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1-(4-Fluorophenyl)-2-{4-phenyl-5-[(1*H*-1,2,4-triazol-1-yl)methyl]-4*H*-1,2,4-triazol-3-ylsulfanyl}ethanone

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.102
Data-to-parameter ratio = 15.1

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

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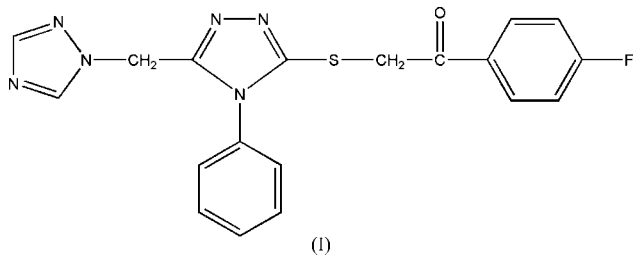
The crystal structure of the title compound, $C_{19}H_{15}FN_6OS$, is stabilized by a weak intermolecular C—H···N hydrogen-bond interaction.

Comment

The triazole motif appears frequently in the structures of various natural products and biologically active compounds. Some 1,4-disubstituted thiosemicarbazide, 1,2,4-triazoline-3-thione and 1,2,4-triazole-3-thiole derivatives are of interest because of their bioactivities, including antibacterial (Goswami *et al.*, 1984), antifungal (Eid *et al.*, 1994) and antitubercular (Kalyoncuoğlu *et al.*, 1992) properties.



(I)

In the title molecule, (I), atoms S1, N4, N5, N6, C4 and C5 are coplanar (plane *p*1). Atom C3 lies in the plane of the triazole ring (N1/N2/N3/C1/C2; plane *p*2). The dihedral angles formed by the C6–C11 phenyl ring, the C14–C19 benzene ring and *p*2 with *p*1 are 85.22 (9), 38.03 (7) and 86.82 (8)°, respectively. There is a weak C—H···N intermolecular hydrogen-bond interaction stabilizing the crystal structure (Table 2).

Experimental

A mixture of 5-[(1*H*-1,2,4-triazol-1-yl)methyl]-4-phenyl-2*H*-1,2,4-triazole-3(4*H*)-thione (0.01 mol), 2-chloro-1-(4-fluorophenyl)-ethanone (0.01 mol) and potassium carbonate (0.01 mol) was stirred in acetone (30 ml) for 4 h at 327 K to afford the title compound (3.03 g, yield 76.8%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Crystal data

$C_{19}H_{15}FN_6OS$
M_r = 394.43
Monoclinic, $P2_1/c$
a = 11.838 (3) Å
b = 14.976 (3) Å
c = 10.611 (3) Å
β = 95.996 (4)°
V = 1870.9 (8) Å^3
Z = 4
D_x = 1.400 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2159 reflections
θ = 2.8–22.4°
μ = 0.21 mm^{-1}
T = 294 (2) K
Block, colourless
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.951, T_{max} = 0.964
10428 measured reflections
3823 independent reflections
2178 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 26.4°
$h = -14 \rightarrow 14$
$k = -18 \rightarrow 13$
$l = -11 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.102
S = 1.00
3823 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0323P)^2 + 0.5833P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C5	1.742 (2)	N3—C3	1.452 (3)
S1—C12	1.806 (2)	N4—C6	1.436 (3)
C5—S1—C12	97.37 (11)	N4—C5—S1	121.22 (16)
N3—C3—C4	111.99 (17)	C7—C6—N4	119.1 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12B···N1^{i}	0.97	2.44	3.400 (3)	171

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

All H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, and included in the final cycles of refinement using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

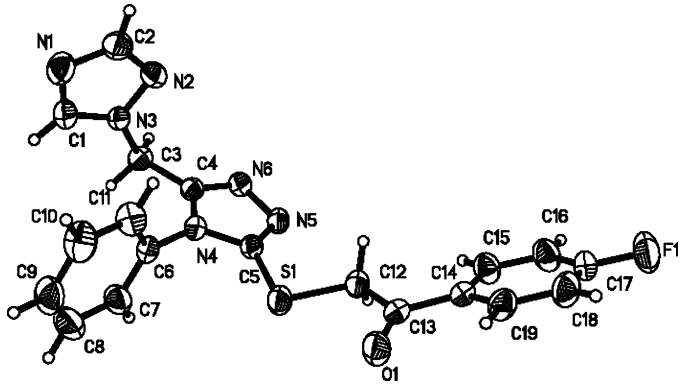


Figure 1
View of the title compound, with displacement ellipsoids drawn at the 40% probability level.

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*.

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