
| C2—C3—H3 | 120.6 | C12—C11—H11 | 121.1 |
| C5—C4—C3 | 119.78 (16) | C10—C11—H11 | 121.1 |
| C5—C4—N1 | 116.72 (14) | N4—C12—N3 | 114.66 (13) |
| C3—C4—N1 | 123.49 (16) | N4—C12—C11 | 123.98 (13) |
| C6—C5—C4 | 120.67 (18) | N3—C12—C11 | 121.34 (13) |
| C6—C5—H5 | 119.7 | C7—N1—C4 | 129.45 (13) |
| C4—C5—H5 | 119.7 | C7—N1—H1 | 115.3 |
| C1—C6—C5 | 118.4 (2) | C4—N1—H1 | 115.3 |
| C1—C6—H6 | 120.8 | C9—N2—C10 | 114.92 (12) |
| C5—C6—H6 | 120.8 | C9—N3—C12 | 115.35 (11) |
| O1—C7—N1 | 125.03 (14) | C12—N4—H4A | 120.0 |
| O1—C7—C8 | 121.11 (13) | C12—N4—H4B | 120.0 |
| N1—C7—C8 | 113.84 (12) | H4A—N4—H4B | 120.0 |
| C7—C8—S1 | 113.63 (10) | C10—N5—H5A | 120.0 |
| C7—C8—H8A | 108.8 | C10—N5—H5B | 120.0 |
| S1—C8—H8A | 108.8 | H5A—N5—H5B | 120.0 |
| C7—C8—H8B | 108.8 | C9—S1—C8 | 103.11 (7) |
| S1—C8—H8B | 108.8 | | |
| | | | |
| C6—C1—C2—C3 | 0.2 (3) | O1—C7—N1—C4 | -1.5 (2) |
| F1—C1—C2—C3 | 179.92 (18) | C8—C7—N1—C4 | 177.03 (13) |
| C1—C2—C3—C4 | 0.2 (3) | C5—C4—N1—C7 | -176.10 (15) |
| C2—C3—C4—C5 | -0.1 (3) | C3—C4—N1—C7 | 3.0 (2) |
| C2—C3—C4—N1 | -179.19 (16) | N3—C9—N2—C10 | 1.3 (2) |
| C3—C4—C5—C6 | -0.3 (3) | S1—C9—N2—C10 | -178.73 (10) |
| N1—C4—C5—C6 | 178.83 (15) | N5—C10—N2—C9 | -178.64 (15) |
| C2—C1—C6—C5 | -0.6 (3) | C11—C10—N2—C9 | 2.5 (2) |
| F1—C1—C6—C5 | 179.66 (18) | N2—C9—N3—C12 | -4.68 (19) |
| C4—C5—C6—C1 | 0.7 (3) | S1—C9—N3—C12 | 175.34 (9) |
| O1—C7—C8—S1 | 96.18 (14) | N4—C12—N3—C9 | -177.50 (12) |
| N1—C7—C8—S1 | -82.44 (14) | C11—C12—N3—C9 | 4.35 (18) |
| N5—C10—C11—C12 | 178.71 (16) | N3—C9—S1—C8 | -11.34 (11) |
| N2—C10—C11—C12 | -2.5 (2) | N2—C9—S1—C8 | 168.68 (10) |
| C10—C11—C12—N4 | -179.08 (14) | C7—C8—S1—C9 | 91.88 (11) |
| C10—C11—C12—N3 | -1.1 (2) | | |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------------------------|-------|-------------|-------------|---------------|
| N1—H1 \cdots N3 | 0.86 | 2.25 | 2.990 (2) | 145 |
| C3—H3 \cdots O1 | 0.93 | 2.31 | 2.903 (2) | 121 |
| N5—H5A \cdots N2 ⁱ | 0.86 | 2.29 | 3.139 (2) | 169 |

| | | | | |
|---------------------------|------|------|-------------|-----|
| N4—H4A···O1 ⁱⁱ | 0.86 | 2.23 | 2.9852 (18) | 146 |
| C2—H2···F1 ⁱⁱⁱ | 0.93 | 2.48 | 3.404 (3) | 172 |

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