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3′-Methyl-2-[5-(4-methylphenoxymethyl)-4-phenyl-4*H*-1,2,4-triazol-5-ylsulfanyl]-acetanilide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.113
Data-to-parameter ratio = 15.3

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

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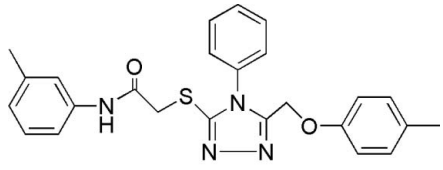
In the crystal structure of the title compound, $C_{25}H_{24}N_4O_2S$, intermolecular N—H···N and C—H···N hydrogen bonds and C—H···π interactions link the molecules into a two-dimensional network parallel to the *bc* plane.

Comment

During the last few decades, considerable attention has been devoted to 1,2,4-triazole derivatives because of their comprehensive bioactivities, such as antimicrobial (Gulerman *et al.*, 2001), anti-inflammatory (Maxwell *et al.*, 1994), analgesic (Turan *et al.*, 1999), antitumor (Demirbas & Demirbas, 2002), antihypertensive (Paulvannan *et al.*, 2000), anticonvulsant (Husain *et al.*, 1987) and antiviral activities (Kritsanida *et al.*, 2002). The broad biological activities that the 1,2,4-triazoles show may be due to the presence of the N═C—S unit (Omar *et al.*, 1986). In a continuation of our previous work on the syntheses and biological activities of 1,2,4-triazole derivatives (Liu *et al.*, 2006), we report here the synthesis and crystal structure of the title compound, (I) (Fig. 1).



(I)

The triazole ring, the C1–C6 benzene ring, the C12–C17 phenyl ring and the C19–C24 benzene ring are planar, with r.m.s. deviations of 0.006, 0.003, 0.004 and 0.008 Å, respectively. The C1–C6, C12–C17 and C19–C24 planes form dihedral angles of 29.7 (1), 79.2 (1) and 70.4 (1)°, respectively, with the N1–N3/C10/C11 plane.

Two types of hydrogen bonds, *viz*. N—H···N and C—H···N, and C—H···π interactions involving the C1–C6

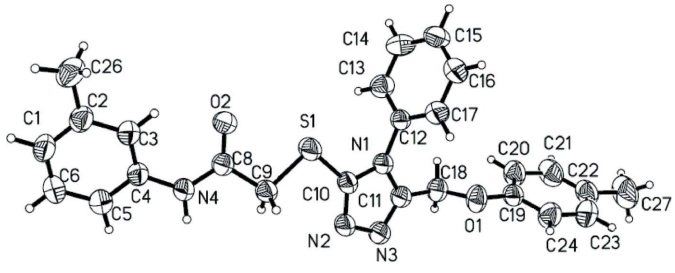


Figure 1
A plot of (I), with displacement ellipsoids drawn at the 50% probability level.

benzene ring are observed in the crystal structure (Table 1 and Fig. 2). The hydrogen bonds link the molecules into a two-dimensional network parallel to the *bc* plane (Fig. 3).

Experimental

N-(3-Methylphenyl)-2-chloroacetanilide (3 mmol) was added to a solution of 3-(4-methylphenoxymethyl)-4-phenyl-1,2,4-triazole (3 mmol) in ethanol (15 ml) and NaOH (3 mmol), and the mixture was refluxed for 1.5 h. After the mixture had been cooled to room temperature, the crude product was filtered and washed with distilled water (3 × 10 ml). Pure compound (I) was obtained by recrystallization from ethanol. Colourless single crystals were obtained by slow evaporation of an ethanol solution of (I) after about two weeks.

Crystal data

$C_{25}H_{24}N_4O_2S$
M_r = 444.54
Monoclinic, $P2_1/c$
a = 16.8947 (18) Å
b = 8.2884 (9) Å
c = 17.2401 (17) Å
β = 106.382 (4)°
V = 2316.1 (4) Å^3
Z = 4
D_x = 1.275 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 294 (2) K
Block, colourless
0.30 × 0.27 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*, Bruker, 1998)
T_{min} = 0.951, T_{max} = 0.972
13217 measured reflections
4892 independent reflections
3186 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 26.7°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.113
S = 1.12
4892 reflections
320 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.048P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0027 (8)

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C1–C6 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···N3^{i}	0.89 (2)	2.09 (2)	2.982 (2)	176 (2)
C14—H14···N2^{ii}	0.93	2.62	3.329 (3)	134
C17—H17···*Cg*1^{iii}	0.93	2.72	3.508 (2)	143

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

Atoms H1, H3–H6, H9*A* and H9*B* were located in a difference map and were refined isotropically [N—H = 0.89 (2) Å and C—H = 0.94 (2)–0.99 (2) Å]. The remaining H atoms were positioned geometrically, with C—H distances in the range 0.93–0.97 Å, and refined using a riding model, with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for the other H atoms.

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

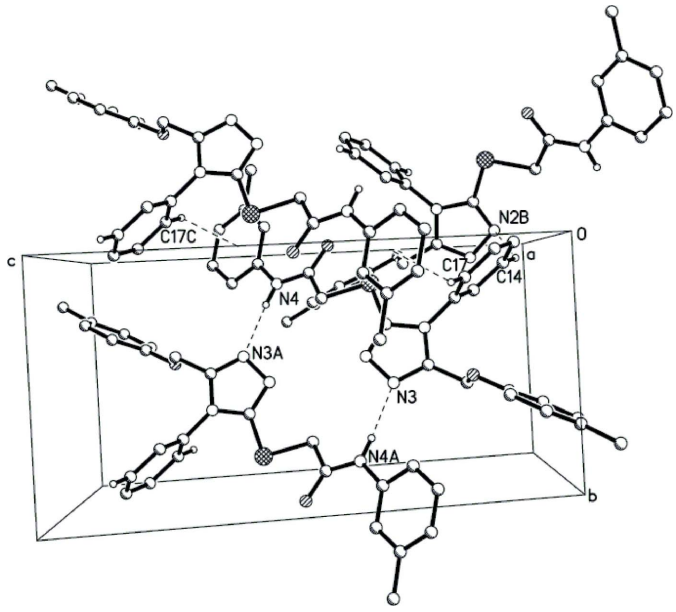


Figure 2
Part of the crystal structure of (I), showing N—H···N, C—H···N and C—H···π interactions as dashed lines. Only the H atoms involved in the interactions are shown. Atoms labelled with the suffixes *A*, *B* and *C* are generated by the symmetry operations $(1-x, 1-y, 1-z)$, $(1-x, -\frac{1}{2}+y, \frac{1}{2}-z)$ and $(1-x, -y, 1-z)$, respectively.

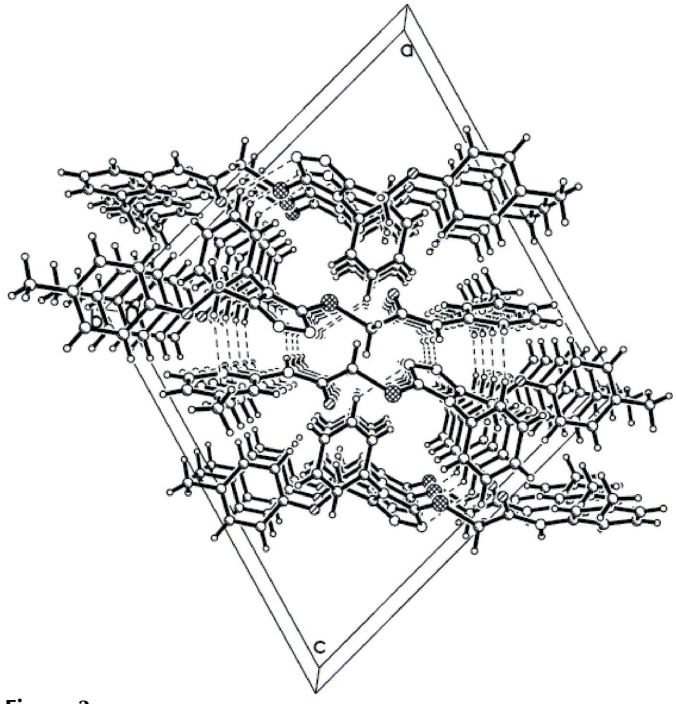


Figure 3
The crystal structure of (I). Hydrogen bonds are shown as dashed lines.

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