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## Key indicators

Single-crystal X-ray study  
 $T = 100\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$   
 $R$  factor = 0.040  
 $wR$  factor = 0.073  
Data-to-parameter ratio = 18.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.3-Benzyl-4-(4-chlorophenyl)-1*H*-1,2,4-triazole-5(4*H*)-thioneIn the title molecule,  $\text{C}_{15}\text{H}_{12}\text{ClN}_3\text{S}$ , the dihedral angles made by the substituted phenyl and benzyl rings with the triazole ring are  $81.39(10)$  and  $63.59(10)^\circ$ , respectively. The crystal structure is stabilized by  $\text{N}-\text{H}\cdots\text{S}$ ,  $\text{C}-\text{H}\cdots\text{Cl}$  and  $\text{C}-\text{H}\cdots\pi$  interactions.

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## Comment

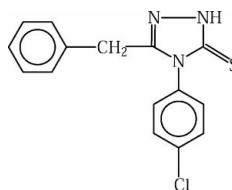
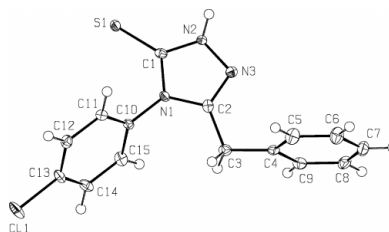
Derivatives of 1,2,4-triazole are known to exhibit anti-inflammatory (Unangst *et al.*, 1992; Mullican *et al.*, 1993), antiviral, analgesic (Sughen & Yoloye, 1978), antimicrobial (Shams El-Dine & Hazzaa, 1974; Misato *et al.*, 1977; Cansız *et al.*, 2001), anticonvulsant (Stillings *et al.*, 1986) and anti-depressant activity (Kane *et al.*, 1988), the last being usually explored by the forced swim test (Porsolt *et al.*, 1977; Vamvakides, 1990). Among the pharmacological profiles of 1,2,4-triazoles, their antimicrobial, anticonvulsant and anti-depressant properties seem to be the best documented. In addition, some studies have been published on the electronic structures and thiol–thione tautomeric equilibrium of heterocyclic thione derivatives (Aydoğan *et al.*, 2002; Charistos *et al.*, 1994). We have synthesized several new compounds. One of these new derivatives is the title compound, (I), reported here.A view of the molecule of (I), including the atomic numbering scheme, is shown in Fig. 1. The  $\text{N}=\text{C}$  [ $1.307(2)\text{ \AA}$ ],  $\text{S}=\text{C}$  [ $1.688(2)\text{ \AA}$ ] and  $\text{Cl}-\text{C}$  [ $1.742(2)\text{ \AA}$ ] bond lengths are close to the values reported in the literature (Öztürk *et al.*, 2004).The title compound, (I), contains three planar rings. One is the triazole ring (*A*), the others are benzene rings *B* (*C4*–*C9*)

Figure 1

An ORTEP-3 (Farrugia, 1997) drawing of (I), with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

and C (C10–C15). In the triazole ring, the maximum deviation from planarity is  $-0.005$  (1) Å for atom N1 (Nardelli, 1995). The dihedral angles between rings A/B, A/C and B/C are  $81.39$  (10),  $63.59$  (10) and  $45.15$  (10)°, respectively.

In the crystal structure, the molecules are linked by intermolecular N–H···S, C–H···Cl and C–H··· $\pi$  interactions, resulting in a three-dimensional network structure (Fig. 2). The geometry of these interactions is listed in Table 2.

## Experimental

A stirred mixture of 1-phenylacetyl-4-(4-chlorophenyl)thiosemicarbazide (1 mmol) and sodium hydroxide (40 mg, 1 mmol, as a 2 N solution) was refluxed for 4 h. After cooling, the solution was acidified with hydrochloric acid and the precipitate was filtered off. The precipitate was then crystallized from ethanol (yield 73%, m.p. 460–461 K). IR  $\nu$  (cm<sup>-1</sup>): 3354, 3292 (N–H), 2980 (CH), 1606 (C=N), 1535, 1260, 1050, 950 (N–C=S, amide I, II, III and IV bands). <sup>1</sup>H NMR:  $\delta$  3.84 (s, 2H, CH<sub>2</sub>), 6.94–7.42 (m, 9H, Ar–H), 12.96 (s, 1H, SH or NH). Calculated for C<sub>15</sub>H<sub>12</sub>ClN<sub>3</sub>S: C 59.70, H 4.01, N 13.92, S 10.62%; found: C 59.58, H 4.07, N 14.00, S 10.58%.

### Crystal data

C <sub>15</sub> H <sub>12</sub> ClN <sub>3</sub> S	$D_x = 1.404$ Mg m <sup>-3</sup>
$M_r = 301.80$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 124 reflections
$a = 9.181$ (5) Å	$\theta = 6.0$ – $20.0^\circ$
$b = 17.803$ (5) Å	$\mu = 0.41$ mm <sup>-1</sup>
$c = 9.231$ (5) Å	$T = 100$ K
$\beta = 108.882$ (5)°	Block, colorless
$V = 1427.6$ (12) Å <sup>3</sup>	$0.25 \times 0.21 \times 0.18$ mm
$Z = 4$	

### Data collection

Bruker–Nonius KappaCCD diffractometer	3388 independent reflections
$\omega$ scans	2378 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	$R_{int} = 0.079$
$T_{min} = 0.905$ , $T_{max} = 0.930$	$\theta_{max} = 28.0^\circ$
18622 measured reflections	$h = -12 \rightarrow 12$
	$k = -23 \rightarrow 22$
	$l = -12 \rightarrow 12$

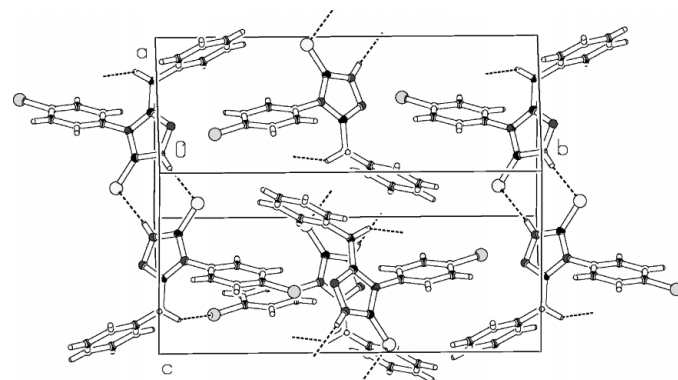
### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0253P)^2 + 0.481P]$
$R[F^2 > 2\sigma(F^2)] = 0.040$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.073$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.26$ e Å <sup>-3</sup>
3388 reflections	$\Delta\rho_{min} = -0.26$ e Å <sup>-3</sup>
181 parameters	
H-atom parameters constrained	

**Table 1**

Selected geometric parameters (Å, °).

Cl1–C13	1.742 (2)	N1–C10	1.445 (2)
S1–C1	1.688 (2)	N2–N3	1.381 (2)
N1–C1	1.379 (2)	N2–C1	1.333 (2)
N1–C2	1.387 (2)	N3–C2	1.307 (2)
C1–N1–C2	107.89 (14)	N3–C2–C3	125.08 (16)
C1–N1–C10	124.39 (14)	N1–C2–N3	110.74 (16)
C2–N1–C10	127.57 (15)	N1–C2–C3	124.14 (16)
N3–N2–C1	113.89 (15)	N1–C10–C11	118.84 (16)
N2–N3–C2	103.92 (14)	N1–C10–C15	119.67 (16)
N1–C1–N2	103.55 (15)	Cl1–C13–C14	118.97 (15)
S1–C1–N1	127.14 (14)	Cl1–C13–C12	118.79 (14)
S1–C1–N2	129.28 (14)		



**Figure 2**

A packing diagram of (I), illustrating the hydrogen-bonding network (dashed lines).

**Table 2**

Hydrogen-bonding geometry (Å, °).

D–H···A	D–H	H···A	D···A	D–H···A
N2–H2···S1 <sup>i</sup>	0.86	2.38	3.237 (2)	175
C3–H3B···Cl1 <sup>ii</sup>	0.97	2.81	3.540 (3)	133
C3–H3B···Cg1 <sup>iii</sup>	0.97	2.99	3.648 (3)	126
C12–H12···Cg1 <sup>iv</sup>	0.93	3.00	3.535 (3)	118
C15–H15···Cg2 <sup>v</sup>	0.93	2.74	3.616 (3)	158

Symmetry codes: (i)  $1 - x, -y, 1 - z$ ; (ii)  $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$ ; (iii)  $-x, -y, 2 - z$ ; (iv)  $\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$ ; (v)  $-x, -y, 1 - z$ . Cg1 and Cg2 denote the centroids of ring B (C4–C9) and the triazole ring, respectively.

All H atoms were positioned geometrically and treated as riding on their parent atoms, with N–H = 0.86 Å and C–H = 0.93 and 0.97 Å for aromatic and methylene H atoms, respectively. The  $U_{iso}(H)$  values were set equal to  $1.2U_{eq}(C,N)$ .

Data collection: COLLECT (Nonius, 1999); cell refinement: EvalCCD (Duisenberg *et al.*, 2003); data reduction: EvalCCD; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

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