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# 3-Benzamidomethyl-4-[(*E*)-2-chlorobenzylideneamino]-1*H*-1,2,4-triazole-5(4*H*)-thione

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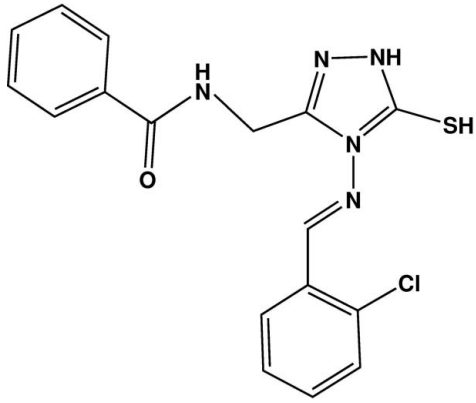
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.001 Å; $R$ factor = 0.033; $wR$ factor = 0.098; data-to-parameter ratio = 31.9.

In the title compound, $C_{17}H_{14}ClN_5OS$, the dihedral angles formed by the two benzene rings with the triazole ring are 66.88 (3) and 19.16 (3)°, and the benzene rings are inclined to each other with a dihedral angle of 78.40 (3)°. Intermolecular N—H···O hydrogen bonds link the molecules into layers parallel to the (100) planes, and centrosymmetric $\pi$–$\pi$ stacking interactions [centroid–centroid distance = 3.7717 (5) Å] are formed between benzene rings in neighbouring layers.

## Related literature

For pharmaceutical and other applications of triazole compounds, see: Almasirad *et al.* (2004); Al-Soud *et al.* (2003); Amir & Shikha (2004); Kalluraya *et al.* (1996); Kawashima *et al.* (1987).

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## Experimental

### Crystal data

$C_{17}H_{14}ClN_5OS$
$M_r$ = 371.84
Monoclinic, $P2_1/c$
$a$ = 17.0185 (6) Å
$b$ = 8.0905 (3) Å
$c$ = 12.8292 (5) Å
$\beta$ = 105.962 (2)°
$V$ = 1698.32 (11) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.36 mm$^{-1}$
$T$ = 100.0 (1) K
0.70 × 0.48 × 0.15 mm

### Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.785, $T_{max}$ = 0.949
57891 measured reflections
7463 independent reflections
6349 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.098
$S$ = 1.09
7463 reflections
234 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.59 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H1N3···O1$^{i}$ | 0.85 (1) | 1.89 (1) | 2.7362 (10) | 175 (1) |
| N1—H1N1···O1$^{ii}$ | 0.84 (1) | 2.29 (1) | 2.9450 (10) | 134 (2) |

Symmetry codes: (i) $x, -y+\frac{5}{2}, z-\frac{1}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; 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* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2320).

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# supporting information

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# 3-Benzamidomethyl-4-[(*E*)-2-chlorobenzylideneamino]-1*H*-1,2,4-triazole-5(4*H*)-thione

**Hoong-Kun Fun, Samuel Robinson Jebas, Jyothi N. Rao and B. Kalluraya**

## S1. Comment

1,2,4-Triazoles and their derivatives represent a rapidly developing field in modern heterocyclic chemistry, in part due to their antibacterial, antifungal, antitubercular, anticancer (Kalluraya *et al.*, 1996), antitumor (Al-Soud *et al.*, 2003), anticonvulsant (Almasirad *et al.*, 2004), anti-inflammatory, and analgesic properties (Amir & Shikha, 2004). Certain 1,2,4-triazoles also find applications in the preparation of photographic plates, polymers, and as analytical agents (Kawashima *et al.*, 1986). In continuation of our interest in the synthesis of chemically and biologically important heterocycles, we report here a substituted 1,2,4-triazole Schiff base.

In the title compound (Fig. 1), the dihedral angles formed by the triazole (N2/N3/C10/N4/C9) ring with the two benzene rings (C1–C6; C12–C17) are 66.88 (3)° and 19.16 (3)° respectively. The benzene rings (C1–C6; C12–C17) form a dihedral angle of 78.40 (3)°, indicating that they are inclined to each other. The structure contains intermolecular N—H···O hydrogen bonds (see Table), linking the molecules into two-dimensional networks parallel to the (100) planes (Fig. 2). Between layers, $\pi$—$\pi$ stacking interactions are formed between inversion-related benzene rings (C12–C17 and its symmetry equivalent 2-*x*, 2-*y*, 1-*z*) with centroid-centroid distance 3.7717 (5) Å.

## S2. Experimental

The title compound was obtained by refluxing *N*-[(4-amino-5-sulfanyl-4*H*-1, 2,4-triazol-3-yl)methyl]benzamide (0.01 mol) and 2-chlorobenzaldehyde (0.01 mol) in ethanol (30 ml) with 3 drops of concentrated sulfuric acid for 5 h. The solid product obtained was collected by filtration, washed with ethanol and dried. The product was then recrystallized using ethanol.

## S3. Refinement

The amino H atoms were located in a difference map and refined with restraints of N—H = 0.85 (1) Å. The remaining H atoms were positioned geometrically [C—H = 0.93Å (aromatic) or 0.97Å (methylene)] and refined using a riding model, with $U_{iso}$(H) = 1.2 $U_{eq}$(C).

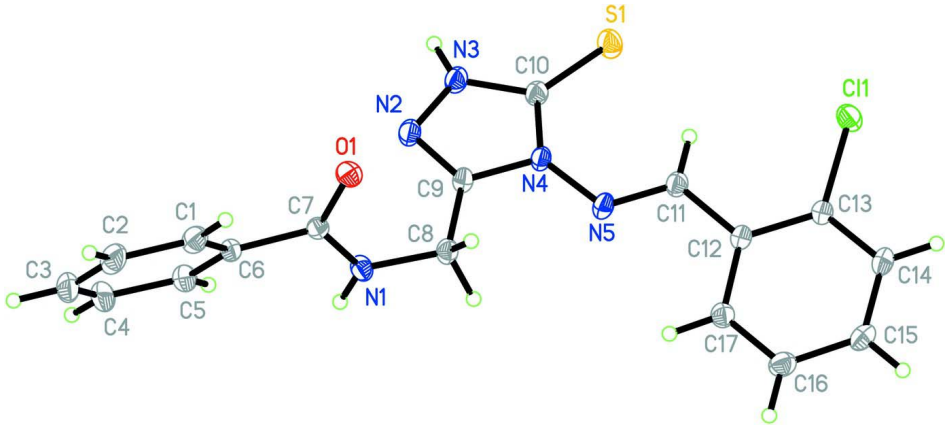


**Figure 1**

The molecular structure of the title compound, showing 50% probability displacement ellipsoids for non-H atoms.

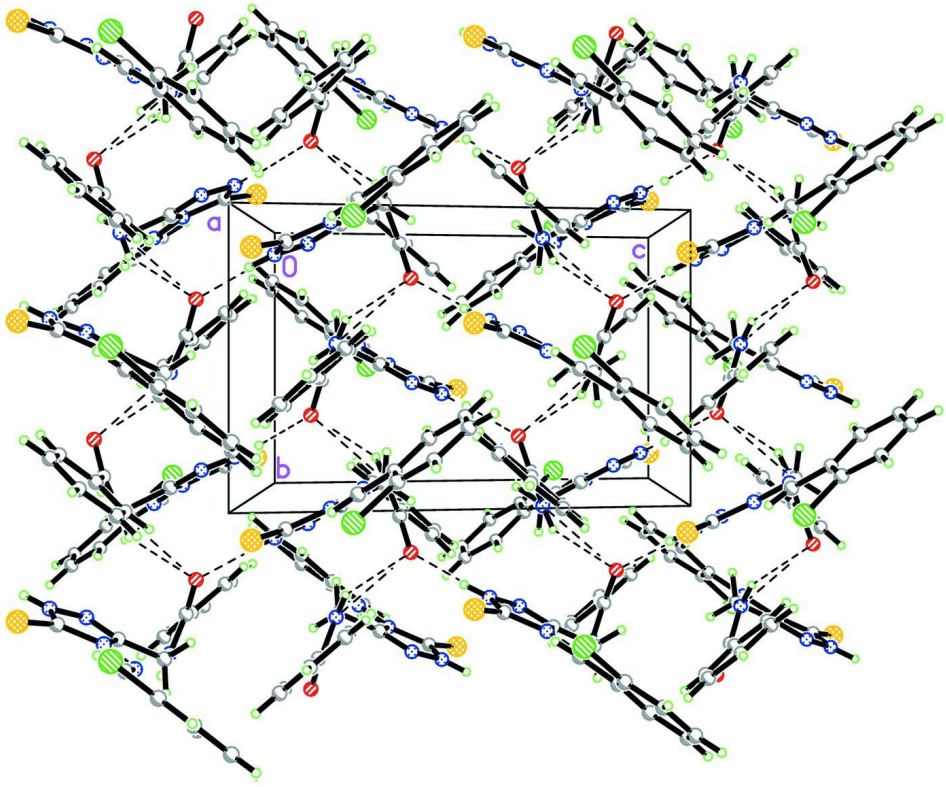


**Figure 2**

Projection down the *a* axis onto one two-dimensional hydrogen-bond network.

**3-Benzamidomethyl-4-[(*E*)-2-chlorobenzylideneamino]-1*H*-1,2,4- triazole-5(4*H*)-thione**

*Crystal data*

$C_{17}H_{14}ClN_5OS$
$M_r = 371.84$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 17.0185\ (6)$ Å
$b = 8.0905\ (3)$ Å
$c = 12.8292\ (5)$ Å
$\beta = 105.962\ (2)°$
$V = 1698.32\ (11)$ Å$^3$
$Z = 4$

$F(000) = 768$
$D_x = 1.454$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9004 reflections
$\theta = 2.6–26.3°$
$\mu = 0.36$ mm$^{-1}$
$T = 100$ K
Plate, colourless
0.70 × 0.48 × 0.15 mm

*Data collection*

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.785$, $T_{max} = 0.949$
57891 measured reflections
7463 independent reflections
6349 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 35.0°$, $\theta_{min} = 1.2°$
$h = -27 \rightarrow 27$
$k = -12 \rightarrow 13$
$l = -20 \rightarrow 20$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.098$
$S = 1.09$
7463 reflections
234 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.4785P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.59$ e Å$^{-3}$
$\Delta\rho_{min} = -0.23$ e Å$^{-3}$

*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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 1.007210 (13) | 1.03657 (3) | 0.261198 (17) | 0.02066 (5) |
| S1 | 0.757666 (14) | 1.12198 (3) | 0.021681 (19) | 0.02205 (6) |
| O1 | 0.52774 (4) | 1.20878 (8) | 0.36983 (5) | 0.01823 (12) |
| N1 | 0.52114 (5) | 0.94734 (9) | 0.30979 (6) | 0.01683 (13) |
| N2 | 0.56478 (5) | 1.09220 (10) | 0.13014 (6) | 0.01817 (13) |
| N3 | 0.60840 (5) | 1.13484 (10) | 0.05794 (6) | 0.01859 (14) |
| N4 | 0.69550 (4) | 1.02508 (9) | 0.19194 (6) | 0.01486 (12) |
| N5 | 0.75857 (4) | 0.95136 (10) | 0.26923 (6) | 0.01636 (13) |
| C1 | 0.37543 (6) | 1.16562 (13) | 0.41825 (8) | 0.02102 (16) |
| H1A | 0.4129 | 1.2333 | 0.4659 | 0.025* |
| C2 | 0.29456 (7) | 1.16030 (15) | 0.42187 (9) | 0.0288 (2) |

| | | | | |
|---|---|---|---|---|
| H2A | 0.2779 | 1.2232 | 0.4726 | 0.035* |
| C3 | 0.23860 (7) | 1.06069 (16) | 0.34943 (11) | 0.0332 (3) |
| H3A | 0.1846 | 1.0569 | 0.3522 | 0.040* |
| C4 | 0.26273 (6) | 0.96688 (15) | 0.27305 (10) | 0.0308 (2) |
| H4A | 0.2247 | 0.9019 | 0.2241 | 0.037* |
| C5 | 0.34392 (6) | 0.96984 (12) | 0.26950 (8) | 0.02199 (17) |
| H5A | 0.3603 | 0.9064 | 0.2188 | 0.026* |
| C6 | 0.40030 (5) | 1.06870 (11) | 0.34268 (7) | 0.01574 (14) |
| C7 | 0.48744 (5) | 1.07999 (10) | 0.34185 (6) | 0.01337 (13) |
| C8 | 0.60617 (5) | 0.94817 (11) | 0.30987 (7) | 0.01689 (14) |
| H8A | 0.6263 | 0.8354 | 0.3162 | 0.020* |
| H8B | 0.6376 | 1.0090 | 0.3727 | 0.020* |
| C9 | 0.61919 (5) | 1.02410 (10) | 0.20985 (7) | 0.01548 (14) |
| C10 | 0.68828 (5) | 1.09511 (11) | 0.09059 (7) | 0.01650 (14) |
| C11 | 0.83182 (5) | 0.96240 (11) | 0.26128 (7) | 0.01659 (14) |
| H11A | 0.8436 | 1.0204 | 0.2048 | 0.020* |
| C12 | 0.89642 (5) | 0.87989 (10) | 0.34477 (6) | 0.01453 (13) |
| C13 | 0.97907 (5) | 0.90723 (10) | 0.35310 (6) | 0.01472 (13) |
| C14 | 1.04079 (5) | 0.83357 (11) | 0.43414 (7) | 0.01758 (15) |
| H14A | 1.0954 | 0.8540 | 0.4387 | 0.021* |
| C15 | 1.01981 (6) | 0.72926 (11) | 0.50811 (7) | 0.01963 (16) |
| H15A | 1.0606 | 0.6804 | 0.5630 | 0.024* |
| C16 | 0.93781 (6) | 0.69731 (12) | 0.50042 (7) | 0.02018 (16) |
| H16A | 0.9240 | 0.6264 | 0.5497 | 0.024* |
| C17 | 0.87707 (5) | 0.77125 (11) | 0.41949 (7) | 0.01766 (14) |
| H17A | 0.8226 | 0.7487 | 0.4145 | 0.021* |
| H1N3 | 0.5848 (9) | 1.1788 (19) | −0.0026 (9) | 0.034 (4)* |
| H1N1 | 0.4932 (9) | 0.8627 (15) | 0.2855 (13) | 0.040 (4)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.01679 (9) | 0.02638 (11) | 0.01858 (9) | −0.00361 (7) | 0.00446 (7) | 0.00349 (7) |
| S1 | 0.01723 (10) | 0.03144 (12) | 0.01831 (10) | 0.00069 (8) | 0.00629 (7) | 0.00525 (8) |
| O1 | 0.0181 (3) | 0.0162 (3) | 0.0190 (3) | −0.0035 (2) | 0.0027 (2) | −0.0028 (2) |
| N1 | 0.0142 (3) | 0.0155 (3) | 0.0217 (3) | −0.0019 (2) | 0.0065 (2) | −0.0035 (2) |
| N2 | 0.0139 (3) | 0.0220 (3) | 0.0183 (3) | 0.0027 (3) | 0.0040 (2) | 0.0024 (3) |
| N3 | 0.0147 (3) | 0.0234 (3) | 0.0168 (3) | 0.0032 (3) | 0.0030 (2) | 0.0044 (3) |
| N4 | 0.0115 (3) | 0.0184 (3) | 0.0143 (3) | 0.0024 (2) | 0.0029 (2) | 0.0018 (2) |
| N5 | 0.0130 (3) | 0.0202 (3) | 0.0147 (3) | 0.0035 (2) | 0.0020 (2) | 0.0013 (2) |
| C1 | 0.0211 (4) | 0.0247 (4) | 0.0198 (4) | 0.0061 (3) | 0.0098 (3) | 0.0049 (3) |
| C2 | 0.0242 (5) | 0.0374 (5) | 0.0302 (5) | 0.0127 (4) | 0.0163 (4) | 0.0145 (4) |
| C3 | 0.0160 (4) | 0.0428 (6) | 0.0430 (6) | 0.0060 (4) | 0.0117 (4) | 0.0218 (5) |
| C4 | 0.0146 (4) | 0.0349 (6) | 0.0396 (6) | −0.0037 (4) | 0.0015 (4) | 0.0115 (4) |
| C5 | 0.0158 (4) | 0.0223 (4) | 0.0255 (4) | −0.0022 (3) | 0.0017 (3) | 0.0029 (3) |
| C6 | 0.0135 (3) | 0.0171 (3) | 0.0170 (3) | 0.0011 (3) | 0.0049 (3) | 0.0037 (3) |
| C7 | 0.0137 (3) | 0.0147 (3) | 0.0115 (3) | −0.0003 (2) | 0.0032 (2) | 0.0006 (2) |
| C8 | 0.0138 (3) | 0.0203 (4) | 0.0173 (3) | 0.0020 (3) | 0.0055 (3) | 0.0012 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.0125 (3) | 0.0175 (3) | 0.0165 (3) | 0.0018 (3) | 0.0040 (3) | 0.0000 (3) |
| C10 | 0.0148 (3) | 0.0184 (3) | 0.0155 (3) | 0.0009 (3) | 0.0029 (3) | 0.0014 (3) |
| C11 | 0.0134 (3) | 0.0196 (4) | 0.0160 (3) | 0.0014 (3) | 0.0028 (3) | 0.0018 (3) |
| C12 | 0.0126 (3) | 0.0161 (3) | 0.0143 (3) | 0.0014 (2) | 0.0027 (2) | −0.0004 (2) |
| C13 | 0.0135 (3) | 0.0161 (3) | 0.0143 (3) | 0.0009 (3) | 0.0032 (2) | −0.0006 (2) |
| C14 | 0.0135 (3) | 0.0193 (4) | 0.0180 (3) | 0.0028 (3) | 0.0011 (3) | −0.0015 (3) |
| C15 | 0.0192 (4) | 0.0188 (4) | 0.0184 (3) | 0.0046 (3) | 0.0008 (3) | 0.0018 (3) |
| C16 | 0.0218 (4) | 0.0196 (4) | 0.0187 (4) | 0.0020 (3) | 0.0048 (3) | 0.0038 (3) |
| C17 | 0.0160 (3) | 0.0196 (4) | 0.0177 (3) | 0.0008 (3) | 0.0051 (3) | 0.0016 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C13 | 1.7393 (9) | C4—C5 | 1.3951 (14) |
| S1—C10 | 1.6726 (9) | C4—H4A | 0.930 |
| O1—C7 | 1.2449 (10) | C5—C6 | 1.3951 (13) |
| N1—C7 | 1.3340 (11) | C5—H5A | 0.930 |
| N1—C8 | 1.4468 (11) | C6—C7 | 1.4887 (11) |
| N1—H1N1 | 0.84 (1) | C8—C9 | 1.4930 (12) |
| N2—C9 | 1.2984 (11) | C8—H8A | 0.970 |
| N2—N3 | 1.3807 (11) | C8—H8B | 0.970 |
| N3—C10 | 1.3467 (11) | C11—C12 | 1.4677 (12) |
| N3—H1N3 | 0.85 (1) | C11—H11A | 0.930 |
| N4—C9 | 1.3797 (11) | C12—C13 | 1.3987 (11) |
| N4—N5 | 1.3804 (10) | C12—C17 | 1.4047 (12) |
| N4—C10 | 1.3924 (11) | C13—C14 | 1.3924 (12) |
| N5—C11 | 1.2816 (11) | C14—C15 | 1.3879 (13) |
| C1—C2 | 1.3905 (14) | C14—H14A | 0.930 |
| C1—C6 | 1.3999 (13) | C15—C16 | 1.3958 (13) |
| C1—H1A | 0.930 | C15—H15A | 0.930 |
| C2—C3 | 1.3904 (19) | C16—C17 | 1.3836 (12) |
| C2—H2A | 0.930 | C16—H16A | 0.930 |
| C3—C4 | 1.3879 (19) | C17—H17A | 0.930 |
| C3—H3A | 0.930 | | |
| | | | |
| C7—N1—C8 | 120.72 (7) | N1—C8—H8A | 109.0 |
| C7—N1—H1N1 | 121.3 (12) | C9—C8—H8A | 109.0 |
| C8—N1—H1N1 | 117.8 (12) | N1—C8—H8B | 109.0 |
| C9—N2—N3 | 103.64 (7) | C9—C8—H8B | 109.0 |
| C10—N3—N2 | 114.49 (7) | H8A—C8—H8B | 107.8 |
| C10—N3—H1N3 | 124.6 (11) | N2—C9—N4 | 111.50 (7) |
| N2—N3—H1N3 | 120.8 (11) | N2—C9—C8 | 127.53 (8) |
| C9—N4—N5 | 117.35 (7) | N4—C9—C8 | 120.96 (7) |
| C9—N4—C10 | 108.21 (7) | N3—C10—N4 | 102.12 (7) |
| N5—N4—C10 | 134.27 (7) | N3—C10—S1 | 127.13 (7) |
| C11—N5—N4 | 119.60 (7) | N4—C10—S1 | 130.74 (7) |
| C2—C1—C6 | 119.76 (10) | N5—C11—C12 | 117.39 (8) |
| C2—C1—H1A | 120.1 | N5—C11—H11A | 121.3 |
| C6—C1—H1A | 120.1 | C12—C11—H11A | 121.3 |

| | | | |
|---|---|---|---|
| C3—C2—C1 | 119.87 (10) | C13—C12—C17 | 117.80 (7) |
| C3—C2—H2A | 120.1 | C13—C12—C11 | 121.30 (7) |
| C1—C2—H2A | 120.1 | C17—C12—C11 | 120.90 (8) |
| C4—C3—C2 | 120.50 (10) | C14—C13—C12 | 121.71 (8) |
| C4—C3—H3A | 119.7 | C14—C13—Cl1 | 118.16 (6) |
| C2—C3—H3A | 119.7 | C12—C13—Cl1 | 120.13 (6) |
| C3—C4—C5 | 120.11 (11) | C15—C14—C13 | 119.19 (8) |
| C3—C4—H4A | 119.9 | C15—C14—H14A | 120.4 |
| C5—C4—H4A | 119.9 | C13—C14—H14A | 120.4 |
| C6—C5—C4 | 119.47 (10) | C14—C15—C16 | 120.29 (8) |
| C6—C5—H5A | 120.3 | C14—C15—H15A | 119.9 |
| C4—C5—H5A | 120.3 | C16—C15—H15A | 119.9 |
| C5—C6—C1 | 120.28 (8) | C17—C16—C15 | 119.94 (8) |
| C5—C6—C7 | 122.17 (8) | C17—C16—H16A | 120.0 |
| C1—C6—C7 | 117.52 (8) | C15—C16—H16A | 120.0 |
| O1—C7—N1 | 120.84 (8) | C16—C17—C12 | 121.04 (8) |
| O1—C7—C6 | 121.35 (8) | C16—C17—H17A | 119.5 |
| N1—C7—C6 | 117.81 (7) | C12—C17—H17A | 119.5 |
| N1—C8—C9 | 112.71 (7) | | |

| | | | |
|---|---|---|---|
| C9—N2—N3—C10 | 0.01 (11) | C10—N4—C9—C8 | 176.80 (8) |
| C9—N4—N5—C11 | −173.61 (8) | N1—C8—C9—N2 | 3.33 (13) |
| C10—N4—N5—C11 | 11.79 (14) | N1—C8—C9—N4 | −175.30 (7) |
| C6—C1—C2—C3 | −0.94 (15) | N2—N3—C10—N4 | −1.18 (10) |
| C1—C2—C3—C4 | −0.30 (16) | N2—N3—C10—S1 | 177.48 (7) |
| C2—C3—C4—C5 | 1.02 (16) | C9—N4—C10—N3 | 1.84 (9) |
| C3—C4—C5—C6 | −0.50 (15) | N5—N4—C10—N3 | 176.80 (9) |
| C4—C5—C6—C1 | −0.73 (14) | C9—N4—C10—S1 | −176.74 (7) |
| C4—C5—C6—C7 | −178.80 (8) | N5—N4—C10—S1 | −1.79 (15) |
| C2—C1—C6—C5 | 1.45 (13) | N4—N5—C11—C12 | −179.19 (7) |
| C2—C1—C6—C7 | 179.61 (8) | N5—C11—C12—C13 | −169.43 (8) |
| C8—N1—C7—O1 | 1.88 (12) | N5—C11—C12—C17 | 10.21 (12) |
| C8—N1—C7—C6 | −178.27 (7) | C17—C12—C13—C14 | −1.71 (12) |
| C5—C6—C7—O1 | 148.96 (9) | C11—C12—C13—C14 | 177.95 (8) |
| C1—C6—C7—O1 | −29.16 (12) | C17—C12—C13—Cl1 | 178.51 (6) |
| C5—C6—C7—N1 | −30.88 (12) | C11—C12—C13—Cl1 | −1.83 (11) |
| C1—C6—C7—N1 | 151.00 (8) | C12—C13—C14—C15 | 0.51 (13) |
| C7—N1—C8—C9 | −83.83 (10) | Cl1—C13—C14—C15 | −179.70 (7) |
| N3—N2—C9—N4 | 1.23 (10) | C13—C14—C15—C16 | 0.73 (13) |
| N3—N2—C9—C8 | −177.50 (8) | C14—C15—C16—C17 | −0.71 (14) |
| N5—N4—C9—N2 | −177.97 (7) | C15—C16—C17—C12 | −0.54 (14) |
| C10—N4—C9—N2 | −2.04 (10) | C13—C12—C17—C16 | 1.72 (13) |
| N5—N4—C9—C8 | 0.86 (12) | C11—C12—C17—C16 | −177.94 (8) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H1*N*3···O1$^{i}$ | 0.85 (1) | 1.89 (1) | 2.7362 (10) | 175 (1) |

| | | | | |
|---|---|---|---|---|
| N1—H1*N*1···O1$^{ii}$ | 0.84 (1) | 2.29 (1) | 2.9450 (10) | 134 (2) |

Symmetry codes: (i) $x$, $-y+5/2$, $z-1/2$; (ii) $-x+1$, $y-1/2$, $-z+1/2$.