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## Structure Reports

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## 3-[(Furan-2-yl)carbonyl]-1-(pyrimidin-2-yl)thiourea

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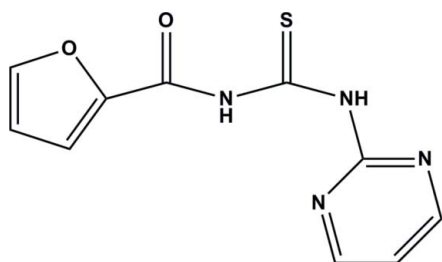
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Key indicators: single-crystal X-ray study;  $T = 123$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.038;  $wR$  factor = 0.108; data-to-parameter ratio = 13.2.

The title compound,  $\text{C}_{10}\text{H}_8\text{N}_4\text{O}_2\text{S}$ , was synthesized from furoyl isothiocyanate and 2-aminopyrimidine in dry acetone. The two N—H groups are in an *anti* conformation with respect to each other and one N—H group is *anti* to the C=S group while the other is *syn*. The amide C=S and the C=O groups are *syn* to each other. The mean plane of the central thiourea fragment forms dihedral angles of 13.50 (14) and 5.03 (11)° with the furan and pyrimidine rings, respectively. The dihedral angle between the furan and pyrimidine rings is 18.43 (10)°. The molecular conformation is stabilized by an intramolecular N—H...N hydrogen bond generating an  $S(6)$  ring motif. In the crystal, molecules are linked by pairs of N—H...N and weak C—H...S hydrogen bonds to form inversion dimers.

## Related literature

For a general background to the biological activity of thiourea, see: Koketsu & Ishihara (2006). For heterocyclic derivatives, metal complexes and molecular electronics, see: Zeng *et al.* (2003); D'hooghe *et al.* (2005); Aly *et al.* (2007); Duque *et al.* (2009). For related structures, see: Singh *et al.* (2012); Koch (2001); Hassan *et al.* (2007); Pérez *et al.* (2008); Yan & Xue (2008).



## Experimental

## Crystal data

$\text{C}_{10}\text{H}_8\text{N}_4\text{O}_2\text{S}$   
 $M_r = 248.26$   
 Monoclinic,  $P2_1/n$   
 $a = 5.6962$  (2) Å  
 $b = 21.0530$  (7) Å  
 $c = 8.7901$  (3) Å  
 $\beta = 95.559$  (3)°  
 $V = 1049.17$  (6) Å<sup>3</sup>  
 $Z = 4$   
 Cu  $K\alpha$  radiation  
 $\mu = 2.74$  mm<sup>-1</sup>  
 $T = 123$  K  
 $0.40 \times 0.22 \times 0.11$  mm

## Data collection

Agilent Xcalibur (Ruby, Gemini) diffractometer  
 Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)  
 $T_{\min} = 0.421$ ,  $T_{\max} = 1.000$   
 6957 measured reflections  
 2028 independent reflections  
 1951 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.028$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$   
 $wR(F^2) = 0.108$   
 $S = 1.04$   
 2028 reflections  
 154 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.46$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.21$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1B}\cdots\text{N3}$	0.86	1.89	2.6240 (18)	142
$\text{N2}-\text{H2B}\cdots\text{N4}^i$	0.86	2.21	3.0726 (19)	175
$\text{C10}-\text{H10A}\cdots\text{S1}^i$	0.93	2.76	3.5536 (17)	144

Symmetry code: (i)  $-x + 2, -y + 1, -z + 1$ .

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5548).

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## supporting information

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### 3-[(Furan-2-yl)carbonyl]-1-(pyrimidin-2-yl)thiourea

Durga P. Singh, Seema Pratap, Sushil K. Gupta and Ray J. Butcher

#### S1. Comment

Thiourea and its derivatives are known to exhibit a wide variety of biological activities (Koketsu & Ishihara, 2006). These are also widely used as precursors or intermediates towards the synthesis of a variety of heterocyclic compounds (Zeng *et al.*, 2003; D'hooghe, *et al.*, 2005). In addition, aroylthioureas have applications in metal complexes and molecular electronics (Aly *et al.*, 2007; Duque *et al.*, 2009). The structure of a related compound was recently published (Yan & Xue, 2008) in which the molecule showed excellent herbicidal activity.

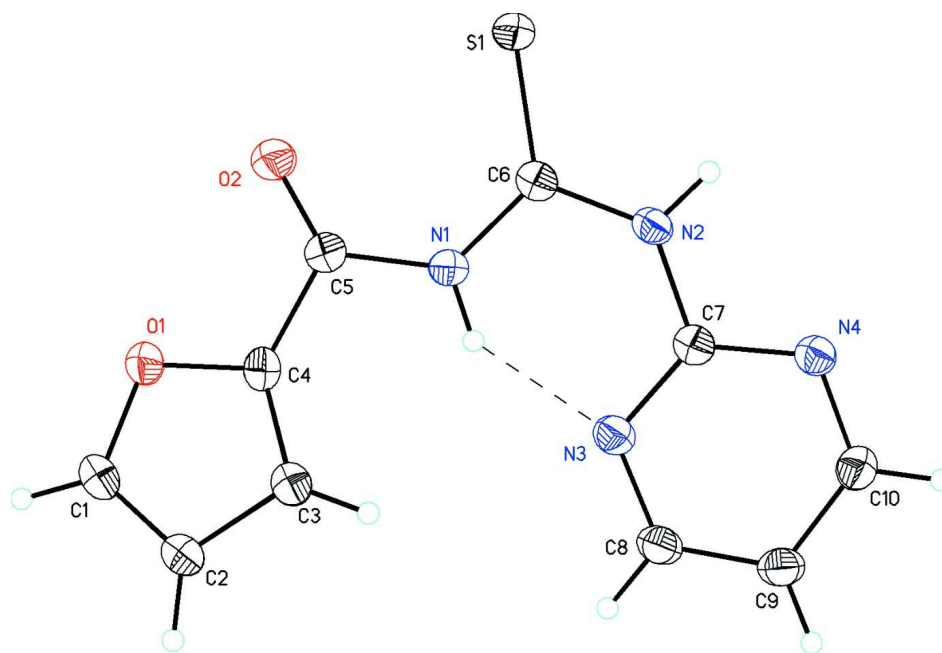
In view of the biological importance of thiourea and its furoic acid derivatives, the structure of the title compound was determined. In the title compound (Fig. 1), the conformation of the two N—H bonds are *anti* to each other, and one of them is *anti* to the C=S and the other is *syn* in the urea moiety. Furthermore, the amide C=S and the C=O groups are *syn* to each other, similar to the *syn* conformation observed in 1-furoyl-3-methyl-3-phenylthiourea (Pérez *et al.*, 2008) and in *N*-(2-furoyl)-*N*-(6-methyl-2-pyridyl)thiourea (Hassan *et al.*, 2007). The bond lengths and angles in the title compound are comparable to other thiourea derivatives (Koch 2001; Pérez *et al.*, 2008; Singh *et al.*, 2012). The C6—S1 and C5—O2 bonds show typical double-bond character. However, the C—N bond lengths, C5—N1, C6—N1, C6—N2 are shorter than the normal C—N single-bond length of about 1.48 Å. These results can be explained by the existence of resonance in this part of the molecule. The central thiourea fragment (O2/C5/N1/C6/N2) makes dihedral angle of 13.50 (14)° with furan ring (O1/C1/C2/C3/C4) and 5.03 (11)° with pyrimidine ring (C7/N3/C8/C9/C10/N4), respectively. The dihedral angle between the mean planes of the furan and pyrimidine rings is 18.43 (10)°. The molecular geometry is stabilized by an intramolecular N—H⋯N hydrogen bond generating an S(6) ring motif. In the crystal, molecules are linked by pairs of N—H⋯N and weak C—H⋯S hydrogen bonds (Table 1) forming centrosymmetric dimers (Fig. 2).

#### S2. Experimental

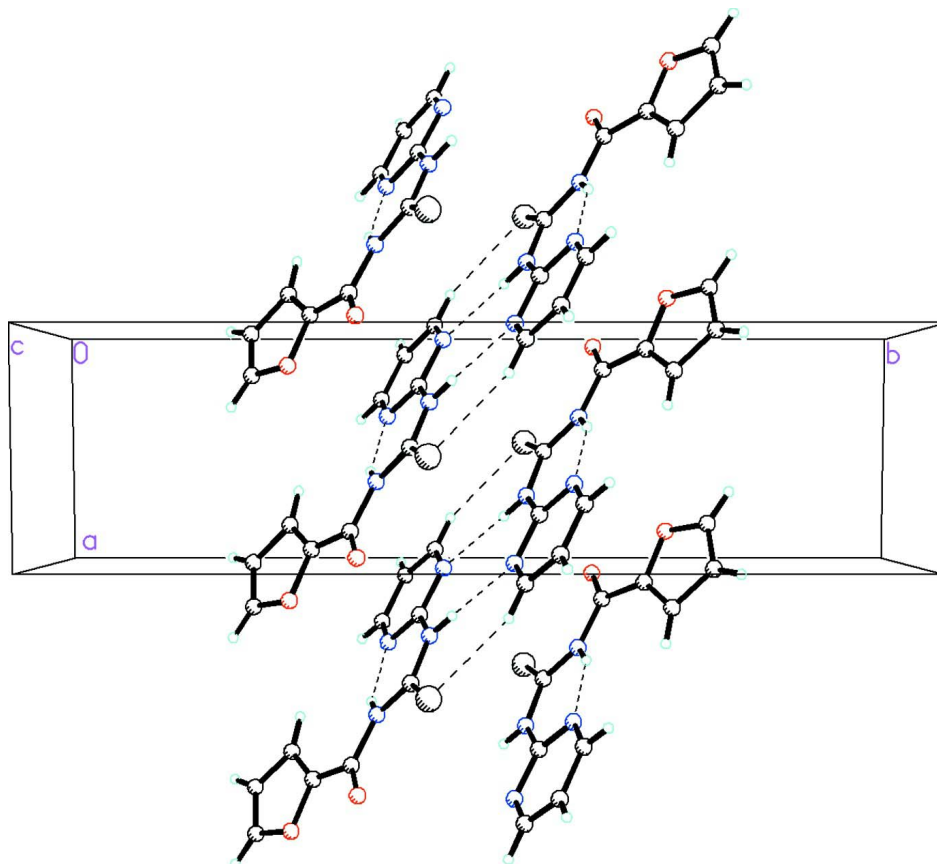
A solution of 2-thiophenecarbonyl chloride (0.01 mol) in anhydrous acetone (80 ml) was added dropwise to a suspension of ammonium thiocyanate (0.01 mol) in anhydrous acetone (50 ml) and the reaction mixture was refluxed for 50 minutes. After cooling to room temperature, a solution of 4-chloroaniline (0.01 mol) in dry acetone (25 ml) was added and the resulting mixture refluxed for 2 h. The reaction mixture was poured into five times its volume of cold water, upon which the thiourea precipitated. The resulting solid product was crystallized from acetone yielding yellow colour X-ray quality single crystals. Yield: 80%; M.P.: 455 - 456 K). Anal. Calc. for C<sub>10</sub>H<sub>8</sub>N<sub>4</sub>O<sub>2</sub>S (%): C, 48.38; H, 3.25; N, 22.57. Found: C, 48.49; H, 3.28; N, 22.50.

#### S3. Refinement

All H atoms were placed in calculated positions and refined using a riding-model approximation with C—H = 0.93 Å, N—H = 0.86 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ .

**Figure 1**

The molecular structure of the title compound showing 30% probability displacement ellipsoids. Dashed lines indicate an intramolecular N—H $\cdots$ N hydrogen bond.

**Figure 2**

Crystal packing for the title compound viewed along the *c* axis. Dashed lines indicate intermolecular N—H...N and C—H...S hydrogen bonds.

### 3-[(Furan-2-yl)carbonyl]-1-(pyrimidin-2-yl)thiourea

#### Crystal data

$C_{10}H_8N_4O_2S$   
 $M_r = 248.26$   
 Monoclinic,  $P2_1/n$   
 Hall symbol: -P 2yn  
 $a = 5.6962$  (2) Å  
 $b = 21.0530$  (7) Å  
 $c = 8.7901$  (3) Å  
 $\beta = 95.559$  (3)°  
 $V = 1049.17$  (6) Å<sup>3</sup>  
 $Z = 4$

$F(000) = 512$   
 $D_x = 1.572$  Mg m<sup>-3</sup>  
 Cu  $K\alpha$  radiation,  $\lambda = 1.54178$  Å  
 Cell parameters from 4415 reflections  
 $\theta = 4.2\text{--}72.7^\circ$   
 $\mu = 2.74$  mm<sup>-1</sup>  
 $T = 123$  K  
 Plate, colorless  
 $0.40 \times 0.22 \times 0.11$  mm

#### Data collection

Agilent Xcalibur (Ruby, Gemini)  
 diffractometer  
 Radiation source: Enhance (Cu) X-ray Source  
 Graphite monochromator  
 Detector resolution: 10.5081 pixels mm<sup>-1</sup>  
 $\omega$  scans

Absorption correction: multi-scan  
 (*CrysAlis PRO*; Agilent, 2011)  
 $T_{\min} = 0.421$ ,  $T_{\max} = 1.000$   
 6957 measured reflections  
 2028 independent reflections  
 1951 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.028$

$\theta_{\max} = 72.8^\circ$ ,  $\theta_{\min} = 4.2^\circ$   
 $h = -6 \rightarrow 5$

$k = -25 \rightarrow 25$   
 $l = -10 \rightarrow 9$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.038$   
 $wR(F^2) = 0.108$   
 $S = 1.04$   
 2028 reflections  
 154 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0735P)^2 + 0.4136P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.46 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.21 \text{ e } \text{Å}^{-3}$

Special details

**Experimental.** FT IR (selected, KBr,  $\text{cm}^{-1}$ ): 3424, 3207 [ $\nu(\text{N}-\text{H})$ ]; 1712 [amide-I,  $\text{C}=\text{O}$ ]; 1586, 1556 [ $\nu(\text{C}=\text{C})$ ]; 1505[thioureido-I], 1327 [thioureido-II], 1177 [thioureido-III], 763 [thioureido-IV].  $^1\text{H}$  NMR (300 MHz,  $\text{dms}\text{-d}_6$ ):  $\delta$  14.08 (s, 1H, H-bonded N-H); 11.90 (s, 1H, free N-H); 8.80 (d,  $J = 7.1$  Hz, 2H, pyrimidine CH); 8.05 (d,  $J = 7.5$  Hz, 1H, furan CH); 7.50 (d,  $J = 7.8$  Hz, 1H, pyrimidine CH); 7.30 (t,  $J_1(\text{H},\text{H}) = 6.8$  Hz,  $J_2(\text{H},\text{H}) = 7.1$  Hz, 1H, pyrimidine CH); 6.76 (t,  $J(\text{H},\text{H}) = 7.8$  Hz, 1H, furan CH).  $^{13}\text{C}$  NMR (75 MHz,  $\text{dms}\text{-d}_6$ ):  $\delta$  177.4, 158.5, 157.1, 155.4, 147.6, 146.4, 117.6, 117.1, 112.9.

**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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{Å}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.47026 (7)	0.555126 (18)	0.19269 (4)	0.02308 (17)
O1	-0.1466 (2)	0.71757 (6)	0.45239 (14)	0.0270 (3)
O2	0.0499 (2)	0.63600 (6)	0.26198 (14)	0.0283 (3)
N1	0.3619 (2)	0.61674 (6)	0.44577 (15)	0.0214 (3)
H1B	0.4047	0.6248	0.5403	0.026*
N2	0.7006 (2)	0.55592 (6)	0.46685 (16)	0.0201 (3)
H2B	0.7901	0.5300	0.4235	0.024*
N3	0.6446 (2)	0.60768 (6)	0.69888 (15)	0.0234 (3)
N4	0.9782 (2)	0.54126 (7)	0.67136 (15)	0.0216 (3)
C1	-0.1833 (3)	0.76232 (8)	0.5596 (2)	0.0285 (4)
H1A	-0.3194	0.7867	0.5597	0.034*
C2	0.0017 (3)	0.76645 (8)	0.6641 (2)	0.0304 (4)
H2A	0.0183	0.7937	0.7478	0.036*
C3	0.1690 (3)	0.72089 (8)	0.6224 (2)	0.0288 (4)
H3A	0.3162	0.7124	0.6737	0.035*
C4	0.0718 (3)	0.69251 (7)	0.49378 (18)	0.0214 (3)
C5	0.1539 (3)	0.64564 (7)	0.38553 (18)	0.0204 (3)
C6	0.5082 (3)	0.57705 (7)	0.37439 (17)	0.0192 (3)

C7	0.7750 (3)	0.56938 (7)	0.61922 (18)	0.0196 (3)
C8	0.7219 (3)	0.61687 (8)	0.84626 (19)	0.0257 (4)
H8A	0.6344	0.6426	0.9055	0.031*
C9	0.9258 (3)	0.58957 (8)	0.91292 (19)	0.0261 (4)
H9A	0.9775	0.5958	1.0154	0.031*
C10	1.0498 (3)	0.55213 (8)	0.81814 (19)	0.0250 (4)
H10A	1.1902	0.5336	0.8591	0.030*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0259 (3)	0.0236 (3)	0.0195 (3)	0.00267 (13)	0.00100 (17)	-0.00364 (13)
O1	0.0233 (6)	0.0286 (6)	0.0280 (6)	0.0067 (5)	-0.0032 (5)	-0.0046 (5)
O2	0.0252 (6)	0.0347 (7)	0.0245 (6)	0.0026 (5)	-0.0006 (5)	-0.0060 (5)
N1	0.0242 (7)	0.0215 (6)	0.0182 (6)	0.0022 (5)	0.0012 (5)	-0.0023 (5)
N2	0.0232 (7)	0.0180 (6)	0.0195 (7)	0.0021 (5)	0.0041 (5)	-0.0022 (5)
N3	0.0273 (7)	0.0210 (6)	0.0218 (7)	0.0036 (5)	0.0024 (5)	-0.0017 (5)
N4	0.0224 (7)	0.0207 (6)	0.0217 (7)	0.0005 (5)	0.0026 (5)	-0.0017 (5)
C1	0.0292 (9)	0.0246 (8)	0.0315 (9)	0.0081 (6)	0.0023 (7)	-0.0038 (6)
C2	0.0315 (9)	0.0282 (9)	0.0304 (9)	0.0086 (7)	-0.0025 (7)	-0.0094 (7)
C3	0.0264 (8)	0.0286 (8)	0.0303 (9)	0.0072 (7)	-0.0030 (7)	-0.0073 (7)
C4	0.0198 (7)	0.0201 (7)	0.0240 (8)	0.0013 (6)	0.0010 (6)	0.0024 (6)
C5	0.0212 (7)	0.0194 (7)	0.0206 (7)	-0.0026 (6)	0.0023 (6)	0.0006 (6)
C6	0.0219 (7)	0.0152 (7)	0.0210 (7)	-0.0023 (5)	0.0042 (6)	0.0003 (5)
C7	0.0224 (8)	0.0163 (7)	0.0205 (8)	-0.0012 (6)	0.0037 (6)	0.0014 (6)
C8	0.0316 (9)	0.0240 (8)	0.0218 (8)	0.0038 (6)	0.0041 (6)	-0.0034 (6)
C9	0.0323 (9)	0.0253 (8)	0.0202 (8)	0.0011 (6)	0.0000 (6)	-0.0034 (6)
C10	0.0241 (8)	0.0258 (9)	0.0245 (9)	0.0022 (6)	-0.0011 (7)	0.0002 (6)

*Geometric parameters (Å, °)*

S1—C6	1.6565 (15)	N4—C7	1.340 (2)
O1—C1	1.363 (2)	C1—C2	1.332 (3)
O1—C4	1.3679 (19)	C1—H1A	0.9300
O2—C5	1.203 (2)	C2—C3	1.425 (2)
N1—C6	1.3739 (19)	C2—H2A	0.9300
N1—C5	1.390 (2)	C3—C4	1.349 (2)
N1—H1B	0.8600	C3—H3A	0.9300
N2—C6	1.373 (2)	C4—C5	1.478 (2)
N2—C7	1.394 (2)	C8—C9	1.375 (2)
N2—H2B	0.8600	C8—H8A	0.9300
N3—C7	1.339 (2)	C9—C10	1.389 (2)
N3—C8	1.341 (2)	C9—H9A	0.9300
N4—C10	1.335 (2)	C10—H10A	0.9300
C1—O1—C4	106.22 (13)	O1—C4—C5	115.00 (14)
C6—N1—C5	128.64 (13)	O2—C5—N1	126.67 (15)
C6—N1—H1B	115.7	O2—C5—C4	122.34 (15)

C5—N1—H1B	115.7	N1—C5—C4	110.98 (13)
C6—N2—C7	130.81 (13)	N2—C6—N1	114.28 (13)
C6—N2—H2B	114.6	N2—C6—S1	120.16 (11)
C7—N2—H2B	114.6	N1—C6—S1	125.56 (12)
C7—N3—C8	116.43 (14)	N3—C7—N4	126.26 (14)
C10—N4—C7	115.33 (14)	N3—C7—N2	119.48 (14)
C2—C1—O1	110.97 (15)	N4—C7—N2	114.26 (13)
C2—C1—H1A	124.5	N3—C8—C9	122.41 (15)
O1—C1—H1A	124.5	N3—C8—H8A	118.8
C1—C2—C3	106.41 (15)	C9—C8—H8A	118.8
C1—C2—H2A	126.8	C8—C9—C10	116.07 (15)
C3—C2—H2A	126.8	C8—C9—H9A	122.0
C4—C3—C2	106.46 (15)	C10—C9—H9A	122.0
C4—C3—H3A	126.8	N4—C10—C9	123.46 (15)
C2—C3—H3A	126.8	N4—C10—H10A	118.3
C3—C4—O1	109.94 (14)	C9—C10—H10A	118.3
C3—C4—C5	134.87 (15)		
C4—O1—C1—C2	0.5 (2)	C7—N2—C6—S1	177.23 (12)
O1—C1—C2—C3	-0.5 (2)	C5—N1—C6—N2	-179.49 (14)
C1—C2—C3—C4	0.3 (2)	C5—N1—C6—S1	1.3 (2)
C2—C3—C4—O1	0.0 (2)	C8—N3—C7—N4	-2.3 (2)
C2—C3—C4—C5	174.44 (18)	C8—N3—C7—N2	177.72 (14)
C1—O1—C4—C3	-0.26 (18)	C10—N4—C7—N3	1.7 (2)
C1—O1—C4—C5	-175.93 (14)	C10—N4—C7—N2	-178.32 (13)
C6—N1—C5—O2	8.1 (3)	C6—N2—C7—N3	2.0 (2)
C6—N1—C5—C4	-171.00 (14)	C6—N2—C7—N4	-177.98 (14)
C3—C4—C5—O2	-165.63 (19)	C7—N3—C8—C9	1.0 (2)
O1—C4—C5—O2	8.6 (2)	N3—C8—C9—C10	0.6 (2)
C3—C4—C5—N1	13.5 (3)	C7—N4—C10—C9	0.2 (2)
O1—C4—C5—N1	-172.23 (12)	C8—C9—C10—N4	-1.3 (2)
C7—N2—C6—N1	-2.0 (2)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1B $\cdots$ N3	0.86	1.89	2.6240 (18)	142
N2—H2B $\cdots$ N4 <sup>i</sup>	0.86	2.21	3.0726 (19)	175
C10—H10A $\cdots$ S1 <sup>i</sup>	0.93	2.76	3.5536 (17)	144

Symmetry code: (i)  $-x+2, -y+1, -z+1$ .