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

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.037
wR factor = 0.102
Data-to-parameter ratio = 10.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_9H_{10}N_4OS$, the whole molecule is almost planar, with a dihedral angle of 6.9 (1)° between the planes of the triazole and phenyl rings. The molecules are interconnected into a three-dimensional network *via* intermolecular interactions.

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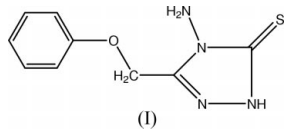
Comment

In recent years, much attention has been focused on the 1,2,4-triazole group, which exhibits fungicidal and plant-growth regulating activities, and which shows antibacterial activity against the *Puccinia* recondite and root-growth regulation for cucumber (Zhao *et al.*, 1998). Derivatives of 1,2,4-triazole containing the 3-aryloxymethyl moiety possess strong biological activities (Shi *et al.*, 2001). In this paper, we report the crystal structure of the title compound, (I) (Fig. 1).



(I)

The bond lengths and angles in (I) are comparable with those observed in related structures (Puviarasan *et al.*, 1999; Govindasamy *et al.*, 1999). The N2—C2 [1.294 (2) Å] bond shows double-bond character, while the other N—C bonds have a character intermediate between single and double (Table 1). The C2—C3 bond [1.487 (3) Å] is longer than the corresponding values in previous structures [1.476 (2) and 1.474 (3) Å], because of π-conjugation effects in the latter. The triazole ring is planar, with atoms N4 and S1 twisted from the plane by 0.017 (1) and 0.037 (8) Å, respectively. The N4—N1—C2—C3 and N4—N1—C1—S1 torsion angles are −1.1 (3) and 1.7 (3)°, respectively. The whole molecule is almost planar, with a dihedral angle of 6.9 (1)° between the planes of the triazole and phenyl rings.

In the crystal structure of (I), the molecules are interconnected into columns by C6—H6···N2 and N4—

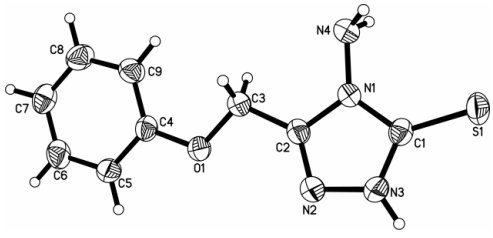


Figure 1
View of (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme.

H1N4···S1 hydrogen bonds (Fig. 2). Weak intermolecular N4—H2N4···N2 and N3—H1N3···S1 interactions link these columns to form a three-dimensional network (Table 2).

Experimental

The title compound was prepared according to the literature method of Zhang *et al.* (1993). The solid product was collected by filtration and single crystals of (I) suitable for crystallographic analysis were obtained by slow evaporation of the filtrate at room temperature.

Crystal data

$C_9H_{10}N_4OS$	D_x = 1.468 Mg m^{-3}
M_r = 222.27	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 1851 reflections
a = 11.251 (2) Å	θ = 1.6–25.0°
b = 6.0066 (12) Å	μ = 0.30 mm^{-1}
c = 15.148 (3) Å	T = 293 (2) K
β = 100.69 (3)°	Block, colourless
V = 1006.0 (3) Å^3	0.34 × 0.22 × 0.18 mm
Z = 4	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	1756 independent reflections
	1559 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.0083
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 25.0°
	$h = -13 \rightarrow 0$
T_{min} = 0.905, T_{max} = 0.948	$k = -7 \rightarrow 0$
3507 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 0.5065P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.037	
$wR(F^2)$ = 0.102	
S = 1.09	$(\Delta/\sigma)_{max} < 0.001$
1756 reflections	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
176 parameters	$\Delta\rho_{min}$ = −0.34 e Å^{-3}
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å, °).

S1—C1	1.6815 (18)	N2—C2	1.294 (2)
N1—C1	1.366 (2)	N2—N3	1.391 (2)
N1—C2	1.372 (2)	N3—C1	1.338 (3)
N1—N4	1.399 (2)	C2—C3	1.487 (3)
C1—N1—C2	108.99 (15)	N3—C1—S1	129.88 (14)
C1—N1—N4	128.50 (15)	N1—C1—S1	127.30 (15)
C2—N1—N4	122.45 (15)	N2—C2—N1	111.02 (16)
C2—N2—N3	103.57 (15)	N2—C2—C3	128.86 (17)
C1—N3—N2	113.54 (15)	N1—C2—C3	120.12 (16)
N3—C1—N1	102.81 (15)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H1N3···S1^{i}	0.88 (2)	2.59 (2)	3.3882 (18)	151 (2)
N4—H1N4···S1^{ii}	0.94 (3)	2.77 (3)	3.452 (2)	130 (3)
N4—H2N4···N2^{iii}	0.86 (3)	2.32 (3)	3.150 (3)	162 (2)
C6—H6···N2^{iv}	0.94 (2)	2.60 (2)	3.381 (3)	141 (2)

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

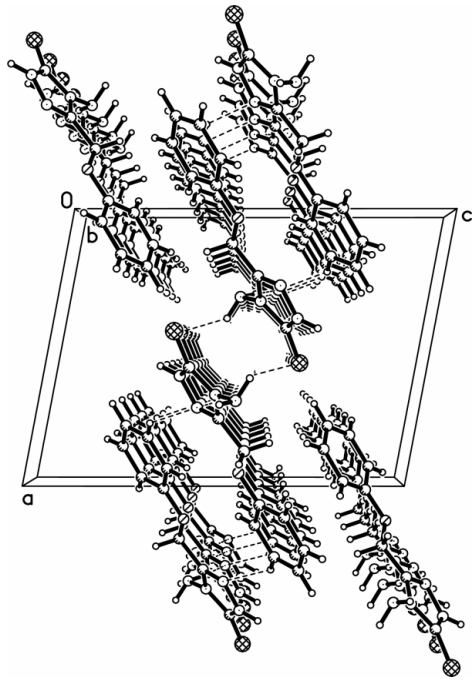


Figure 2
Packing diagram of the title compound, showing the columns of molecules. Hydrogen bonds are indicated by dashed lines.

All H atoms were located in a difference Fourier map and refined isotropically.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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