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

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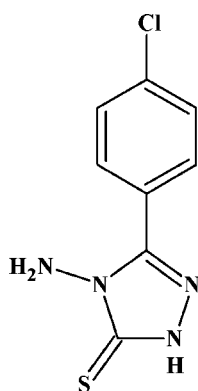
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; disorder in main residue; R factor = 0.080; wR factor = 0.236; data-to-parameter ratio = 10.5.

In the title compound, $\text{C}_8\text{H}_7\text{ClN}_4\text{S}$, the benzene ring is statistically disordered over two conformations rotated about the $\text{Cl}-\text{C}\cdots\text{C}-\text{C}$ axis, which subtend dihedral angles of 24.7 (3) and 9.9 (2) ° with respect to the triazole ring. An intramolecular $\text{C}-\text{H}\cdots\text{N}$ close contact occurs. In the crystal, $\text{N}-\text{H}\cdots\text{N}$ and $\text{N}-\text{H}\cdots\text{S}$ hydrogen bonds link the molecules into (001) sheets: $R_2^2(8)$ and $R_2^2(10)$ graph-set motifs result. Weak $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds and aromatic $\pi-\pi$ stacking interactions [shortest centroid-centroid separation = 3.681 (7) Å] complete the structure.

Related literature

For a related structure and background references, see: Natarajan & Mathews (2011). For a related structure, see: Ambalavanan *et al.* (2003).



Experimental

Crystal data

 $\text{C}_8\text{H}_7\text{ClN}_4\text{S}$ $M_r = 226.69$

Triclinic, $P\bar{1}$
 $a = 6.0765$ (9) Å
 $b = 8.0268$ (7) Å
 $c = 10.9873$ (16) Å
 $\alpha = 72.501$ (10)°
 $\beta = 87.597$ (10)°
 $\gamma = 67.88$ (2)°

$V = 471.94$ (12) Å³
 $Z = 2$
 Cu $K\alpha$ radiation
 $\mu = 5.35$ mm⁻¹
 $T = 293$ K
 $0.24 \times 0.18 \times 0.12$ mm

Data collection

Enraf-Nonius CAD-4 diffractometer
 Absorption correction: part of the refinement model (ΔF) (*SHELXA*; Sheldrick, 2008)
 $T_{\text{min}} = 0.146$, $T_{\text{max}} = 0.618$

1912 measured reflections
 1818 independent reflections
 1670 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.054$
 3 standard reflections every 60 min
 intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.080$
 $wR(F^2) = 0.236$
 $S = 1.09$
 1818 reflections
 173 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.62$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.51$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C4B}-\text{H4B}\cdots\text{N4}$	0.93	2.32	2.98	128
$\text{N3}-\text{H3}\cdots\text{S1}^{\text{i}}$	0.86	2.55	3.332 (3)	152
$\text{C5B}-\text{H5B}\cdots\text{N4}^{\text{ii}}$	0.93	2.72	3.582 (8)	155
$\text{C8A}-\text{H8A}\cdots\text{N4}^{\text{iii}}$	0.93	2.53	3.416 (9)	158
$\text{C7B}-\text{H7B}\cdots\text{N2}^{\text{iv}}$	0.93	2.64	3.541 (10)	162
$\text{N4}-\text{H4C}\cdots\text{S1}^{\text{v}}$	0.91 (6)	2.70 (6)	3.552 (4)	155 (5)
$\text{N4}-\text{H4D}\cdots\text{N2}^{\text{vi}}$	0.96 (7)	2.42 (7)	3.349 (5)	164 (5)

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

Data collection: *CAD-4 EXPRESS* (Enraf-Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* and *PLATON*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6583).

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supplementary materials

Acta Cryst. (2012). E68, o443 [doi:10.1107/S1600536812000785]

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

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Comment

As part of our ongoing studies of 1,2,4-triazole derivatives (Natarajan & Mathews, 2011), we now describe the title compound.

The title molecule (Fig.1) contains the rings 1,2,4-triazole and 4-chlorophenyl. All the bond lengths and bond angles are well agreed with previously reported structure (Ambalavanan *et al.*, 2003; Natarajan and Mathews, 2011). The phenyl ring substituted on the atom C2 shows rotational disorder by the atoms of C4, C5, C7 & C8. The rotational disorder of phenyl ring results in two phenyl ring orientations A (C3/C4A/C5A/C6/C7A/C8A) and B (C3/C4B/C5B/CB/C7B/C8B) with respect to 1,2,4-triazole ring. The dihedral angles of these phenyl rings with triazole moiety are 24.7 (3) and 9.9 (2)°, respectively for phenyl rings A and B.

The packing diagram of the title compound viewed down *a* axis is shown in Fig. 2. The crystal structure is stabilized by the intra and intermolecular hydrogen bonds namely N—H⋯N, C—H⋯N and N—H⋯S. One of them (N—H⋯S) is involved in self-complementary interactions of triazole rings and forms $R_2^2(8)$ and $R_2^2(10)$ types graph set motifs. The motif, $R_2^2(10)$ is formed by the dimer interactions between the symmetry related 1,2,4-triazole-3-thione moieties and it is connected by the motif $R_2^2(8)$ along the *b* axis in the unit cell packing. In addition, three $\pi\cdots\pi$ weak interactions { $Cg1\cdots Cg1=3.681(7)$ Å, $Cg1\cdots Cg2=3.691(7)$ Å & $Cg2\cdots Cg2=3.701(7)$ Å ($2-x, 1-y, -z$); *Cg* is the centroid of the rings; $Cg1=C3/C4A/C5A/C6/C7A/C8A$ and $Cg2=C3/C4B/C5B/C6/C7B/C8B$ } are also helping to consolidate the molecules in crystal packing. The detailed geometry of the non-bonded interactions is presented in Table 1.

Experimental

A mixture of β -4-chlorophenyldithiocarbazine potassium salt (0.1 mol) and hydrazine hydrate (0.25 mol) was heated on an oil-bath at 150° C for 5 h (until evolution of H₂S gas in the reaction). The reaction mixture was then cooled and poured into the cold water and then acidified with conc. HCl. The filtered product was washed extensively with cold water and recrystallized using ethanol to yield yellow needles.

Refinement

The primary amine H atoms were derived from the Fourier map and the remaining H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å for aromatic Hs and for N—H = 0.86 Å. The U_{iso} values were constrained to be 1.2U_{eq} of the carrier atom for the aromatic C—H and N—H hydrogen atoms.

Figures

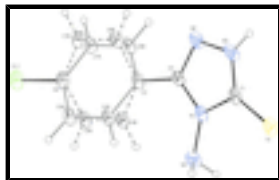


Fig. 1. ORTEP diagram of the title molecule with displacement ellipsoid drawn at 30% probability level.

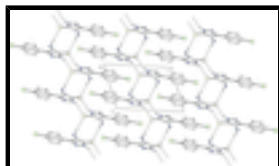


Fig. 2. A unit cell packing of the crystal structure of the title compound viewed down *a* axis. Dashed lines are indicating the hydrogen bonds between the molecules.

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

Crystal data

$C_8H_7ClN_4S$	$Z = 2$
$M_r = 226.69$	$F(000) = 232$
Triclinic, $P\bar{1}$	$D_x = 1.595 \text{ Mg m}^{-3}$
$a = 6.0765 (9) \text{ \AA}$	Cu $K\alpha$ radiation, $\lambda = 1.54184 \text{ \AA}$
$b = 8.0268 (7) \text{ \AA}$	Cell parameters from 25 reflections
$c = 10.9873 (16) \text{ \AA}$	$\theta = 1\text{--}60^\circ$
$\alpha = 72.501 (10)^\circ$	$\mu = 5.35 \text{ mm}^{-1}$
$\beta = 87.597 (10)^\circ$	$T = 293 \text{ K}$
$\gamma = 67.88 (2)^\circ$	Needle, yellow
$V = 471.94 (12) \text{ \AA}^3$	$0.24 \times 0.18 \times 0.12 \text{ mm}$

Data collection

Enraf–Nonius CAD-4 diffractometer	1670 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{\text{int}} = 0.054$
graphite	$\theta_{\text{max}} = 72.5^\circ$, $\theta_{\text{min}} = 4.2^\circ$
ω scans	$h = -6 \rightarrow 7$
Absorption correction: part of the refinement model (ΔF) (SHELXA; Sheldrick, 2008)	$k = -9 \rightarrow 9$
$T_{\text{min}} = 0.146$, $T_{\text{max}} = 0.618$	$l = -9 \rightarrow 13$
1912 measured reflections	3 standard reflections every 60 min
1818 independent reflections	intensity decay: none

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$$R[F^2 > 2\sigma(F^2)] = 0.080$$

$$wR(F^2) = 0.236$$

$$S = 1.09$$

1818 reflections

173 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.1913P)^2 + 0.1469P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\max} = 0.62 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.51 \text{ e } \text{\AA}^{-3}$$

Extinction correction: *SHELXL97* (Sheldrick, 2008),

$$F_c^* = kF_c[1+0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$$

Extinction coefficient: 0.031 (8)

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>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Cl1	0.91511 (17)	0.68117 (13)	-0.30339 (8)	0.0585 (5)	
S1	0.31850 (16)	0.79307 (13)	0.50686 (8)	0.0534 (5)	
N1	0.5022 (5)	0.7466 (4)	0.2844 (2)	0.0404 (7)	
N2	0.7683 (6)	0.8756 (5)	0.2550 (3)	0.0569 (9)	
N3	0.6640 (6)	0.8820 (5)	0.3677 (3)	0.0596 (9)	
H3	0.7032	0.9292	0.4196	0.072*	
N4	0.3603 (7)	0.6528 (5)	0.2662 (3)	0.0541 (8)	
C1	0.4998 (6)	0.8091 (5)	0.3885 (3)	0.0453 (8)	
C2	0.6627 (5)	0.7938 (4)	0.2044 (3)	0.0407 (7)	
C3	0.7171 (5)	0.7637 (4)	0.0791 (3)	0.0395 (7)	
C4A	0.5509 (19)	0.7474 (19)	0.0004 (9)	0.0404 (19)	0.50 (2)
H4A	0.4041	0.7494	0.0291	0.048*	0.50 (2)
C5A	0.6105 (19)	0.7284 (18)	-0.1214 (9)	0.048 (2)	0.50 (2)
H5A	0.5020	0.7227	-0.1757	0.057*	0.50 (2)
C4B	0.631 (2)	0.661 (2)	0.0331 (10)	0.041 (2)	0.50 (2)
H4B	0.5303	0.6072	0.0799	0.050*	0.50 (2)
C5B	0.694 (2)	0.636 (2)	-0.0856 (10)	0.047 (3)	0.50 (2)
H5B	0.6401	0.5606	-0.1156	0.056*	0.50 (2)
C6	0.8321 (6)	0.7185 (4)	-0.1578 (3)	0.0437 (8)	
C7A	0.9891 (19)	0.737 (2)	-0.0863 (8)	0.047 (2)	0.50 (2)
H7A	1.1338	0.7384	-0.1168	0.057*	0.50 (2)

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C8A	0.9324 (19)	0.755 (2)	0.0335 (8)	0.047 (2)	0.50 (2)
H8A	1.0451	0.7608	0.0850	0.057*	0.50 (2)
C7B	0.9186 (19)	0.831 (2)	-0.1110 (9)	0.046 (2)	0.50 (2)
H7B	1.0154	0.8880	-0.1592	0.056*	0.50 (2)
C8B	0.8574 (18)	0.856 (2)	0.0063 (8)	0.041 (2)	0.50 (2)
H8B	0.9085	0.9321	0.0371	0.050*	0.50 (2)
H4C	0.394 (11)	0.538 (9)	0.327 (6)	0.095 (19)*	
H4D	0.198 (12)	0.724 (9)	0.277 (6)	0.096 (18)*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0650 (7)	0.0717 (7)	0.0365 (6)	-0.0151 (5)	0.0119 (4)	-0.0289 (4)
S1	0.0548 (7)	0.0735 (7)	0.0408 (6)	-0.0209 (5)	0.0126 (4)	-0.0356 (5)
N1	0.0407 (14)	0.0474 (13)	0.0337 (13)	-0.0068 (10)	0.0014 (10)	-0.0258 (11)
N2	0.0591 (18)	0.090 (2)	0.0414 (16)	-0.0351 (16)	0.0129 (13)	-0.0406 (15)
N3	0.0627 (19)	0.098 (2)	0.0446 (16)	-0.0400 (17)	0.0151 (14)	-0.0490 (17)
N4	0.0587 (19)	0.073 (2)	0.0469 (17)	-0.0299 (15)	0.0138 (14)	-0.0360 (15)
C1	0.0451 (17)	0.0584 (17)	0.0326 (15)	-0.0081 (14)	0.0023 (12)	-0.0295 (13)
C2	0.0359 (15)	0.0500 (16)	0.0358 (15)	-0.0072 (12)	-0.0010 (11)	-0.0238 (12)
C3	0.0373 (15)	0.0435 (14)	0.0330 (14)	-0.0024 (11)	0.0001 (11)	-0.0213 (11)
C4A	0.033 (4)	0.049 (5)	0.035 (4)	-0.003 (4)	0.001 (3)	-0.023 (3)
C5A	0.050 (4)	0.051 (5)	0.033 (4)	-0.005 (4)	-0.003 (3)	-0.018 (4)
C4B	0.041 (4)	0.053 (6)	0.034 (4)	-0.012 (4)	0.008 (3)	-0.027 (4)
C5B	0.052 (5)	0.057 (6)	0.038 (4)	-0.016 (5)	0.004 (4)	-0.030 (4)
C6	0.0419 (16)	0.0468 (15)	0.0338 (16)	-0.0026 (13)	0.0028 (12)	-0.0188 (12)
C7A	0.047 (4)	0.054 (6)	0.040 (4)	-0.014 (4)	0.003 (3)	-0.020 (4)
C8A	0.045 (4)	0.055 (6)	0.045 (4)	-0.012 (4)	-0.004 (3)	-0.028 (4)
C7B	0.045 (4)	0.048 (6)	0.040 (4)	-0.011 (4)	0.010 (3)	-0.016 (4)
C8B	0.041 (4)	0.048 (6)	0.042 (4)	-0.012 (4)	0.006 (3)	-0.030 (4)

Geometric parameters (\AA , $^\circ$)

C11—C6	1.735 (3)	C4A—C5A	1.410 (9)
S1—C1	1.675 (3)	C4A—H4A	0.9300
N1—C2	1.368 (4)	C5A—C6	1.368 (9)
N1—C1	1.378 (4)	C5A—H5A	0.9300
N1—N4	1.394 (4)	C4B—C5B	1.395 (9)
N2—C2	1.311 (4)	C4B—H4B	0.9300
N2—N3	1.373 (4)	C5B—C6	1.346 (9)
N3—C1	1.315 (5)	C5B—H5B	0.9300
N3—H3	0.8572	C6—C7A	1.339 (9)
N4—H4C	0.91 (6)	C6—C7B	1.421 (10)
N4—H4D	0.96 (7)	C7A—C8A	1.381 (10)
C2—C3	1.471 (4)	C7A—H7A	0.9300
C3—C4B	1.344 (8)	C8A—H8A	0.9300
C3—C8A	1.365 (9)	C7B—C8B	1.377 (10)
C3—C8B	1.405 (9)	C7B—H7B	0.9300
C3—C4A	1.423 (8)	C8B—H8B	0.9300

C2—N1—C1	108.7 (3)	C6—C5A—H5A	120.8
C2—N1—N4	127.1 (3)	C4A—C5A—H5A	120.8
C1—N1—N4	124.3 (3)	C3—C4B—C5B	119.3 (7)
C2—N2—N3	104.2 (3)	C3—C4B—H4B	120.4
C1—N3—N2	114.0 (3)	C5B—C4B—H4B	120.4
C1—N3—H3	123.3	C6—C5B—C4B	121.7 (6)
N2—N3—H3	122.7	C6—C5B—H5B	119.1
N1—N4—H4C	113 (4)	C4B—C5B—H5B	119.1
N1—N4—H4D	109 (4)	C7A—C6—C5B	112.0 (5)
H4C—N4—H4D	104 (5)	C7A—C6—C5A	123.0 (5)
N3—C1—N1	103.3 (3)	C5B—C6—C5A	30.8 (4)
N3—C1—S1	131.5 (3)	C7A—C6—C7B	28.6 (3)
N1—C1—S1	125.2 (3)	C5B—C6—C7B	119.2 (5)
N2—C2—N1	109.8 (3)	C5A—C6—C7B	113.4 (5)
N2—C2—C3	122.3 (3)	C7A—C6—C11	118.0 (4)
N1—C2—C3	127.9 (3)	C5B—C6—C11	121.1 (4)
C4B—C3—C8A	110.6 (5)	C5A—C6—C11	119.0 (4)
C4B—C3—C8B	121.1 (5)	C7B—C6—C11	119.7 (4)
C8A—C3—C8B	30.7 (3)	C6—C7A—C8A	118.8 (7)
C4B—C3—C4A	28.1 (3)	C6—C7A—H7A	120.6
C8A—C3—C4A	117.7 (5)	C8A—C7A—H7A	120.6
C8B—C3—C4A	111.9 (5)	C3—C8A—C7A	122.4 (6)
C4B—C3—C2	122.7 (4)	C3—C8A—H8A	118.8
C8A—C3—C2	119.7 (4)	C7A—C8A—H8A	118.8
C8B—C3—C2	116.1 (4)	C8B—C7B—C6	119.3 (7)
C4A—C3—C2	122.6 (4)	C8B—C7B—H7B	120.3
C5A—C4A—C3	119.5 (6)	C6—C7B—H7B	120.3
C5A—C4A—H4A	120.2	C7B—C8B—C3	119.3 (6)
C3—C4A—H4A	120.2	C7B—C8B—H8B	120.4
C6—C5A—C4A	118.3 (6)	C3—C8B—H8B	120.4
C2—N2—N3—C1	-0.2 (5)	C2—C3—C4B—C5B	-178.8 (6)
N2—N3—C1—N1	1.7 (4)	C3—C4B—C5B—C6	-2.7 (14)
N2—N3—C1—S1	-177.0 (3)	C4B—C5B—C6—C7A	31.8 (11)
C2—N1—C1—N3	-2.5 (3)	C4B—C5B—C6—C5A	-86.1 (12)
N4—N1—C1—N3	178.0 (3)	C4B—C5B—C6—C7B	1.1 (11)
C2—N1—C1—S1	176.3 (2)	C4B—C5B—C6—C11	178.4 (7)
N4—N1—C1—S1	-3.2 (4)	C4A—C5A—C6—C7A	-4.1 (11)
N3—N2—C2—N1	-1.4 (4)	C4A—C5A—C6—C5B	73.4 (10)
N3—N2—C2—C3	178.1 (3)	C4A—C5A—C6—C7B	-34.8 (9)
C1—N1—C2—N2	2.5 (4)	C4A—C5A—C6—C11	176.3 (5)
N4—N1—C2—N2	-178.0 (3)	C5B—C6—C7A—C8A	-28.2 (10)
C1—N1—C2—C3	-176.9 (3)	C5A—C6—C7A—C8A	4.5 (11)
N4—N1—C2—C3	2.5 (5)	C7B—C6—C7A—C8A	82.8 (12)
N2—C2—C3—C4B	172.1 (9)	C11—C6—C7A—C8A	-175.9 (6)
N1—C2—C3—C4B	-8.5 (9)	C4B—C3—C8A—C7A	32.1 (10)
N2—C2—C3—C8A	24.1 (9)	C8B—C3—C8A—C7A	-84.4 (11)
N1—C2—C3—C8A	-156.5 (8)	C4A—C3—C8A—C7A	2.2 (11)
N2—C2—C3—C8B	-10.5 (7)	C2—C3—C8A—C7A	-176.4 (7)

supplementary materials

N1—C2—C3—C8B	168.9 (7)	C6—C7A—C8A—C3	-3.5 (13)
N2—C2—C3—C4A	-154.4 (7)	C7A—C6—C7B—C8B	-83.4 (12)
N1—C2—C3—C4A	25.0 (8)	C5B—C6—C7B—C8B	-0.8 (10)
C4B—C3—C4A—C5A	-83.7 (11)	C5A—C6—C7B—C8B	33.1 (9)
C8A—C3—C4A—C5A	-1.8 (10)	C11—C6—C7B—C8B	-178.1 (5)
C8B—C3—C4A—C5A	31.6 (9)	C6—C7B—C8B—C3	2.0 (11)
C2—C3—C4A—C5A	176.8 (6)	C4B—C3—C8B—C7B	-3.6 (10)
C3—C4A—C5A—C6	2.6 (11)	C8A—C3—C8B—C7B	74.2 (9)
C8A—C3—C4B—C5B	-28.3 (10)	C4A—C3—C8B—C7B	-33.5 (9)
C8B—C3—C4B—C5B	3.9 (11)	C2—C3—C8B—C7B	178.9 (6)
C4A—C3—C4B—C5B	82.2 (13)		

Hydrogen-bond geometry (\AA , $^\circ$)

<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>
C4B—H4B \cdots N4	0.93	2.32	2.98	128
N3—H3 \cdots S1 ⁱ	0.86	2.55	3.332 (3)	152
C5B—H5B \cdots N4 ⁱⁱ	0.93	2.72	3.582 (8)	155
C8A—H8A \cdots N4 ⁱⁱⁱ	0.93	2.53	3.416 (9)	158
C7B—H7B \cdots N2 ^{iv}	0.93	2.64	3.541 (10)	162
N4—H4C \cdots S1 ^v	0.91 (6)	2.70 (6)	3.552 (4)	155 (5)
N4—H4D \cdots N2 ^{vi}	0.96 (7)	2.42 (7)	3.349 (5)	164 (5)

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

Fig. 1

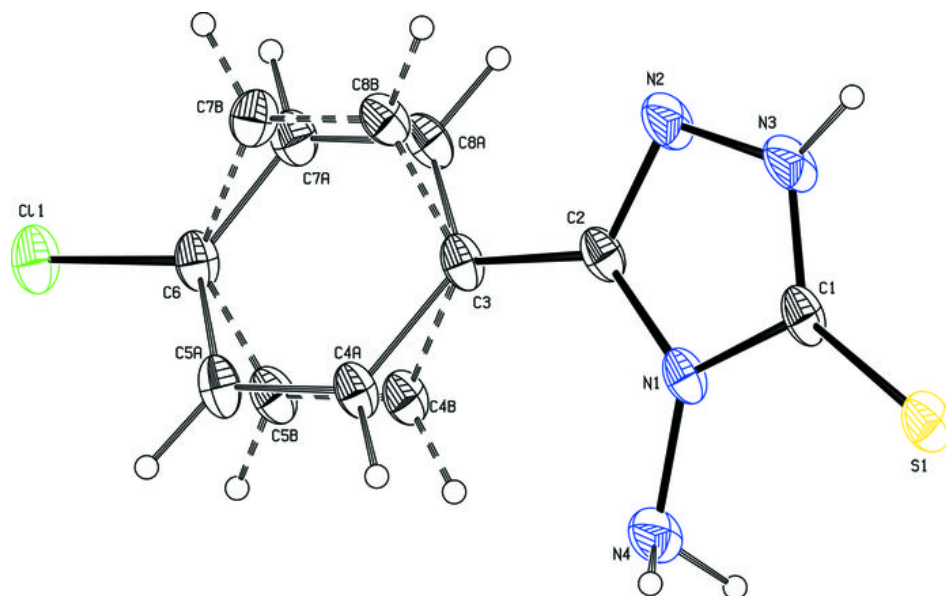


Fig. 2

