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## Structure Reports

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4-[(*E*)-(4-Chlorobenzylidene)amino]-3-methyl-1*H*-1,2,4-triazole-5(4*H*)-thioneB. K. Sarojini,<sup>a,b</sup> P. S. Manjula,<sup>a</sup> Manpreet Kaur,<sup>c</sup> Brian J. Anderson<sup>d</sup> and Jerry P. Jasinski<sup>d\*</sup>

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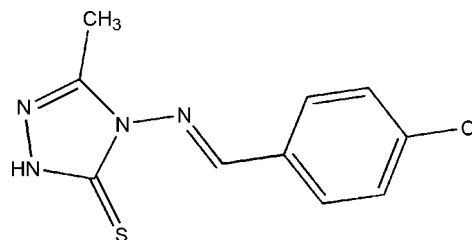
Received 8 December 2013; accepted 11 December 2013

Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.043;  $wR$  factor = 0.120; data-to-parameter ratio = 15.0.

In the title compound,  $\text{C}_{10}\text{H}_9\text{ClN}_4\text{S}$ , the dihedral angle between the mean planes of the phenyl and 1*H*-1,2,4-triazole-5(4*H*)-thione rings is  $25.3(9)^\circ$ . The latter ring is essentially planar, with maximum deviations of 0.010 and  $-0.010$  Å for the ring N atom in the 4-position and ring C atom bearing the methyl group, respectively. An intramolecular  $\text{C}-\text{H}\cdots\text{S}$  contact occurs. In the crystal, pairs of weak  $\text{N}-\text{H}\cdots\text{S}$  interactions link the molecules into inversion dimers in the *ac* plane, forming  $R_2^2(8)$  graph-set motifs. In addition, weak  $\pi-\pi$  interactions [centroid-centroid distances =  $3.3463(14)$  and  $3.6127(13)$  Å] are observed.

## Related literature

For the chemistry of Schiff base compounds, see: Dubey & Vaid (1991); Yadav *et al.* (1994). For the use of Schiff bases containing different donor atoms in analytical applications and metal coordination, see: Galic *et al.* (2001); Wyrzykiewicz & Prukah (1998); Reddy & Lirgappa (1994). Many compounds containing S and N atoms are antihypertensive (Wei *et al.*, 1981,1982), analgesic (Thieme *et al.*, 1973*a,b*), antiinflammatory (Dornow *et al.*, 1964), sedative (Barrera *et al.*, 1985), or fungicidal (Malik *et al.*, 2011). For the crystal structures of related Schiff bases, see: Jeyaseelan *et al.* (2012); Devarajegowda *et al.* (2012); Vinduvahini *et al.* (2011); Almutairi *et al.* (2012); Kubicki *et al.* (2012); Praveen *et al.* (2012); Kant *et al.* (2012); Ding *et al.* (2009). For the crystal structures of Schiff bases reported by our group, see: Sarojini *et al.* (2007*a,b*). For standard bond lengths, see: Allen *et al.* (1987). For  $\pi-\pi$  stacking, see: Grimme (2008).



## Experimental

## Crystal data

$\text{C}_{10}\text{H}_9\text{ClN}_4\text{S}$   
 $M_r = 252.72$   
 Triclinic,  $P\bar{1}$   
 $a = 7.0718(8)$  Å  
 $b = 7.2901(8)$  Å  
 $c = 11.8434(7)$  Å  
 $\alpha = 92.778(7)^\circ$   
 $\beta = 94.986(7)^\circ$   
 $\gamma = 109.752(10)^\circ$   
 $V = 570.50(10)$  Å<sup>3</sup>  
 $Z = 2$   
 Cu  $K\alpha$  radiation  
 $\mu = 4.49$  mm<sup>-1</sup>  
 $T = 173$  K  
 $0.42 \times 0.08 \times 0.06$  mm

## Data collection

Agilent Gemini EOS diffractometer  
 Absorption correction: multi-scan  
 (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)  
 $T_{\min} = 0.544$ ,  $T_{\max} = 1.000$   
 3413 measured reflections  
 2195 independent reflections  
 1860 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.030$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.120$   
 $S = 1.02$   
 2195 reflections  
 146 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.34$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.39$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> — <i>H</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i> ⋯ <i>A</i>
<i>N</i> 4— <i>H</i> 4⋯ <i>S</i> 1 <sup>i</sup>	0.86	2.43	3.2926 (19)	176
<i>Cl</i> 1— <i>H</i> 1⋯ <i>S</i> 1	0.93	2.62	3.199 (2)	121

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL2012* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

BKS and PSM gratefully acknowledge the Department of Chemistry, P. A. College of Engineering, for providing research facilities. JPJ acknowledges the NSF-MRI program (grant No. CHE-1039027) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QM2102).

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## supporting information

*Acta Cryst.* (2014). E70, o57–o58 [https://doi.org/10.1107/S1600536813033527]

**4-[(*E*)-(4-Chlorobenzylidene)amino]-3-methyl-1*H*-1,2,4-triazole-5(4*H*)-thione****B. K. Sarojini, P. S. Manjula, Manpreet Kaur, Brian J. Anderson and Jerry P. Jasinski****S1. Comment**

During the last few decades, there has been a considerable interest in the chemistry of Schiff base compounds (Dubey & Vaid, 1991; Yadav *et al.*, 1994). Schiff bases, containing different donor atoms, also find use in analytical applications and metal coordination (Galic *et al.*, 2001; Wyrzykiewicz & Pruka, 1998; Reddy & Lirgappa, 1994). Since many compounds containing sulfur and nitrogen atoms are antihypertensive (Wei *et al.*, 1981,1982), analgesic (Thieme *et al.*, 1973*a,b*), antiinflammatory (Dornow *et al.*, 1964), sedative (Barrera *et al.*,1985), or fungicidal (Malik *et al.*, 2011), synthesis of the corresponding heterocyclic compounds could be of interest from the viewpoint of chemical reactivity and biological activity. The crystal structures of some of the related Schiff bases viz: 3-ethyl-4-[(*E*)-(4-fluorobenzylidene)amino]-1*H*-1,2,4-triazole-5(4*H*)-thione (Jeyaseelan *et al.*, 2012); 4-[(*E*)-(4-fluorobenzylidene)amino]-3-methyl-1*H*-1,2,4-triazole-5(4*H*)-thione (Devarajegowda *et al.*, 2012); 3-[2-(2,6-dichloro-anilino)benzyl]-4-[(4-methoxybenzylidene)amino]-1*H*-1,2,4-triazole-5(4*H*)-thione (Vinduvahini *et al.*, 2011); 3-(adamantan-1-yl)-1-[(4-ethylpiperazin-1-yl)methyl]-4-[(*E*)-(4-hydroxy-benzylidene)amino]-1*H*-1,2,4-triazole-5(4*H*)-thione (Almutairi *et al.*, 2012); 4-[(2*E*)-2-[1-(4-Methoxyphenyl)ethylidene]hydrazinyl]-8-(trifluoromethyl)quinoline (Kubicki *et al.*, 2012); (*E*)-*N'*-(4-Methoxybenzylidene)-2-*m*-tolylacetohydrazide (Praveen *et al.*, 2012); (1*Z*)-1-[(2*E*)-3-(4-bromophenyl)-1-(4-fluorophenyl)prop-2-en-1-ylidene]-2-(2,4-dinitrophenyl)hydrazine (Kant *et al.*, 2012); (*E*)-3-(2-ethoxyphenyl)-4-(2-fluorobenzylideneamino)-1*H*-1,2,4-triazole-5(4*H*)-thione (Ding *et al.*,2009) have been reported. Crystal structures of some of the Schiff bases were also reported from our group (Sarojini *et al.*, 2007*a,b*). In continuation of our work on the synthesis of acetamides derivatives, we report herein the crystal structure of the title compound, C<sub>10</sub>H<sub>9</sub>ClN<sub>4</sub>S, (I).

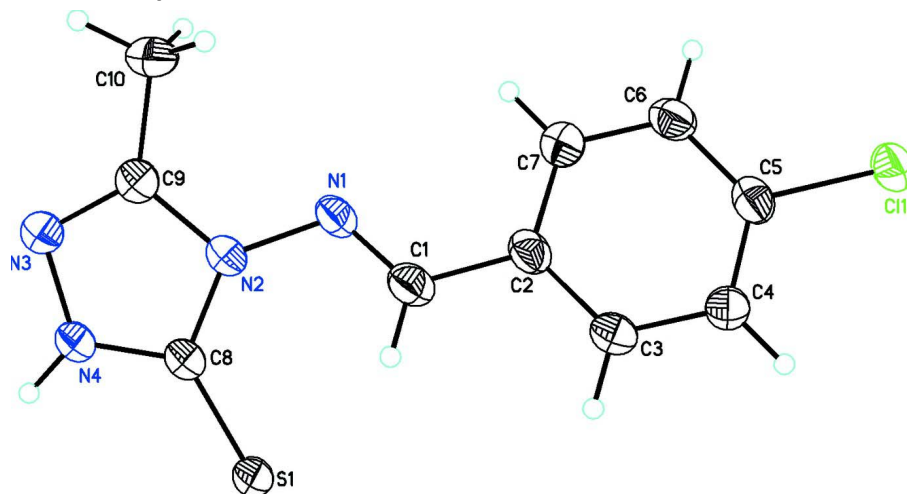
In the title compound, (I), C<sub>10</sub>H<sub>9</sub>ClN<sub>4</sub>S, the dihedral angle between the mean planes of the phenyl ring and the 1*H*-1,2,4-triazole-5(4*H*)-thione ring is 25.3 (9)° (Fig.1). The 1,2,4-triazole-5(4*H*)-thione ring is essentially planar with a maximum deviation of 0.010Å and -0.010Å for the N2 nitrogen and C9 carbon atom, respectively. Bond lengths and bond angles are in normal ranges (Allen *et al.*, 1987).In the crystal, weak N4—H4···S1 intermolecular interactions forming R<sub>2</sub><sup>2</sup>(8) graph set motifs link the molecules into dimers diagonally in the ac plane (Fig. 2). In addition, weak Cg—Cg π—π intermolecular interactions are observed which may contribute to crystal packing (Cg1—Cg1 = 3.3463 (14)Å; -x, 1-y, -z; Cg2—Cg2 = 3.6127 (13)Å; 1-x, 2-y, 1-z; Cg1 = N2/C81/N4/N3/C9; Cg2 = C2—C7) (Grimme, 1987). No classical hydrogen bonds were observed.

**S2. Experimental**

To a suspension of 4-chlorobenzaldehyde (1.405 g, 0.01 mol) in ethanol (15 ml), 4-amino-5-methyl-2,4-dihydro-3*H*-1,2,4-triazole- 3-thione (0.01 mol, 1.3 g) was added and heated to get a clear solution. To this a few drops of conc.H<sub>2</sub>SO<sub>4</sub> was added as a catalyst and refluxed for 36 h on a water bath. The precipitate formed was filtered and recrystallized from methanol to get the titled compound. The single crystals were grown from methanol (M.P.:463 - 465 K).

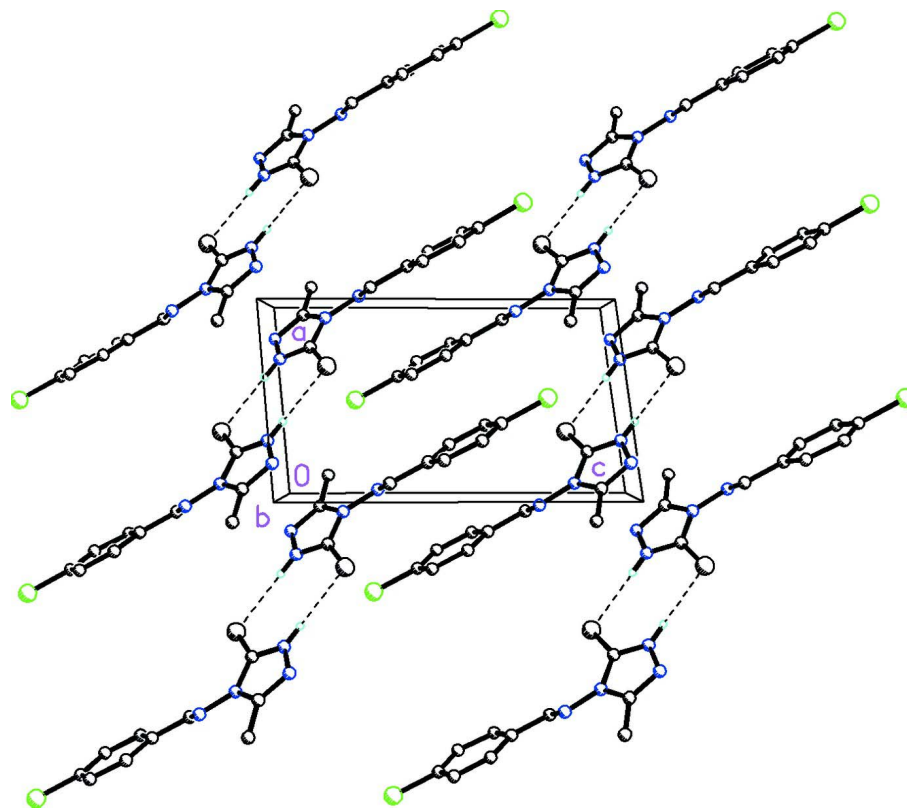
### S3. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with Atom—H lengths of 0.93 Å (CH), 0.96 Å (CH<sub>3</sub>) or 0.86 Å (NH). Isotropic displacement parameters for these atoms were set to 1.2 (CH, NH) or 1.5 (CH<sub>3</sub>) times  $U_{eq}$  of the parent atom. Idealised Me refined as rotating groups.



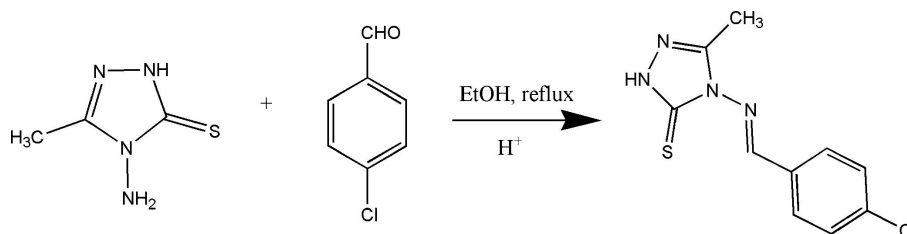
**Figure 1**

ORTEP drawing of (I) (C<sub>10</sub>H<sub>9</sub>ClN<sub>4</sub>S) showing the labeling scheme with 50% probability displacement ellipsoids.



**Figure 2**

Molecular packing for (I) viewed along the *b* axis. Dashed lines indicate weak N4—H4...S1 intermolecular interactions forming  $R_2^2(8)$  graph set motifs linking the molecules into dimers diagonally in the *ac* plane. H atoms not involved in hydrogen bonding have been removed for clarity.



**Figure 3**

Synthesis scheme for (I).

#### 4-[(*E*)-(4-Chlorobenzylidene)amino]-3-methyl-1*H*-1,2,4-triazole-5(4*H*)-thione

##### Crystal data

$C_{10}H_9ClN_4S$

$M_r = 252.72$

Triclinic,  $P\bar{1}$

$a = 7.0718$  (8) Å

$b = 7.2901$  (8) Å

$c = 11.8434$  (7) Å

$\alpha = 92.778$  (7)°

$\beta = 94.986$  (7)°

$\gamma = 109.752$  (10)°

$V = 570.50$  (10) Å<sup>3</sup>

$Z = 2$

$F(000) = 260$

$D_x = 1.471$  Mg m<sup>-3</sup>

Cu  $K\alpha$  radiation,  $\lambda = 1.54184$  Å

Cell parameters from 1400 reflections

$\theta = 3.8$ – $72.2$ °

$\mu = 4.49 \text{ mm}^{-1}$   
 $T = 173 \text{ K}$

Irregular, colourless  
 $0.42 \times 0.08 \times 0.06 \text{ mm}$

*Data collection*

Agilent Gemini EOS  
 diffractometer  
 Radiation source: Enhance (Cu) X-ray Source  
 Detector resolution:  $16.0416 \text{ pixels mm}^{-1}$   
 $\omega$  scans  
 Absorption correction: multi-scan  
 (*CrysAlis PRO* and *CrysAlis RED*; Agilent,  
 2012)  
 $T_{\min} = 0.544$ ,  $T_{\max} = 1.000$

3413 measured reflections  
 2195 independent reflections  
 1860 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.030$   
 $\theta_{\max} = 72.3^\circ$ ,  $\theta_{\min} = 3.8^\circ$   
 $h = -8 \rightarrow 8$   
 $k = -8 \rightarrow 8$   
 $l = -10 \rightarrow 14$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.120$   
 $S = 1.02$   
 2195 reflections  
 146 parameters  
 0 restraints

Primary atom site location: structure-invariant  
 direct methods  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0694P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.34 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.39 \text{ e } \text{Å}^{-3}$

*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 ( $\text{Å}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.50541 (9)	0.96033 (9)	0.77738 (5)	0.03752 (19)
S1	-0.33106 (9)	0.64930 (9)	0.16551 (5)	0.03564 (19)
N1	0.0401 (3)	0.4905 (3)	0.27296 (16)	0.0295 (4)
N2	-0.0729 (3)	0.4344 (3)	0.16664 (15)	0.0287 (4)
N3	-0.1813 (3)	0.2442 (3)	0.00660 (17)	0.0353 (4)
N4	-0.2891 (3)	0.3680 (3)	0.02140 (16)	0.0317 (4)
H4	-0.3862	0.3696	-0.0271	0.038*
C1	0.0775 (3)	0.6667 (3)	0.31206 (19)	0.0311 (5)
H1	0.0364	0.7520	0.2684	0.037*
C2	0.1852 (3)	0.7342 (3)	0.42579 (19)	0.0289 (5)
C3	0.2005 (3)	0.9179 (3)	0.4726 (2)	0.0320 (5)
H3	0.1460	0.9957	0.4301	0.038*
C4	0.2955 (3)	0.9876 (3)	0.5816 (2)	0.0318 (5)
H4A	0.3026	1.1095	0.6131	0.038*
C5	0.3788 (3)	0.8714 (3)	0.64183 (19)	0.0307 (5)
C6	0.3682 (3)	0.6889 (3)	0.5977 (2)	0.0329 (5)
H6	0.4265	0.6136	0.6400	0.039*

C7	0.2703 (3)	0.6195 (3)	0.4903 (2)	0.0333 (5)
H7	0.2606	0.4959	0.4605	0.040*
C8	-0.2301 (3)	0.4851 (3)	0.11732 (19)	0.0291 (5)
C9	-0.0524 (3)	0.2861 (3)	0.0975 (2)	0.0322 (5)
C10	0.1023 (4)	0.1949 (4)	0.1262 (2)	0.0431 (6)
H10A	0.0590	0.1060	0.1837	0.065*
H10B	0.2284	0.2949	0.1541	0.065*
H10C	0.1195	0.1248	0.0594	0.065*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C11	0.0398 (3)	0.0455 (3)	0.0282 (3)	0.0191 (3)	-0.0056 (2)	-0.0031 (2)
S1	0.0364 (3)	0.0421 (3)	0.0329 (3)	0.0242 (3)	-0.0099 (2)	-0.0080 (2)
N1	0.0255 (9)	0.0372 (10)	0.0263 (10)	0.0134 (7)	-0.0047 (7)	0.0010 (7)
N2	0.0270 (9)	0.0321 (9)	0.0274 (10)	0.0132 (7)	-0.0046 (7)	-0.0007 (7)
N3	0.0369 (10)	0.0397 (10)	0.0325 (11)	0.0212 (8)	-0.0063 (8)	-0.0057 (8)
N4	0.0318 (10)	0.0394 (10)	0.0272 (10)	0.0198 (8)	-0.0066 (8)	-0.0030 (8)
C1	0.0260 (10)	0.0337 (11)	0.0334 (12)	0.0113 (8)	-0.0029 (9)	0.0044 (9)
C2	0.0208 (10)	0.0344 (11)	0.0296 (12)	0.0087 (8)	-0.0020 (8)	0.0007 (9)
C3	0.0264 (10)	0.0364 (12)	0.0355 (12)	0.0153 (9)	-0.0017 (9)	0.0010 (9)
C4	0.0282 (10)	0.0353 (11)	0.0339 (12)	0.0152 (9)	-0.0004 (9)	-0.0041 (9)
C5	0.0248 (10)	0.0406 (12)	0.0260 (11)	0.0112 (9)	0.0007 (8)	-0.0001 (9)
C6	0.0331 (11)	0.0350 (11)	0.0328 (12)	0.0155 (9)	-0.0015 (9)	0.0064 (9)
C7	0.0346 (11)	0.0307 (11)	0.0342 (12)	0.0122 (9)	-0.0009 (10)	-0.0001 (9)
C8	0.0284 (10)	0.0330 (11)	0.0269 (11)	0.0138 (8)	-0.0036 (8)	0.0003 (9)
C9	0.0314 (11)	0.0350 (11)	0.0311 (12)	0.0148 (9)	-0.0021 (9)	-0.0024 (9)
C10	0.0420 (14)	0.0460 (14)	0.0481 (16)	0.0288 (12)	-0.0086 (12)	-0.0060 (12)

*Geometric parameters (Å, °)*

C11—C5	1.748 (2)	C2—C7	1.402 (3)
S1—C8	1.689 (2)	C3—H3	0.9300
N1—N2	1.395 (2)	C3—C4	1.390 (3)
N1—C1	1.275 (3)	C4—H4A	0.9300
N2—C8	1.378 (3)	C4—C5	1.377 (3)
N2—C9	1.379 (3)	C5—C6	1.381 (3)
N3—N4	1.378 (2)	C6—H6	0.9300
N3—C9	1.301 (3)	C6—C7	1.379 (3)
N4—H4	0.8600	C7—H7	0.9300
N4—C8	1.333 (3)	C9—C10	1.484 (3)
C1—H1	0.9300	C10—H10A	0.9600
C1—C2	1.463 (3)	C10—H10B	0.9600
C2—C3	1.390 (3)	C10—H10C	0.9600
C1—N1—N2	116.28 (19)	C4—C5—C6	122.1 (2)
C8—N2—N1	131.27 (18)	C6—C5—C11	119.20 (18)
C8—N2—C9	108.25 (18)	C5—C6—H6	120.4

C9—N2—N1	119.99 (18)	C7—C6—C5	119.2 (2)
C9—N3—N4	103.61 (18)	C7—C6—H6	120.4
N3—N4—H4	122.9	C2—C7—H7	119.8
C8—N4—N3	114.29 (18)	C6—C7—C2	120.4 (2)
C8—N4—H4	122.9	C6—C7—H7	119.8
N1—C1—H1	120.1	N2—C8—S1	129.63 (17)
N1—C1—C2	119.8 (2)	N4—C8—S1	127.48 (17)
C2—C1—H1	120.1	N4—C8—N2	102.87 (18)
C3—C2—C1	118.6 (2)	N2—C9—C10	122.4 (2)
C3—C2—C7	118.7 (2)	N3—C9—N2	110.94 (19)
C7—C2—C1	122.6 (2)	N3—C9—C10	126.6 (2)
C2—C3—H3	119.3	C9—C10—H10A	109.5
C4—C3—C2	121.3 (2)	C9—C10—H10B	109.5
C4—C3—H3	119.3	C9—C10—H10C	109.5
C3—C4—H4A	120.9	H10A—C10—H10B	109.5
C5—C4—C3	118.2 (2)	H10A—C10—H10C	109.5
C5—C4—H4A	120.9	H10B—C10—H10C	109.5
C4—C5—C11	118.70 (18)		
C11—C5—C6—C7	-179.28 (17)	C1—C2—C3—C4	178.0 (2)
N1—N2—C8—S1	5.3 (4)	C1—C2—C7—C6	-179.2 (2)
N1—N2—C8—N4	-173.2 (2)	C2—C3—C4—C5	1.4 (3)
N1—N2—C9—N3	174.80 (19)	C3—C2—C7—C6	-0.4 (3)
N1—N2—C9—C10	-6.5 (3)	C3—C4—C5—C11	178.09 (17)
N1—C1—C2—C3	-171.5 (2)	C3—C4—C5—C6	-0.8 (3)
N1—C1—C2—C7	7.2 (3)	C4—C5—C6—C7	-0.4 (4)
N2—N1—C1—C2	176.53 (18)	C5—C6—C7—C2	1.0 (3)
N3—N4—C8—S1	-177.92 (17)	C7—C2—C3—C4	-0.8 (3)
N3—N4—C8—N2	0.6 (3)	C8—N2—C9—N3	2.0 (3)
N4—N3—C9—N2	-1.5 (3)	C8—N2—C9—C10	-179.3 (2)
N4—N3—C9—C10	179.8 (2)	C9—N2—C8—S1	177.00 (18)
C1—N1—N2—C8	-35.9 (3)	C9—N2—C8—N4	-1.5 (2)
C1—N1—N2—C9	153.2 (2)	C9—N3—N4—C8	0.5 (3)

*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—H4 $\cdots$ S1 <sup>i</sup>	0.86	2.43	3.2926 (19)	176
C1—H1 $\cdots$ S1	0.93	2.62	3.199 (2)	121

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