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2-(4-Methylbenzoyl)-*N*-phenyl-2-(1*H*-1,2,4-triazol-1-yl)ethanethioamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.134
Data-to-parameter ratio = 18.3

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

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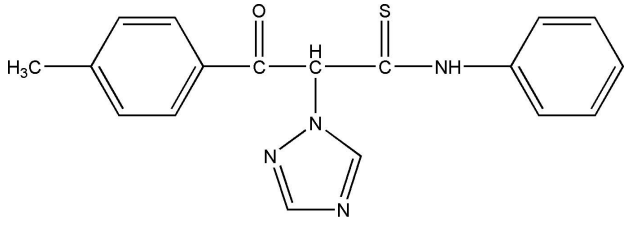
The title compound, $C_{18}H_{16}N_4OS$, crystallizes in space group $P2_1/n$ with two independent molecules in the asymmetric unit. The bond lengths and angles in both molecules are within normal ranges. There are some weak intermolecular hydrogen-bond interactions in the crystal structure, providing stabilization.

Comment

As a type of fungicide, triazole compounds are highly efficient, of low toxicity, low inward absorbence (Xu *et al.*, 2004), and show plant growth regulator activities (Xu *et al.*, 2002). Owing to their important biological activities, these compounds have received a great deal of attention in respect of their syntheses and in the elucidation of their crystal structures. In the search for new triazole compounds with higher biological activities, the title compound, (I), was synthesized.



(I)

Compound (I) crystallizes with two independent molecules in the asymmetric unit (Fig. 1). The bond lengths and angles in both molecules are in agreement with those reported for similar compounds with benzene and triazole rings (Jian *et al.*, 2004). The C=S distance is 0.03 Å shorter than the mean value of 1.660 Å reported by Allen *et al.* (1987). Atoms C2 and C20 lie in the planes of the N2/N3/C18/N4/C17 and N6/N7/C36/N8/C35 triazole rings, respectively. Atoms N1 and N5 lie in the plane of the C11–C16 and C29–C34 benzene rings, respectively.

The most interesting structural feature is the occurrence of weak intermolecular hydrogen-bond interactions involving atoms N4 and N8 of the triazole rings, resulting in the formation of zigzag chains parallel to the *b* axis (Table 2 and Fig. 2).

Experimental

The title compound was prepared by the reaction of 1-*p*-tolyl-2-(1*H*-1,2,4-triazol-1-yl)ethanone (4.02 g, 0.02 mol), phenyl isothiocyanate (2.24 g, 0.02 mol) and potassium hydroxide (2.24 g, 0.04 mol) in 1,4-dioxane solution (30 ml) at room temperature. Single crystals of the

title compound suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Crystal data

$C_{18}H_{16}N_4OS$	D_x = 1.351 Mg m^{-3}
M_r = 336.41	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 2352 reflections
a = 16.151 (2) Å	θ = 2.2–21.0°
b = 11.9923 (14) Å	μ = 0.21 mm^{-1}
c = 18.094 (2) Å	T = 293 (2) K
β = 109.261 (2)°	Block, yellow
V = 3308.4 (7) Å^3	0.22 × 0.18 × 0.16 mm
Z = 8	

Data collection

Bruker SMART CCD area-detector diffractometer	7912 independent reflections
φ and ω scans	4310 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.043
T_{min} = 0.939, T_{max} = 0.967	θ_{max} = 27.9°
21 974 measured reflections	$h = -13 \rightarrow 21$
	$k = -15 \rightarrow 15$
	$l = -23 \rightarrow 21$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0569P)^2 + 0.1446P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.049	
$wR(F^2)$ = 0.134	
S = 1.01	$(\Delta/\sigma)_{max} < 0.001$
7912 reflections	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
433 parameters	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
H-atom parameters constrained	Extinction correction: none

Table 1
Selected geometric parameters (Å, °).

S1—C1	1.6308 (19)	N5—C19	1.331 (2)
S2—C19	1.638 (2)	N5—C29	1.428 (3)
N1—C1	1.328 (2)	O1—C3	1.212 (2)
N1—C11	1.430 (2)	O2—C21	1.212 (2)
C1—N1—C11	124.61 (16)	C2—C1—S1	120.13 (14)
C19—N5—C29	128.97 (17)	N5—C19—S2	127.58 (16)
N1—C1—S1	127.15 (15)	C20—C19—S2	118.43 (14)
C11—N1—C1—C2	−177.16 (18)	C29—N5—C19—S2	2.2 (3)
C11—N1—C1—S1	3.6 (3)	C35—N6—C20—C21	−40.3 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N4^{i}	0.86	2.20	3.012 (2)	158
C2—H2A···N4^{i}	0.98	2.58	3.487 (3)	153
N5—H5A···N8^{ii}	0.86	2.26	3.117 (2)	174
C20—H20A···N8^{ii}	0.98	2.79	3.686 (3)	152

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

All H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.98 Å and N—H distances fixed at 0.86 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2U_{eq}(parent atom).

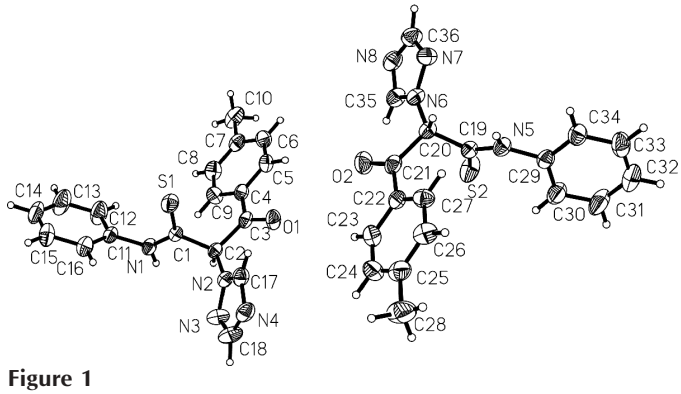


Figure 1
View of the asymmetric unit of the title compound, (I), with displacement ellipsoids drawn at the 40% probability level.

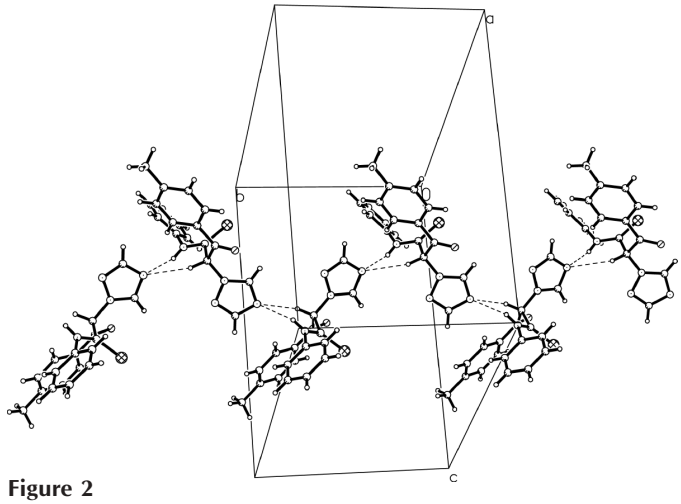


Figure 2
Packing in (I), showing the hydrogen-bonding interactions (dashed lines) involving one independent molecule.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans.* 2, pp. S1–19.

Bruker (1998). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (1999). *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

Jian, F. F., Xiao, H. L., Qin, Y. Q. & Xu, L. Z. (2004). *Acta Cryst.* C**60**, o492–o493.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Xu, L. Z., Jian, F. F., Shi, J. G., Sun, P. P.& Jiao, K. (2004). *Chin. J. Chem.* **22**, 698–701.

Xu, L. Z., Jiao, K., Zhang, S. S. & Kuang, S. P. (2002). *Bull. Korean Chem. Soc.* **23**, 1699–1701.