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

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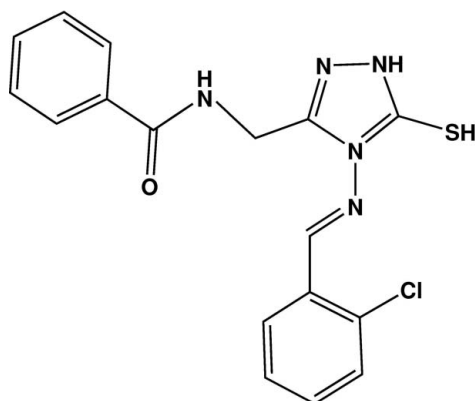
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.001$ Å; R factor = 0.033; wR factor = 0.098; data-to-parameter ratio = 31.9.

In the title compound, $\text{C}_{17}\text{H}_{14}\text{ClN}_5\text{OS}$, 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 $\text{N}-\text{H}\cdots\text{O}$ 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

$\text{C}_{17}\text{H}_{14}\text{ClN}_5\text{OS}$
 $M_r = 371.84$
 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) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.36$ mm⁻¹
 $T = 100.0$ (1) K
 $0.70 \times 0.48 \times 0.15$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$

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
 $\Delta\rho_{\text{max}} = 0.59$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.23$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N3}-\text{H1N3}\cdots\text{O1}^{\text{i}}$	0.85 (1)	1.89 (1)	2.7362 (10)	175 (1)
$\text{N1}-\text{H1N1}\cdots\text{O1}^{\text{ii}}$	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: B12320).

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supplementary materials

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

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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, π — π 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.

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.

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 = 0.93 Å (aromatic) or 0.97 Å (methylene)] and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

Figures

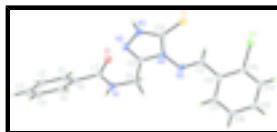


Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids for non-H atoms.

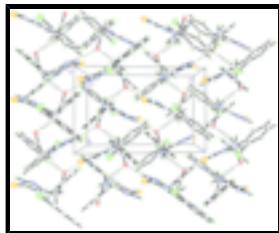


Fig. 2. Projection down the a axis onto one two-dimensional hydrogen-bond network.

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) Å³

$Z = 4$

$F_{000} = 768$

$D_x = 1.454$ 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

$T = 100.0$ (1) K

Plate, colourless

$0.70 \times 0.48 \times 0.15$ mm

Data collection

Bruker SMART APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 100.0$ (1) K

φ and ω 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 $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$

$\theta_{\max} = 35.0$ °

$\theta_{\min} = 1.2$ °

$h = -27$ → 27

$k = -12$ → 13

$l = -20$ → 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

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

234 parameters

$$\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$$

2 restraints

Extinction correction: none

Primary atom site location: structure-invariant direct methods

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	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)

supplementary materials

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 (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	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 (\AA , $^\circ$)

C11—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—C11	118.16 (6)
C2—C3—H3A	119.7	C12—C13—C11	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)

supplementary materials

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—C11	178.51 (6)
C5—C6—C7—N1	-30.88 (12)	C11—C12—C13—C11	-1.83 (11)
C1—C6—C7—N1	151.00 (8)	C12—C13—C14—C15	0.51 (13)
C7—N1—C8—C9	-83.83 (10)	C11—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 (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H1N3 \cdots O1 ⁱ	0.85 (1)	1.89 (1)	2.7362 (10)	175 (1)
N1—H1N1 \cdots O1 ⁱⁱ	0.84 (1)	2.29 (1)	2.9450 (10)	134 (2)

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

Fig. 1

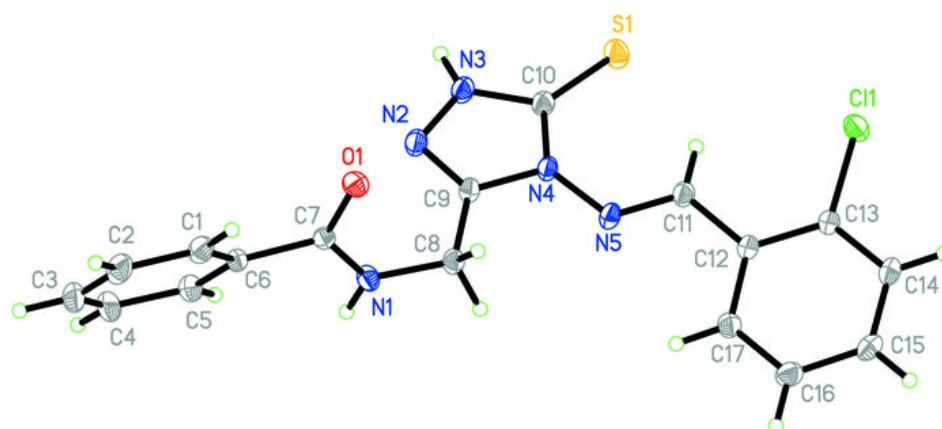


Fig. 2

