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Crystal structure of (*E*)-2-amino-4-methylsulfanyl-6-oxo-1-[[*(*thiophen-2-yl)methylidene]amino]-1,6-dihydropyrimidine-5-carbonitrile

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The title compound, C₁₁H₉N₅OS₂, a 1-thiophen-2-ylmethyleneaminopyrimidine derivative, displays an essentially planar C—NH₂ group. The conformation across the N=C bond linking the pyrimidine and thienyl groups is *E*. The pyrimidine and thienyl ring systems subtend an inter-planar angle of 42.72 (5)°. In the crystal, molecules are linked by N—H···N_{nitrile} and N—H···O=C hydrogen bonds, forming chains parallel to the *b* axis.

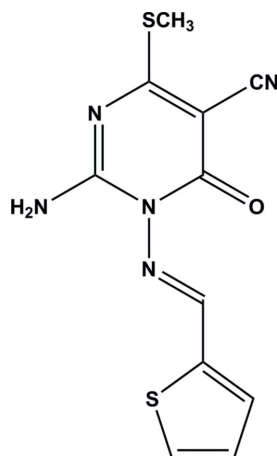
Keywords: crystal structure; pyrimidine; thienyl; N—H···N and N—H···O hydrogen bonds.

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1. Chemical context

Pyrimidines are well known for their biological activities as antimetabolic agents and have attracted much attention from the standpoint of pharmaceutical chemistry. Many drugs, such as 5-fluorouracil, containing a pyrimidine moiety have been developed and used as anticancer agents. It is difficult to find a general method for the introduction of specific substituents into the pyrimidine nucleus directly, and thus many synthetic methods have been developed for the construction of pyrimidine rings bearing potential functional groups (Elgemeie & Sood, 2001). As part of our program directed toward the preparation of potential antimetabolites (Elgemeie & Hussain, 1994), we have recently reported various successful approaches for the syntheses of purine and pyrimidine analogues (Elgemeie, 2003; Elgemeie *et al.*, 2009). Derivatives of these ring systems are interesting as antimetabolic agents in biochemical reactions (Scala *et al.*, 1997).



We report herein on the synthesis and crystal structure of a new 1-thiophen-2-ylmethyleneaminopyrimidine derivative, obtained by reaction of dimethyl *N*-cyanodithioimino-carbonate with 1-cyanoacetyl-4-thiophenemethylidene semi-

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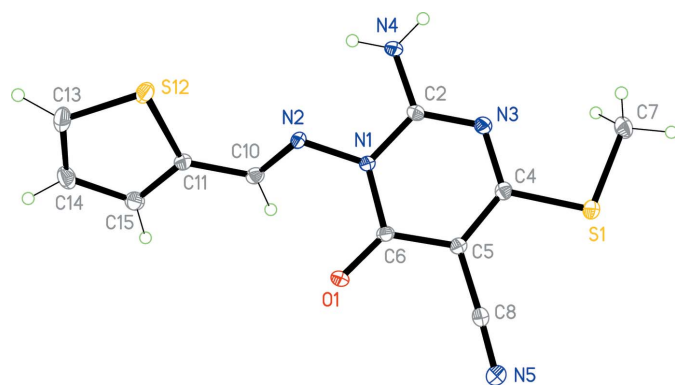


Figure 1

The molecule structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular hydrogen bond, H042...N1, is not shown.

carbazide in dioxane containing KOH at room temperature. To the best of our knowledge, this is the first example of this approach to be reported for *N*-substituted aminopyrimidine derivatives. The X-ray structure determination was undertaken to establish the nature of the product unambiguously.

2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The *E* conformation across the double bond N2=C10 is confirmed, with a bond length of 1.2879 (14) Å. Both ring systems are, as expected, planar (r.m.s. deviations are 0.017 Å for the pyrimidine and 0.001 Å for the thienyl ring). Atom N2 lies 0.189 (2) Å out of the pyrimidine plane; all other immediate substituent atoms lie effectively in the ring plane. Carbon atom C7 of the thiomethyl group is rotated slightly out of the ring plane, with torsion angle N3—C4—S1—C7 being -6.30 (10)°. The inter-planar angle between the rings is 42.72 (5)°; the relative orientation is influenced by the torsion

Table 1

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>
N4—H041...N2	0.827 (18)	2.224 (17)	2.6062 (13)	108.4 (14)
N4—H041...N5 ⁱ	0.827 (18)	2.513 (17)	3.0555 (14)	124.2 (15)
N4—H042...O1 ⁱ	0.823 (17)	2.144 (17)	2.9414 (12)	163.1 (15)
C13—H13...N5 ⁱⁱ	0.95	2.49	3.2722 (15)	139
C10—H10...O1 ⁱⁱⁱ	0.95	2.35	3.2124 (13)	150

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

angles C6—N1—N2—C10 = -51.78 (13), N1—N2—C10—C11 = 174.68 (9) and N2—C10—C11—S12 = 5.22 (15)°. The NH₂ group is planar; the nitrogen atom lies only 0.048 (9) Å out of the plane of its substituents. The intramolecular contact H041...N2 = 2.22 (2) Å may be construed as a hydrogen bond, although the angle at the H atom is necessarily narrow at 108.4 (14)° (Table 1).

3. Supramolecular features

In the crystal, molecules are connected into chains parallel to the *b* axis by the two classical hydrogen bonds, H041...N5 2.51 (2) Å and H042...O1 2.14 (2) Å (Table 1 and Fig. 2), both involving the 2_1 screw operator $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$. The longer of these two contacts forms part of a three-center system with the intramolecular contact H041...N2 (Table 1). The 'weak' hydrogen bond H13...N5 of 2.49 Å, formed *via* the *c* glide operator $x + 1, -y + \frac{3}{2}, z - \frac{1}{2}$, connects the chains to form layers parallel to (102) (Table 1 and Fig. 2).

4. Database survey

A search of the Cambridge Structural Database (Version 5.36, 2014; Groom & Allen, 2014) revealed 42 hits for pyrimidines

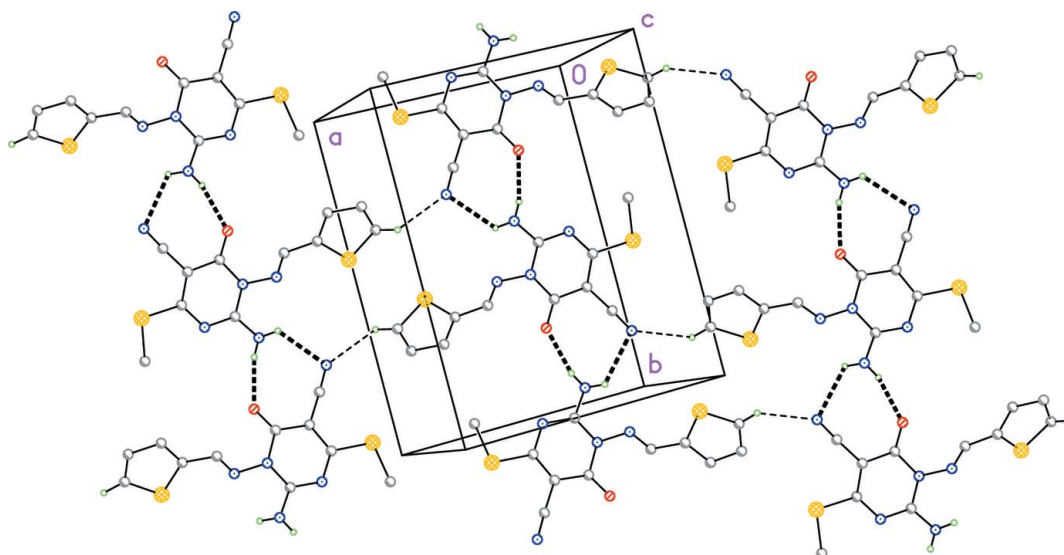


Figure 2

Crystal packing diagram of the title compound, viewed perpendicular to (102). Classical hydrogen bonds are drawn as thick dashed lines and 'weak' hydrogen bonds as thin dashed lines (see Table 1).

with the amino and C=O functions located as for the title compound.

5. Synthesis and crystallization

Dimethyl *N*-cyanodithioiminocarbonate (0.01 mol) was added to a stirred solution of 1-cyanoacetyl-4-thiophenemethylidenesemicarbazide (0.01 mol) in dry dioxane (50 ml), containing potassium hydroxide (0.01 mol), at room temperature. The solution was stirred overnight at room temperature, after which a colourless solid product was collected by filtration and crystallized from ethanol (m.p. 541–542 K), giving colourless block-like crystals.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The NH hydrogen atoms were located in a difference Fourier map and freely refined. The C-bound H atoms were included in calculated positions and treated as riding atoms: C–H = 0.95–0.98 Å with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $1.2U_{\text{eq}}(\text{C})$ for other H atoms. The methyl group was refined as an idealized rigid group, allowed to rotate but not to tip.

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Table 2

Experimental details.

Crystal data	
Chemical formula	$\text{C}_{11}\text{H}_9\text{N}_5\text{OS}_2$
M_r	291.35
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	11.4650 (4), 14.7715 (4), 7.5924 (3)
β (°)	96.397 (3)
V (Å ³)	1277.81 (8)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ^{−1})	0.42
Crystal size (mm)	0.40 × 0.40 × 0.12
Data collection	
Diffractometer	Oxford Diffraction Xcalibur, Eos
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2013)
$T_{\text{min}}, T_{\text{max}}$	0.949, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	40035, 3838, 3400
R_{int}	0.035
$(\sin \theta/\lambda)_{\text{max}}$ (Å ^{−1})	0.719
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.030, 0.078, 1.05
No. of reflections	3838
No. of parameters	181
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ^{−3})	0.45, −0.28

Computer programs: *CrysAlis PRO* (Agilent, 2013), *SHELXS97*, *SHELXL97* and *XP* in *SHELXTL* (Sheldrick, 2008).

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supporting information

Acta Cryst. (2015). E71, 1319-1321 [https://doi.org/10.1107/S205698901501885X]

Crystal structure of (*E*)-2-amino-4-methylsulfanyl-6-oxo-1-[(thiophen-2-yl)methylidene]amino}-1,6-dihydropyrimidine-5-carbonitrile

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Computing details

Data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO* (Agilent, 2013); data reduction: *CrysAlis PRO* (Agilent, 2013); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

(*E*)-2-Amino-4-methylsulfanyl-6-oxo-1-[(thiophen-2-yl)methylidene]amino}-1,6-dihydropyrimidine-5-carbonitrile

Crystal data

C₁₁H₉N₅OS₂

$M_r = 291.35$

Monoclinic, $P2_1/c$

Hall symbol: -P 2yc

$a = 11.4650$ (4) Å

$b = 14.7715$ (4) Å

$c = 7.5924$ (3) Å

$\beta = 96.397$ (3)°

$V = 1277.81$ (8) Å³

$Z = 4$

$F(000) = 600$

$D_x = 1.514$ Mg m⁻³

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

Cell parameters from 11992 reflections

$\theta = 2.8\text{--}30.7^\circ$

$\mu = 0.42$ mm⁻¹

$T = 100$ K

Block, colourless

$0.40 \times 0.40 \times 0.12$ mm

Data collection

Oxford Diffraction Xcalibur, Eos
diffractometer

Radiation source: Enhance (Mo) X-ray Source

Graphite monochromator

Detector resolution: 16.1419 pixels mm⁻¹

ω -scan

Absorption correction: multi-scan

(*CrysAlis Pro*; Agilent, 2013)

$T_{\min} = 0.949$, $T_{\max} = 1.000$

40035 measured reflections

3838 independent reflections

3400 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\max} = 30.7^\circ$, $\theta_{\min} = 2.3^\circ$

$h = -16 \rightarrow 16$

$k = -21 \rightarrow 20$

$l = -10 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.030$

$wR(F^2) = 0.078$

$S = 1.05$

3838 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 atoms treated by a mixture of independent
and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0353P)^2 + 0.5986P]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$$\Delta\rho_{\max} = 0.45 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.28 \text{ e } \text{\AA}^{-3}$$

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

NH H atoms were refined freely. The methyl was refined as an idealized rigid group allowed to rotate but not tip (AFIX 137). Other H atoms were included using a riding model starting from calculated positions.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.18882 (2)	0.570453 (19)	0.93852 (4)	0.01607 (8)
N1	0.53629 (8)	0.58971 (6)	0.73366 (12)	0.01132 (17)
C2	0.48455 (9)	0.50790 (7)	0.76239 (14)	0.01123 (19)
N3	0.37941 (8)	0.50061 (6)	0.82064 (12)	0.01267 (18)
C4	0.32601 (9)	0.57730 (7)	0.86044 (14)	0.01173 (19)
C5	0.37518 (9)	0.66299 (7)	0.84526 (14)	0.0122 (2)
C6	0.48602 (9)	0.67272 (7)	0.77860 (14)	0.01108 (19)
C7	0.15734 (11)	0.45152 (8)	0.91405 (16)	0.0186 (2)
H7A	0.1624	0.4334	0.7910	0.028*
H7B	0.0781	0.4395	0.9450	0.028*
H7C	0.2144	0.4169	0.9929	0.028*
C8	0.31807 (10)	0.74448 (7)	0.88764 (15)	0.0147 (2)
O1	0.53764 (7)	0.74475 (5)	0.75918 (11)	0.01462 (16)
N2	0.65393 (8)	0.58528 (6)	0.69401 (13)	0.01224 (18)
N4	0.54197 (9)	0.43358 (6)	0.72510 (14)	0.01410 (18)
H041	0.6097 (16)	0.4387 (12)	0.699 (2)	0.027 (4)*
H042	0.5115 (14)	0.3849 (11)	0.746 (2)	0.020 (4)*
N5	0.27567 (9)	0.81204 (7)	0.92072 (15)	0.0213 (2)
C10	0.67911 (9)	0.64245 (7)	0.57588 (14)	0.0123 (2)
H10	0.6191	0.6792	0.5165	0.015*
C11	0.79798 (9)	0.65073 (7)	0.53371 (14)	0.0124 (2)
S12	0.91097 (2)	0.58149 (2)	0.62072 (4)	0.01827 (8)
C13	1.01057 (10)	0.64133 (9)	0.51488 (16)	0.0190 (2)
H13	1.0919	0.6273	0.5232	0.023*
C14	0.96003 (11)	0.71124 (8)	0.41744 (16)	0.0189 (2)
H14	1.0022	0.7516	0.3505	0.023*
C15	0.83751 (10)	0.71713 (8)	0.42687 (15)	0.0157 (2)
H15	0.7883	0.7616	0.3666	0.019*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01141 (13)	0.01430 (13)	0.02338 (15)	−0.00065 (9)	0.00585 (10)	−0.00028 (10)
N1	0.0097 (4)	0.0088 (4)	0.0158 (4)	0.0005 (3)	0.0028 (3)	−0.0004 (3)
C2	0.0122 (5)	0.0093 (4)	0.0120 (5)	−0.0008 (4)	0.0002 (4)	−0.0001 (3)
N3	0.0116 (4)	0.0110 (4)	0.0154 (4)	−0.0006 (3)	0.0014 (3)	−0.0001 (3)
C4	0.0099 (4)	0.0130 (5)	0.0121 (5)	−0.0001 (4)	0.0001 (4)	0.0006 (4)
C5	0.0110 (5)	0.0105 (4)	0.0153 (5)	0.0007 (4)	0.0024 (4)	−0.0004 (4)
C6	0.0107 (5)	0.0094 (4)	0.0130 (5)	0.0010 (3)	0.0007 (4)	−0.0008 (4)
C7	0.0168 (5)	0.0164 (5)	0.0235 (6)	−0.0054 (4)	0.0058 (4)	−0.0012 (4)
C8	0.0127 (5)	0.0136 (5)	0.0185 (5)	−0.0014 (4)	0.0045 (4)	0.0010 (4)
O1	0.0142 (4)	0.0086 (3)	0.0217 (4)	−0.0011 (3)	0.0044 (3)	−0.0012 (3)
N2	0.0090 (4)	0.0109 (4)	0.0173 (4)	0.0003 (3)	0.0035 (3)	−0.0014 (3)
N4	0.0134 (4)	0.0079 (4)	0.0214 (5)	−0.0002 (3)	0.0036 (4)	−0.0005 (3)
N5	0.0189 (5)	0.0158 (5)	0.0308 (6)	0.0014 (4)	0.0104 (4)	−0.0002 (4)
C10	0.0123 (5)	0.0115 (4)	0.0130 (5)	0.0009 (4)	0.0008 (4)	−0.0022 (4)
C11	0.0124 (5)	0.0111 (4)	0.0139 (5)	0.0009 (4)	0.0023 (4)	−0.0014 (4)
S12	0.01309 (14)	0.01868 (14)	0.02389 (16)	0.00414 (10)	0.00586 (11)	0.00657 (11)
C13	0.0128 (5)	0.0241 (6)	0.0210 (6)	−0.0025 (4)	0.0058 (4)	−0.0022 (5)
C14	0.0202 (6)	0.0181 (5)	0.0199 (5)	−0.0053 (4)	0.0084 (4)	−0.0004 (4)
C15	0.0181 (5)	0.0140 (5)	0.0158 (5)	0.0001 (4)	0.0048 (4)	0.0000 (4)

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

S1—C4	1.7446 (11)	C11—C15	1.3811 (15)
S1—C7	1.7990 (12)	C11—S12	1.7234 (11)
N1—C2	1.3744 (13)	S12—C13	1.7133 (12)
N1—C6	1.4127 (13)	C13—C14	1.3617 (18)
N1—N2	1.4158 (12)	C14—C15	1.4172 (16)
C2—N4	1.3268 (13)	C7—H7A	0.9800
C2—N3	1.3337 (14)	C7—H7B	0.9800
N3—C4	1.3382 (13)	C7—H7C	0.9800
C4—C5	1.3956 (14)	N4—H041	0.827 (18)
C5—C8	1.4242 (15)	N4—H042	0.823 (17)
C5—C6	1.4265 (14)	C10—H10	0.9500
C6—O1	1.2343 (13)	C13—H13	0.9500
C8—N5	1.1500 (15)	C14—H14	0.9500
N2—C10	1.2879 (14)	C15—H15	0.9500
C10—C11	1.4395 (14)		
C4—S1—C7	101.52 (5)	C10—C11—S12	123.65 (8)
C2—N1—C6	122.00 (9)	C13—S12—C11	91.48 (6)
C2—N1—N2	115.55 (8)	C14—C13—S12	112.37 (9)
C6—N1—N2	121.03 (8)	C13—C14—C15	112.54 (10)
N4—C2—N3	119.49 (10)	C11—C15—C14	112.22 (10)
N4—C2—N1	117.42 (10)	S1—C7—H7A	109.5
N3—C2—N1	123.07 (9)	S1—C7—H7B	109.5

C2—N3—C4	117.37 (9)	H7A—C7—H7B	109.5
N3—C4—C5	123.36 (10)	S1—C7—H7C	109.5
N3—C4—S1	118.70 (8)	H7A—C7—H7C	109.5
C5—C4—S1	117.93 (8)	H7B—C7—H7C	109.5
C4—C5—C8	123.21 (10)	C2—N4—H041	118.5 (12)
C4—C5—C6	120.31 (9)	C2—N4—H042	116.8 (11)
C8—C5—C6	116.44 (9)	H041—N4—H042	123.9 (16)
O1—C6—N1	120.35 (9)	N2—C10—H10	119.9
O1—C6—C5	125.96 (10)	C11—C10—H10	119.9
N1—C6—C5	113.69 (9)	C14—C13—H13	123.8
N5—C8—C5	177.44 (12)	S12—C13—H13	123.8
C10—N2—N1	114.23 (9)	C13—C14—H14	123.7
N2—C10—C11	120.12 (10)	C15—C14—H14	123.7
C15—C11—C10	124.88 (10)	C11—C15—H15	123.9
C15—C11—S12	111.39 (8)	C14—C15—H15	123.9
C6—N1—C2—N4	−176.23 (10)	N2—N1—C6—C5	−169.29 (9)
N2—N1—C2—N4	−9.70 (14)	C4—C5—C6—O1	179.88 (11)
C6—N1—C2—N3	5.62 (16)	C8—C5—C6—O1	2.07 (17)
N2—N1—C2—N3	172.15 (10)	C4—C5—C6—N1	−0.23 (15)
N4—C2—N3—C4	178.49 (10)	C8—C5—C6—N1	−178.04 (9)
N1—C2—N3—C4	−3.40 (16)	C2—N1—N2—C10	141.55 (10)
C2—N3—C4—C5	−0.54 (16)	C6—N1—N2—C10	−51.78 (13)
C2—N3—C4—S1	−179.55 (8)	N1—N2—C10—C11	174.68 (9)
C7—S1—C4—N3	−6.30 (10)	N2—C10—C11—C15	−171.31 (11)
C7—S1—C4—C5	174.63 (9)	N2—C10—C11—S12	5.22 (15)
N3—C4—C5—C8	179.96 (11)	C15—C11—S12—C13	0.11 (9)
S1—C4—C5—C8	−1.01 (15)	C10—C11—S12—C13	−176.84 (10)
N3—C4—C5—C6	2.31 (17)	C11—S12—C13—C14	0.08 (10)
S1—C4—C5—C6	−178.67 (8)	S12—C13—C14—C15	−0.25 (14)
C2—N1—C6—O1	176.40 (10)	C10—C11—C15—C14	176.64 (10)
N2—N1—C6—O1	10.60 (15)	S12—C11—C15—C14	−0.26 (13)
C2—N1—C6—C5	−3.50 (15)	C13—C14—C15—C11	0.33 (15)

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>
N4—H041 \cdots N2	0.827 (18)	2.224 (17)	2.6062 (13)	108.4 (14)
N4—H041 \cdots N5 ⁱ	0.827 (18)	2.513 (17)	3.0555 (14)	124.2 (15)
N4—H042 \cdots O1 ⁱ	0.823 (17)	2.144 (17)	2.9414 (12)	163.1 (15)
C13—H13 \cdots N5 ⁱⁱ	0.95	2.49	3.2722 (15)	139
C10—H10 \cdots O1 ⁱⁱⁱ	0.95	2.35	3.2124 (13)	150

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