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4-Amino-3-(*p*-tolylloxymethyl)-1*H*-1,2,4-triazole-5(4*H*)-thioneHoong-Kun Fun,^{a,*} Jia Hao Goh,^a A. M. Vijesh,^{b,c} S Mahesh Padaki^c and Arun M. Isloor^c

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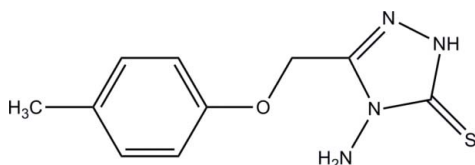
Received 7 July 2009; accepted 14 July 2009

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.001$ Å; R factor = 0.032; wR factor = 0.095; data-to-parameter ratio = 24.4.

In the title triazole compound, $\text{C}_{10}\text{H}_{12}\text{N}_4\text{OS}$, the triazole ring is essentially planar [maximum deviation = 0.009 (1) Å] and forms a dihedral angle of 5.78 (4)° with the benzene ring. In the crystal structure, molecules are linked into dimers by centrosymmetric $\text{N}-\text{H}\cdots\text{S}$ interactions. These dimers are linked into two-molecule-wide tapes by $\text{N}-\text{H}\cdots\text{N}$ and $\text{S}\cdots\text{S}$ [3.2634 (3) Å] interactions. In addition, they are further interconnected by weak $\text{N}-\text{H}\cdots\text{S}$ interactions into sheets parallel to the *ab* plane. The crystal structure is further stabilized by weak intermolecular $\text{C}-\text{H}\cdots\pi$ interactions.

Related literature

For general background and applications of triazole derivatives, see: Amir *et al.* (2008); Kuş *et al.* (2008); Krzysztof *et al.* (2008); Padmavathi *et al.* (2008). For the preparation, see: Conti (1964). For related structures, see: Fun *et al.* (2008, 2009). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

 $\text{C}_{10}\text{H}_{12}\text{N}_4\text{OS}$ $M_r = 236.30$

* Thomson Reuters ResearcherID: A-3561-2009.

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Triclinic, $P\bar{1}$
 $a = 5.9977$ (1) Å
 $b = 6.4002$ (1) Å
 $c = 15.5506$ (2) Å
 $\alpha = 89.352$ (1)°
 $\beta = 83.157$ (1)°
 $\gamma = 65.562$ (1)°

$V = 539.11$ (1) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.28$ mm⁻¹
 $T = 100$ K
 $0.47 \times 0.30 \times 0.09$ mm

Data collection

Bruker SMART APEXII CCD
 area-detector diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2005)
 $T_{\min} = 0.878$, $T_{\max} = 0.975$

19910 measured reflections
 4712 independent reflections
 4228 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.095$
 $S = 1.05$
 4712 reflections
 193 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.59$ e Å⁻³
 $\Delta\rho_{\min} = -0.33$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{N2}-\text{H1N2}\cdots\text{S1}^i$ | 0.930 (13) | 2.412 (13) | 3.3364 (7) | 172.5 (11) |
| $\text{N4}-\text{H1N4}\cdots\text{N1}^{ii}$ | 0.930 (17) | 2.428 (17) | 3.2100 (9) | 141.6 (12) |
| $\text{N4}-\text{H2N4}\cdots\text{S1}^{iii}$ | 0.894 (15) | 2.937 (16) | 3.5456 (7) | 126.8 (12) |
| $\text{C10}-\text{H10C}\cdots\text{Cg2}^{iv}$ | 0.968 (18) | 2.697 (19) | 3.6250 (9) | 160.8 (14) |

Symmetry codes: (i) $-x + 2, -y + 1, -z$; (ii) $x, y - 1, z$; (iii) $-x + 1, -y + 1, -z$; (iv) $-x - 1, -y + 3, -z + 1$. Cg2 is the centroid of the C4-C9 ring.

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2497).

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supporting information

Acta Cryst. (2009). E65, o1918–o1919 [doi:10.1107/S1600536809027664]

4-Amino-3-(*p*-tolylloxymethyl)-1*H*-1,2,4-triazole-5(4*H*)-thione

Hoong-Kun Fun, Jia Hao Goh, A. M. Vijesh, Mahesh Padaki and Arun M. Isloor

S1. Comment

1,2,4-Triazole and its derivatives were reported to exhibit various pharmacological activities such as anti-microbial, analgesic, anti-inflammatory, anti-cancer and anti-oxidant properties (Amir *et al.*, 2008; Kuş *et al.*, 2008; Krzysztof *et al.*, 2008; Padmavathi *et al.*, 2008). Some of the present day drugs such as Ribavirin (anti-viral agent), Rizatriptan (anti-migraine agent), Alprazolam (anxiolytic agent), Fluconazole and Itraconazole (anti-fungal agents) are the best examples for potent molecules possessing the triazole nucleus. The amino and mercapto groups of thio-substituted 1,2,4-triazole serve as readily accessible nucleophilic centers for the preparation of N-bridged heterocycles. In view of their biological importance, we have synthesized the title compound (I) to study its crystal structure.

In (I), Fig. 1, the 1,2,4-triazole ring (C1/C2/N1-N3) is essentially planar, with a maximum deviation of 0.009 (1) Å for atom C1. The 1,2,4-triazole ring makes dihedral angle of 5.78 (4)° with the C4-C9 benzene ring. The bond lengths and angles in the molecule are comparable to those found in closely related structures (Fun *et al.*, 2008, 2009).

In the crystal packing (Fig. 2), centrosymmetrically related molecules are linked into dimers by N2—H1N2···S1 interactions (Table 1). These dimers are linked into two-molecule-wide tapes by N4—H1N4···N1 (Table 1) and by short S1···S1 contacts of 3.2634 (3) Å; symmetry code: 2-x, -y, -z. In addition, these tapes are interconnected into sheets parallel to the *ab* plane by weak N4—H2N4···S1 interactions (Table 1). The crystal structure is further stabilized by weak C···H··· π interactions (Table 1).

S2. Experimental

p-Cresoloxycetyl hydrazine (18.0 g, 0.10 mol) was added slowly to a solution of potassium hydroxide (8.4 g, 0.15 mol) in ethanol (150 ml). The resulting mixture was stirred well until a clear solution was obtained. Carbon disulphide (11.4 g, 0.15 mol) was added drop-wise and the contents were stirred vigorously. Further stirring was continued for 24 h. The resulting mixture was diluted with ether (100 ml) and the precipitate formed was collected by filtration, washed with dry ether and dried at 65 °C under vacuum. It was used for the next step without any purification.

A mixture of the above synthesized potassium dithiocarbazinate (29.4 g, 0.10 mol), hydrazine hydrate (99 %, 0.20 mol) and water (2 ml) was heated gently to boil for 30 minutes. Heating was continued until the evacuation of hydrogen sulphide ceased. The reaction mixture was cooled to room temperature, diluted with water (100 ml) and acidified with HCl. The solid mass that separated was collected by filtration, washed with water and dried. Recrystallization was achieved from ethanol (Conti, 1964). The yield was 14.63 g, 62 %. *M.p.* 461–463 K.

S3. Refinement

All the H atoms were located from difference Fourier map [range of C-H = 0.894 (15) - 1.011 (12) Å] and allowed to refine freely.

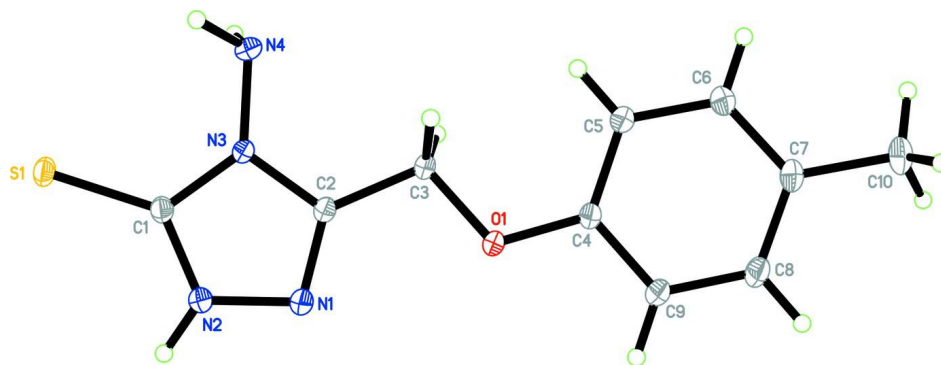
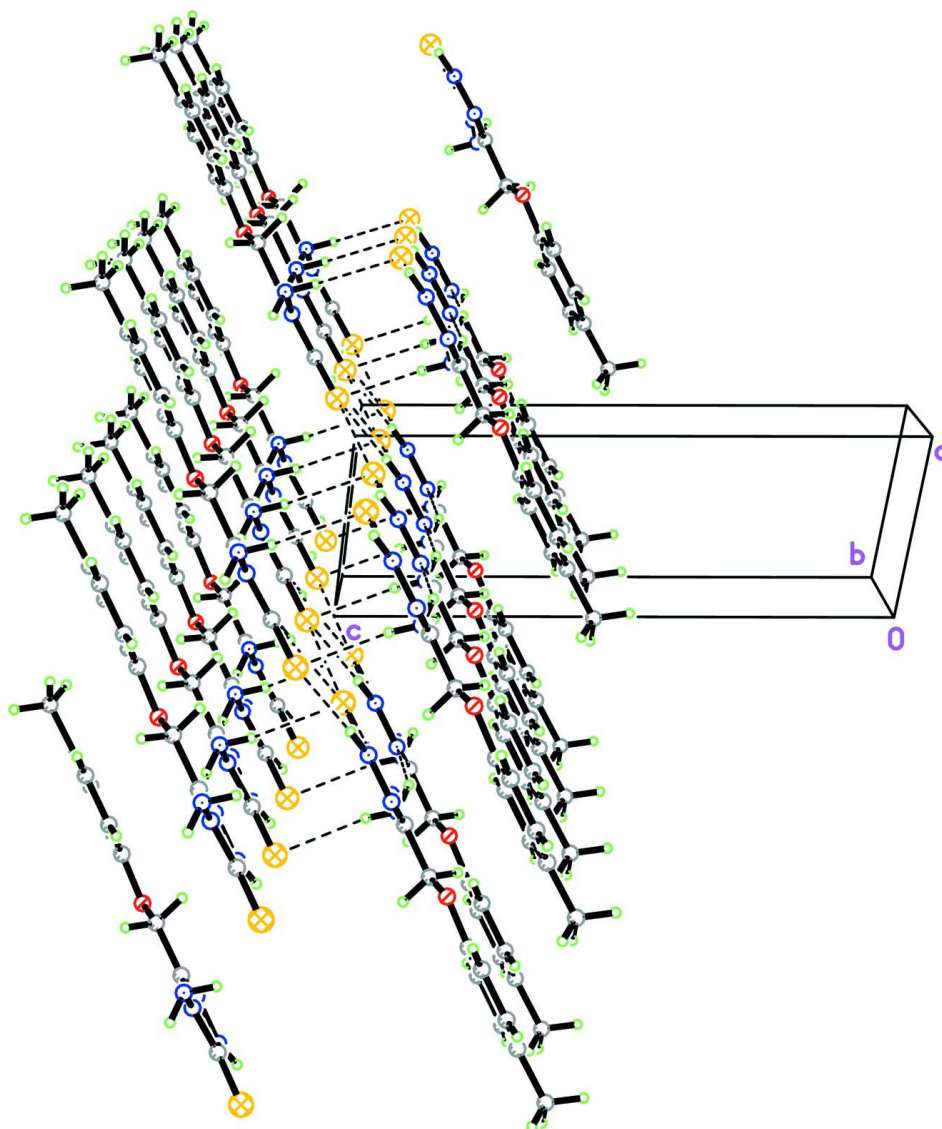


Figure 1

The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

**Figure 2**

Two-molecular-wide tapes connected by N—H⋯S, N—H⋯N and S⋯S interactions. The tapes form sheets parallel to the *ab* plane via weaker N—H⋯S interactions. Intermolecular interactions are shown as dashed bonds.

4-Amino-3-(*p*-tolylloxymethyl)-1*H*-1,2,4-triazole-5(4*H*)-thione

Crystal data

$C_{10}H_{12}N_4OS$

$M_r = 236.30$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 5.9977$ (1) Å

$b = 6.4002$ (1) Å

$c = 15.5506$ (2) Å

$\alpha = 89.352$ (1)°

$\beta = 83.157$ (1)°

$\gamma = 65.562$ (1)°

$V = 539.11$ (1) Å³

$Z = 2$

$F(000) = 248$

$D_x = 1.456$ Mg m⁻³

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

Cell parameters from 9925 reflections

$\theta = 2.6$ – 35.2 °

$\mu = 0.28$ mm⁻¹

$T = 100$ K

Plate, colourless

$0.47 \times 0.30 \times 0.09$ mm

Data collection

Bruker SMART APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2005)

$T_{\min} = 0.878$, $T_{\max} = 0.975$

19910 measured reflections

4712 independent reflections

4228 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$

$\theta_{\max} = 35.0^\circ$, $\theta_{\min} = 2.6^\circ$

$h = -9 \rightarrow 9$

$k = -10 \rightarrow 10$

$l = -25 \rightarrow 24$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.095$

$S = 1.05$

4712 reflections

193 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

$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2 + 0.0513P]$

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

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

$\Delta\rho_{\max} = 0.59 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.33 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1)K.

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.

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|--------------|---------------|----------------------------------|
| S1 | 0.84328 (3) | 0.26155 (3) | 0.040453 (11) | 0.01525 (6) |
| O1 | 0.06661 (10) | 1.12912 (9) | 0.24927 (4) | 0.01568 (10) |
| N1 | 0.49686 (12) | 0.89098 (11) | 0.14036 (4) | 0.01591 (11) |
| N2 | 0.69184 (11) | 0.71323 (11) | 0.09371 (4) | 0.01581 (11) |
| H1N2 | 0.820 (2) | 0.732 (2) | 0.0596 (9) | 0.024 (3)* |
| N3 | 0.43624 (11) | 0.57330 (10) | 0.13942 (4) | 0.01199 (10) |
| N4 | 0.30133 (12) | 0.43979 (11) | 0.15295 (4) | 0.01506 (11) |
| H1N4 | 0.405 (2) | 0.293 (3) | 0.1674 (9) | 0.023 (3)* |
| H2N4 | 0.258 (3) | 0.419 (3) | 0.1018 (10) | 0.035 (4)* |
| C1 | 0.66067 (12) | 0.51754 (12) | 0.09031 (4) | 0.01305 (11) |
| C2 | 0.34451 (12) | 0.79838 (12) | 0.16710 (4) | 0.01274 (11) |
| C3 | 0.09665 (12) | 0.91116 (11) | 0.21854 (5) | 0.01325 (11) |
| H3A | -0.034 (2) | 0.927 (2) | 0.1804 (8) | 0.018 (3)* |
| H3B | 0.086 (2) | 0.808 (2) | 0.2649 (8) | 0.016 (3)* |

| | | | | |
|------|---------------|--------------|-------------|--------------|
| C4 | -0.16049 (12) | 1.26194 (12) | 0.29390 (4) | 0.01307 (12) |
| C5 | -0.34570 (13) | 1.18698 (13) | 0.31707 (5) | 0.01573 (12) |
| H5A | -0.333 (2) | 1.039 (2) | 0.2991 (9) | 0.026 (3)* |
| C6 | -0.56524 (13) | 1.33505 (13) | 0.36639 (5) | 0.01718 (13) |
| H6A | -0.682 (3) | 1.275 (2) | 0.3802 (9) | 0.027 (3)* |
| C7 | -0.60421 (13) | 1.55609 (12) | 0.39238 (5) | 0.01587 (13) |
| C8 | -0.41667 (15) | 1.62850 (13) | 0.36627 (5) | 0.01808 (13) |
| H8A | -0.443 (3) | 1.785 (3) | 0.3837 (9) | 0.028 (3)* |
| C9 | -0.19792 (14) | 1.48515 (12) | 0.31738 (5) | 0.01693 (13) |
| H9A | -0.070 (3) | 1.533 (3) | 0.2975 (10) | 0.031 (4)* |
| C10 | -0.83720 (14) | 1.71372 (15) | 0.44753 (5) | 0.02093 (15) |
| H10A | -0.902 (3) | 1.871 (3) | 0.4283 (11) | 0.042 (4)* |
| H10B | -0.971 (3) | 1.672 (3) | 0.4484 (11) | 0.046 (4)* |
| H10C | -0.807 (3) | 1.720 (3) | 0.5070 (12) | 0.049 (5)* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|---------------|--------------|---------------|
| S1 | 0.01469 (9) | 0.01076 (8) | 0.01619 (9) | -0.00247 (6) | 0.00295 (6) | -0.00124 (6) |
| O1 | 0.0137 (2) | 0.0113 (2) | 0.0208 (2) | -0.00540 (17) | 0.00364 (18) | -0.00495 (18) |
| N1 | 0.0146 (2) | 0.0125 (2) | 0.0193 (3) | -0.0056 (2) | 0.0033 (2) | -0.0034 (2) |
| N2 | 0.0138 (2) | 0.0134 (2) | 0.0194 (3) | -0.0062 (2) | 0.0036 (2) | -0.0032 (2) |
| N3 | 0.0118 (2) | 0.0090 (2) | 0.0141 (2) | -0.00392 (18) | 0.00088 (18) | -0.00093 (18) |
| N4 | 0.0165 (3) | 0.0110 (2) | 0.0186 (3) | -0.0073 (2) | 0.0007 (2) | 0.0000 (2) |
| C1 | 0.0118 (2) | 0.0120 (3) | 0.0136 (3) | -0.0037 (2) | 0.0004 (2) | -0.0002 (2) |
| C2 | 0.0130 (2) | 0.0099 (2) | 0.0139 (3) | -0.0038 (2) | 0.0002 (2) | -0.0013 (2) |
| C3 | 0.0126 (3) | 0.0095 (2) | 0.0156 (3) | -0.0035 (2) | 0.0018 (2) | -0.0025 (2) |
| C4 | 0.0125 (3) | 0.0106 (3) | 0.0143 (3) | -0.0035 (2) | 0.0008 (2) | -0.0015 (2) |
| C5 | 0.0140 (3) | 0.0128 (3) | 0.0195 (3) | -0.0055 (2) | 0.0011 (2) | -0.0024 (2) |
| C6 | 0.0134 (3) | 0.0163 (3) | 0.0199 (3) | -0.0051 (2) | 0.0015 (2) | -0.0026 (2) |
| C7 | 0.0141 (3) | 0.0143 (3) | 0.0147 (3) | -0.0017 (2) | -0.0003 (2) | -0.0011 (2) |
| C8 | 0.0192 (3) | 0.0113 (3) | 0.0204 (3) | -0.0041 (2) | 0.0018 (2) | -0.0028 (2) |
| C9 | 0.0179 (3) | 0.0117 (3) | 0.0201 (3) | -0.0064 (2) | 0.0028 (2) | -0.0026 (2) |
| C10 | 0.0164 (3) | 0.0199 (3) | 0.0193 (3) | -0.0011 (3) | 0.0014 (2) | -0.0041 (3) |

Geometric parameters (Å, °)

| | | | |
|---------|------------|--------|-------------|
| S1—C1 | 1.6812 (7) | C4—C5 | 1.3913 (10) |
| O1—C4 | 1.3746 (8) | C4—C9 | 1.3970 (10) |
| O1—C3 | 1.4119 (9) | C5—C6 | 1.4012 (10) |
| N1—C2 | 1.3080 (9) | C5—H5A | 0.962 (14) |
| N1—N2 | 1.3798 (9) | C6—C7 | 1.3915 (10) |
| N2—C1 | 1.3432 (9) | C6—H6A | 0.930 (14) |
| N2—H1N2 | 0.932 (13) | C7—C8 | 1.4011 (11) |
| N3—C2 | 1.3657 (9) | C7—C10 | 1.5078 (10) |
| N3—C1 | 1.3734 (9) | C8—C9 | 1.3868 (10) |
| N3—N4 | 1.3988 (8) | C8—H8A | 0.984 (14) |
| N4—H1N4 | 0.928 (14) | C9—H9A | 0.959 (14) |

| | | | |
|--------------|-------------|---------------|-------------|
| N4—H2N4 | 0.894 (15) | C10—H10A | 0.975 (17) |
| C2—C3 | 1.4875 (9) | C10—H10B | 0.944 (17) |
| C3—H3A | 1.011 (12) | C10—H10C | 0.968 (18) |
| C3—H3B | 0.986 (12) | | |
| | | | |
| C4—O1—C3 | 115.53 (5) | O1—C4—C9 | 115.49 (6) |
| C2—N1—N2 | 103.33 (6) | C5—C4—C9 | 119.96 (6) |
| C1—N2—N1 | 113.75 (6) | C4—C5—C6 | 119.23 (7) |
| C1—N2—H1N2 | 121.9 (9) | C4—C5—H5A | 122.9 (8) |
| N1—N2—H1N2 | 123.5 (9) | C6—C5—H5A | 117.8 (8) |
| C2—N3—C1 | 108.49 (6) | C7—C6—C5 | 121.82 (7) |
| C2—N3—N4 | 122.95 (6) | C7—C6—H6A | 122.7 (9) |
| C1—N3—N4 | 128.18 (6) | C5—C6—H6A | 115.4 (9) |
| N3—N4—H1N4 | 109.3 (8) | C6—C7—C8 | 117.60 (7) |
| N3—N4—H2N4 | 107.2 (10) | C6—C7—C10 | 122.01 (7) |
| H1N4—N4—H2N4 | 104.5 (13) | C8—C7—C10 | 120.39 (7) |
| N2—C1—N3 | 102.99 (6) | C9—C8—C7 | 121.62 (7) |
| N2—C1—S1 | 130.61 (6) | C9—C8—H8A | 120.1 (8) |
| N3—C1—S1 | 126.40 (5) | C7—C8—H8A | 118.3 (8) |
| N1—C2—N3 | 111.41 (6) | C8—C9—C4 | 119.73 (7) |
| N1—C2—C3 | 127.78 (6) | C8—C9—H9A | 122.7 (9) |
| N3—C2—C3 | 120.78 (6) | C4—C9—H9A | 117.5 (9) |
| O1—C3—C2 | 108.32 (6) | C7—C10—H10A | 112.9 (10) |
| O1—C3—H3A | 110.4 (7) | C7—C10—H10B | 114.7 (11) |
| C2—C3—H3A | 109.3 (7) | H10A—C10—H10B | 104.2 (14) |
| O1—C3—H3B | 113.9 (7) | C7—C10—H10C | 110.4 (11) |
| C2—C3—H3B | 107.8 (7) | H10A—C10—H10C | 107.1 (14) |
| H3A—C3—H3B | 107.0 (10) | H10B—C10—H10C | 107.1 (15) |
| O1—C4—C5 | 124.54 (6) | | |
| | | | |
| C2—N1—N2—C1 | 0.94 (8) | N1—C2—C3—O1 | -11.09 (10) |
| N1—N2—C1—N3 | -1.56 (8) | N3—C2—C3—O1 | 171.04 (6) |
| N1—N2—C1—S1 | 178.86 (6) | C3—O1—C4—C5 | 6.66 (10) |
| C2—N3—C1—N2 | 1.55 (8) | C3—O1—C4—C9 | -174.38 (6) |
| N4—N3—C1—N2 | 174.57 (7) | O1—C4—C5—C6 | 176.82 (7) |
| C2—N3—C1—S1 | -178.85 (5) | C9—C4—C5—C6 | -2.10 (11) |
| N4—N3—C1—S1 | -5.83 (11) | C4—C5—C6—C7 | 0.49 (12) |
| N2—N1—C2—N3 | 0.13 (8) | C5—C6—C7—C8 | 1.01 (11) |
| N2—N1—C2—C3 | -177.90 (7) | C5—C6—C7—C10 | -178.28 (7) |
| C1—N3—C2—N1 | -1.10 (8) | C6—C7—C8—C9 | -0.94 (12) |
| N4—N3—C2—N1 | -174.56 (6) | C10—C7—C8—C9 | 178.36 (7) |
| C1—N3—C2—C3 | 177.09 (6) | C7—C8—C9—C4 | -0.64 (12) |
| N4—N3—C2—C3 | 3.62 (10) | O1—C4—C9—C8 | -176.84 (7) |
| C4—O1—C3—C2 | 176.18 (6) | C5—C4—C9—C8 | 2.18 (12) |

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> |
|------------------------------|-------------|---------------|-----------------------|-------------------------|
| N2—H1N2···S1 ⁱ | 0.930 (13) | 2.412 (13) | 3.3364 (7) | 172.5 (11) |
| N4—H1N4···N1 ⁱⁱ | 0.930 (17) | 2.428 (17) | 3.2100 (9) | 141.6 (12) |
| N4—H2N4···S1 ⁱⁱⁱ | 0.894 (15) | 2.937 (16) | 3.5456 (7) | 126.8 (12) |
| C10—H10C···Cg2 ^{iv} | 0.968 (18) | 2.697 (19) | 3.6250 (9) | 160.8 (14) |

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