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

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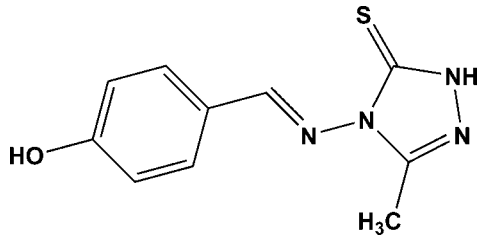
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.054; wR factor = 0.151; data-to-parameter ratio = 13.5.

The title compound, $C_{10}H_{10}N_4OS$, is nearly planar with the mean planes of the hydroxybenzyl and triazole rings inclined at an angle of only 3.2 (7)°. In the crystal, O—H···N hydrogen bonds between the hydroxy group and the triazole ring in concert with weak N—H···S intermolecular interactions between the triazole ring and thione group form chains along [$\bar{2}$10] enclosing $R_2^2(8)$ graph-set motifs. A weak intramolecular C—H···S interaction and intermolecular π–π interactions [centroid–centroid distance = 3.5990 (15) Å] are also observed.

Related literature

For the chemistry of Schiff base compounds, see: Dubey & Vaid (1991); Yadav *et al.* (1994). For uses of Schiff bases in analytical applications and metal coordination, see: Galic *et al.* (2001); Wyrzykiewicz & Prukah (1998); Reddy & Lirgappa (1994). For the chemical and biological activity of Schiff base compounds, see: Barrera *et al.* (1985); Dornow *et al.* (1964); Malik *et al.* (2011); Thieme *et al.* (1973*a*,*b*); Wei & Bell (1982). For related structures see: Kant *et al.* (2012); Praveen *et al.* (2012); Kubicki *et al.* (2012); Jeyaseelan *et al.* (2012); Devarajegowda *et al.* (2012); Vinduvahini *et al.* (2011); Almutairi *et al.* (2012); Ding *et al.* (2009); Sarojini *et al.* (2007*a*,*b*). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{10}H_{10}N_4OS$
M_r = 234.28
Triclinic, $P\overline{1}$
a = 5.7677 (5) Å
b = 7.7233 (8) Å
c = 12.7269 (12) Å
α = 84.104 (8)°
β = 77.719 (8)°
γ = 73.358 (9)°
V = 530.23 (9) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 2.59 mm^{-1}
T = 173 K
0.28 × 0.16 × 0.12 mm

Data collection

Agilent Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)
T_{min} = 0.723, T_{max} = 1.000
3082 measured reflections
1987 independent reflections
1658 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.151
S = 1.05
1987 reflections
147 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N3^{i}	0.84	1.98	2.804 (3)	165
N4—H4···S1^{ii}	0.88	2.46	3.324 (2)	166
C3—H3···S1	0.95	2.49	3.234 (3)	135

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

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

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SJ5405).

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

Balladka K. Sarojini, Padmanabha S. Manjula, B. Narayana 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 & Prukah, 1998; Reddy & Lirgappa, 1994). Since many compounds containing sulfur and nitrogen atoms are antihypertensive (Wei & Bell, 1982), analgesic (Thieme *et al.*, 1973*a*,*b*), anti-inflammatory (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 and biological activity. The crystal structures of some of the related Schiff bases viz: 3-ethyl-4-[(E)-(4-fluorobenzylidene)amino]-1H-1,2,4-triazole-5(4H)-thione (Jeyaseelan *et al.*, 2012); 4-[(E)-(4-fluorobenzylidene)amino]-3-methyl-1H-1,2,4-triazole-5(4H)-thione (Devarajegowda *et al.*, 2012); 3-[2-(2,6-dichloro-anilino)benzyl]-4-[(4-methoxybenzylidene)amino]-1H-1,2,4-triazole-5(4H)-thione (Vinduvahini *et al.*, 2011); 3-(adamantan-1-yl)-1-[(4-ethylpiperazin-1-yl)methyl]-4-[(E)-(4-hydroxy- benzylidene)amino]-1H-1,2,4-triazole-5(4H)-thione (Almutairi *et al.*, 2012); 4-{(2E)-2-[1-(4-Methoxyphenyl)-ethylidene]hydrazinyl}-8-(trifluoromethyl) quinoline (Kubicki *et al.*, 2012); (E)-N′-(4-Methoxybenzylidene)-2-m-tolyl-acetohydrazide (Praveen *et al.*, 2012); (1Z)-1-[(2E)-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)-1H-1,2,4-triazole-5(4H)- thione (Ding *et al.*, 2009) have been reported. Crystal structures of some Schiff bases were also reported by our group (Sarojini *et al.*, 2007*a*,*b*). The present work describes the synthesis and crystal structure of the title compound, (I), $C_{10}H_{10}N_4OS$.

In (I), the molecule is nearly planar with the mean planes of the hydroxybenzyl and triazole rings inclined at an angle of only 3.2 (7)°. (Fig. 1). Bond lengths are in normal ranges (Allen *et al.*, 1987). In the crystal, O—H···N hydrogen bonds between the hydroxy group and triazole ring in concert with weak N—H···S intermolecular interactions between the triazole ring and thione group form infinite polymeric 1-dimensional chains along [-2 1 0] displaying $R_2^2(8)$ graph set motifs (Fig. 2). As the chains are extended, additional graph set motifs [$R_4^4(28)$, $R_4^4(30)$, $R_4^4(32)$, $R_6^6(50)$, $R_6^6(52)$ & $R_6^6(54)$] are also formed. A weak C—H···S intramolecular interaction (Table 1) and weak $\pi\cdots\pi$ intermolecular interactions (Cg1–Cg2 = 3.5990 (15)Å, 1+x, y, z; (Cg1 and Cg2 are the centroids of the N2/C1/N3/N4/C2 and C4–C9 rings respectively) are also observed.

S2. Experimental

To a suspension of 4-hydroxy benzaldehyde (1.22g, 0.01mol) in ethanol (15ml), 4-amino-5-methyl-2,4-dihydro-3H-1,2,4-triazole-3-thione (0.01mol, 1.3g) was added and heated to get a clear solution. To this a few drops of conc. H_2SO_4 was added as a catalyst and refluxed for 36 hr. on a water bath (Fig. 3). The precipitate formed was filtered and recrystallized from methanol to get the title compound, (I). Single crystals were grown from methanol by the slow evaporation method (m.p. 505–507 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 0.95Å (CH), 0.98Å (CH_3), 0.84Å (OH) or 0.88Å (NH). Isotropic displacement parameters for these atoms were set to 1.2 (CH, NH) or 1.5 (CH_3, OH) times U_{eq} of the parent atom. Idealised Me and tetrahedral OH (O1(H1))were refined as rotating groups.

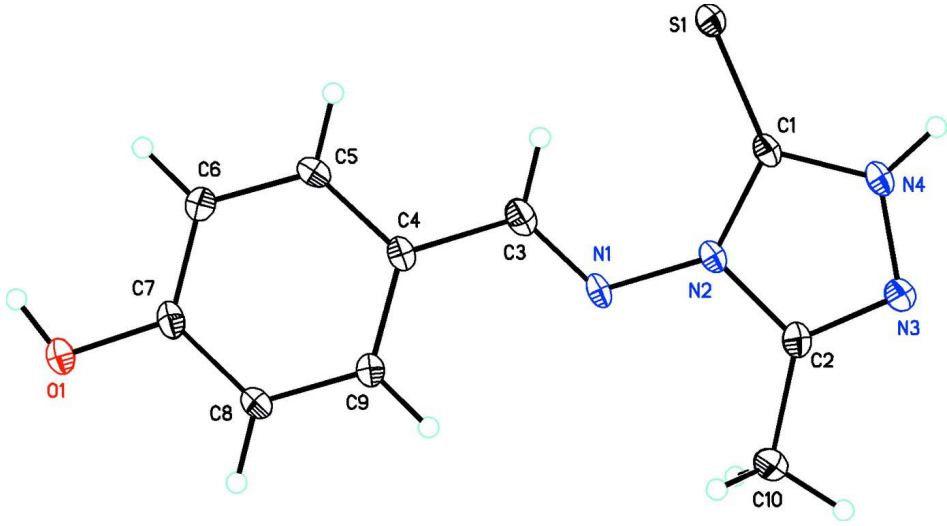

Figure 1

ORTEP drawing of (I), $C_{10}H_{10}N_4OS$, showing the labeling scheme with 30% probability displacement ellipsoids.

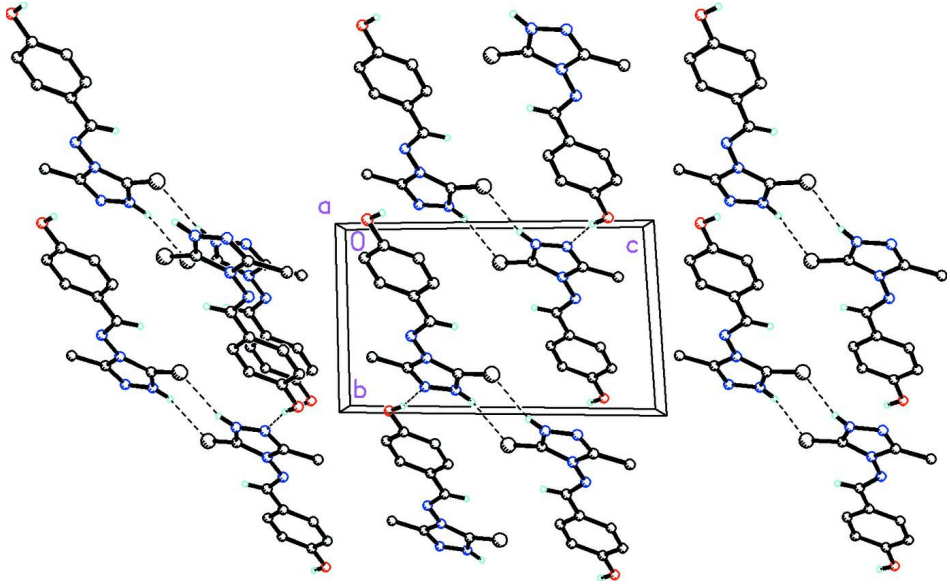

Figure 2

Molecular packing for (I) viewed along the *b* axis. Dashed lines indicate O—H···N hydogen bonds between the hydroxy group and triazole ring and weak S—H···S intermolecular interactions between the triazole ring and thione group forming infinite polymeric 1-dimensional chains along [$\bar{2}$10] and displaying $R_2^2(8)$ graph-set motifs. H atoms not involved in hydrogen bonding or weak intermolecular interactions have been removed for clarity.

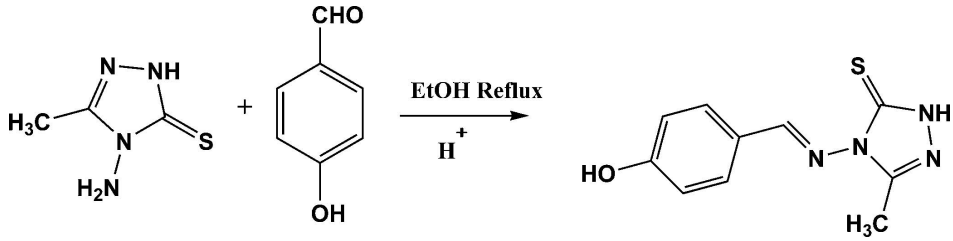

Figure 3

Reaction scheme.

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

Crystal data

$C_{10}H_{10}N_4OS$
$M_r = 234.28$
Triclinic, $P\overline{1}$
$a = 5.7677$ (5) Å
$b = 7.7233$ (8) Å
$c = 12.7269$ (12) Å
$\alpha = 84.104$ (8)°
$\beta = 77.719$ (8)°
$\gamma = 73.358$ (9)°
$V = 530.23$ (9) Å^3
$Z = 2$
$F(000) = 244$
$D_x = 1.467$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 1294 reflections
$\theta = 6.0$–$71.1°$
$\mu = 2.59$ mm^{-1}
$T = 173$ K
Prism, colourless
0.28 × 0.16 × 0.12 mm

Data collection

Agilent Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)
$T_{min} = 0.723$, $T_{max} = 1.000$
3082 measured reflections
1987 independent reflections
1658 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 71.3°$, $\theta_{min} = 3.6°$
$h = -6 \rightarrow 7$
$k = -8 \rightarrow 9$
$l = -11 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.151$
$S = 1.05$
1987 reflections
147 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0895P)^2 + 0.0331P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ 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}
S1	1.11567 (12)	0.19885 (9)	0.52135 (5)	0.0379 (3)
O1	−0.1143 (3)	0.9783 (3)	0.86418 (16)	0.0377 (5)
H1	−0.2048	1.0077	0.8180	0.057*
N1	0.9248 (4)	0.4001 (3)	0.76560 (17)	0.0283 (5)
N2	1.1501 (4)	0.2819 (3)	0.72431 (16)	0.0256 (4)
N3	1.5264 (4)	0.1215 (3)	0.73740 (18)	0.0307 (5)
N4	1.4752 (4)	0.1066 (3)	0.63900 (17)	0.0300 (5)
H4	1.5835	0.0420	0.5881	0.036*
C1	1.2477 (4)	0.1981 (3)	0.6267 (2)	0.0265 (5)
C2	1.3255 (4)	0.2280 (3)	0.7878 (2)	0.0287 (5)
C3	0.7774 (5)	0.4764 (3)	0.7032 (2)	0.0318 (6)
H3	0.8179	0.4491	0.6293	0.038*
C4	0.5459 (4)	0.6061 (3)	0.7454 (2)	0.0276 (5)
C5	0.3644 (5)	0.6680 (4)	0.6829 (2)	0.0322 (6)
H5	0.3944	0.6250	0.6126	0.039*
C6	0.1427 (5)	0.7901 (3)	0.7209 (2)	0.0316 (6)
H6	0.0210	0.8298	0.6773	0.038*
C7	0.0976 (4)	0.8550 (3)	0.8236 (2)	0.0289 (5)
C8	0.2773 (5)	0.7967 (3)	0.8869 (2)	0.0327 (6)
H8	0.2482	0.8420	0.9566	0.039*
C9	0.4976 (5)	0.6732 (3)	0.8483 (2)	0.0324 (6)
H9	0.6186	0.6329	0.8923	0.039*
C10	1.2826 (5)	0.2836 (4)	0.9004 (2)	0.0384 (6)
H10A	1.1664	0.2240	0.9467	0.058*
H10B	1.2139	0.4151	0.9029	0.058*
H10C	1.4392	0.2481	0.9259	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0299 (4)	0.0437 (4)	0.0324 (4)	0.0105 (3)	−0.0096 (3)	−0.0190 (3)
O1	0.0277 (10)	0.0413 (11)	0.0346 (10)	0.0111 (8)	−0.0076 (8)	−0.0141 (8)
N1	0.0209 (10)	0.0271 (10)	0.0295 (11)	0.0057 (8)	−0.0011 (8)	−0.0113 (8)
N2	0.0212 (10)	0.0252 (9)	0.0255 (10)	0.0022 (8)	−0.0022 (8)	−0.0090 (8)
N3	0.0262 (11)	0.0329 (11)	0.0286 (11)	0.0026 (9)	−0.0061 (8)	−0.0104 (8)
N4	0.0229 (10)	0.0309 (10)	0.0295 (11)	0.0047 (8)	−0.0016 (8)	−0.0127 (8)
C1	0.0229 (11)	0.0252 (11)	0.0257 (11)	0.0025 (9)	−0.0016 (9)	−0.0085 (9)
C2	0.0223 (12)	0.0283 (12)	0.0314 (13)	0.0013 (9)	−0.0059 (10)	−0.0056 (10)
C3	0.0280 (13)	0.0294 (12)	0.0313 (13)	0.0013 (10)	−0.0011 (10)	−0.0077 (10)
C4	0.0224 (12)	0.0270 (11)	0.0280 (12)	0.0022 (9)	−0.0030 (9)	−0.0066 (9)
C5	0.0322 (13)	0.0355 (13)	0.0240 (12)	0.0016 (11)	−0.0048 (10)	−0.0121 (10)
C6	0.0265 (13)	0.0353 (13)	0.0291 (13)	0.0022 (10)	−0.0093 (10)	−0.0056 (10)
C7	0.0218 (12)	0.0258 (11)	0.0334 (13)	0.0021 (9)	−0.0024 (10)	−0.0063 (10)
C8	0.0293 (13)	0.0347 (13)	0.0300 (13)	0.0033 (11)	−0.0070 (10)	−0.0154 (11)
C9	0.0251 (13)	0.0350 (13)	0.0324 (13)	0.0060 (10)	−0.0099 (10)	−0.0118 (11)

C10	0.0342 (15)	0.0457 (15)	0.0285 (13)	0.0058 (12)	−0.0087 (11)	−0.0133 (12)

Geometric parameters (Å, º)

S1—C1	1.675 (2)	C4—C5	1.396 (4)
O1—H1	0.8400	C4—C9	1.401 (4)
O1—C7	1.354 (3)	C5—H5	0.9500
N1—N2	1.388 (3)	C5—C6	1.378 (4)
N1—C3	1.267 (3)	C6—H6	0.9500
N2—C1	1.392 (3)	C6—C7	1.394 (4)
N2—C2	1.374 (3)	C7—C8	1.393 (4)
N3—N4	1.369 (3)	C8—H8	0.9500
N3—C2	1.295 (3)	C8—C9	1.379 (3)
N4—H4	0.8800	C9—H9	0.9500
N4—C1	1.334 (3)	C10—H10A	0.9800
C2—C10	1.488 (4)	C10—H10B	0.9800
C3—H3	0.9500	C10—H10C	0.9800
C3—C4	1.454 (3)		
C7—O1—H1	109.5	C4—C5—H5	119.3
C3—N1—N2	119.5 (2)	C6—C5—C4	121.4 (2)
N1—N2—C1	133.6 (2)	C6—C5—H5	119.3
C2—N2—N1	118.42 (19)	C5—C6—H6	120.1
C2—N2—C1	108.01 (19)	C5—C6—C7	119.7 (2)
C2—N3—N4	104.1 (2)	C7—C6—H6	120.1
N3—N4—H4	122.8	O1—C7—C6	122.3 (2)
C1—N4—N3	114.5 (2)	O1—C7—C8	117.8 (2)
C1—N4—H4	122.8	C8—C7—C6	119.8 (2)
N2—C1—S1	130.18 (18)	C7—C8—H8	120.1
N4—C1—S1	127.45 (18)	C9—C8—C7	119.9 (2)
N4—C1—N2	102.3 (2)	C9—C8—H8	120.1
N2—C2—C10	123.3 (2)	C4—C9—H9	119.5
N3—C2—N2	111.1 (2)	C8—C9—C4	121.1 (2)
N3—C2—C10	125.6 (2)	C8—C9—H9	119.5
N1—C3—H3	120.2	C2—C10—H10A	109.5
N1—C3—C4	119.6 (2)	C2—C10—H10B	109.5
C4—C3—H3	120.2	C2—C10—H10C	109.5
C5—C4—C3	120.1 (2)	H10A—C10—H10B	109.5
C5—C4—C9	118.0 (2)	H10A—C10—H10C	109.5
C9—C4—C3	121.9 (2)	H10B—C10—H10C	109.5
O1—C7—C8—C9	−179.1 (2)	C2—N2—C1—S1	175.0 (2)
N1—N2—C1—S1	−4.7 (4)	C2—N2—C1—N4	−2.0 (3)
N1—N2—C1—N4	178.3 (2)	C2—N3—N4—C1	−0.9 (3)
N1—N2—C2—N3	−178.6 (2)	C3—N1—N2—C1	−12.7 (4)
N1—N2—C2—C10	2.8 (4)	C3—N1—N2—C2	167.6 (2)
N1—C3—C4—C5	−169.2 (2)	C3—C4—C5—C6	179.6 (2)
N1—C3—C4—C9	11.1 (4)	C3—C4—C9—C8	179.7 (3)

N2—N1—C3—C4	−177.4 (2)	C4—C5—C6—C7	0.5 (4)
N3—N4—C1—S1	−175.24 (19)	C5—C4—C9—C8	0.0 (4)
N3—N4—C1—N2	1.9 (3)	C5—C6—C7—O1	178.4 (3)
N4—N3—C2—N2	−0.5 (3)	C5—C6—C7—C8	0.3 (4)
N4—N3—C2—C10	178.1 (3)	C6—C7—C8—C9	−0.9 (4)
C1—N2—C2—N3	1.6 (3)	C7—C8—C9—C4	0.7 (4)
C1—N2—C2—C10	−177.0 (2)	C9—C4—C5—C6	−0.6 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N3^{i}	0.84	1.98	2.804 (3)	165
N4—H4···S1^{ii}	0.88	2.46	3.324 (2)	166
C3—H3···S1	0.95	2.49	3.234 (3)	135

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