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2-(2-Fluoro-5-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) = 0.005 Å
R factor = 0.064
wR factor = 0.110
Data-to-parameter ratio = 15.5

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

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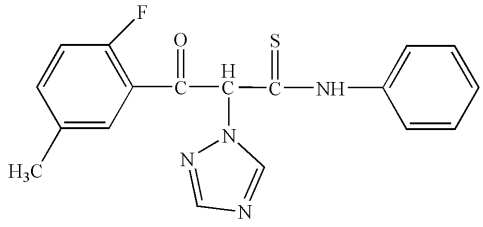
The structure of the title compound, $C_{18}H_{15}FN_4OS$, is stabilized by hydrogen-bonding interactions between the NH group and one of the triazole N atoms of a symmetry-related molecule, resulting in chains parallel to the *b* axis.

Comment

Recently, compounds containing the 1*H*-1,2,4-triazole group have attracted much interest owing to their fungicidal and plant-growth-regulating activities (Xu *et al.*, 2002), as well as their antibacterial activity against *Puccinia recondite* and root-growth regulation for cucumber (Zhao *et al.*, 1998). In order to search for new triazole compounds with higher bioactivity, we synthesized and characterized the title compound, (I) (Fig. 1).



(I)

The bond lengths and angles in (I) agree with those reported in other phenyl and triazole rings (Ji *et al.*, 2002). The C—S bond length is close to the typical C=S bond length. The C—F bond length [1.361 (4) Å] is typical of values found in a related compound with fluorine attached to a benzene ring

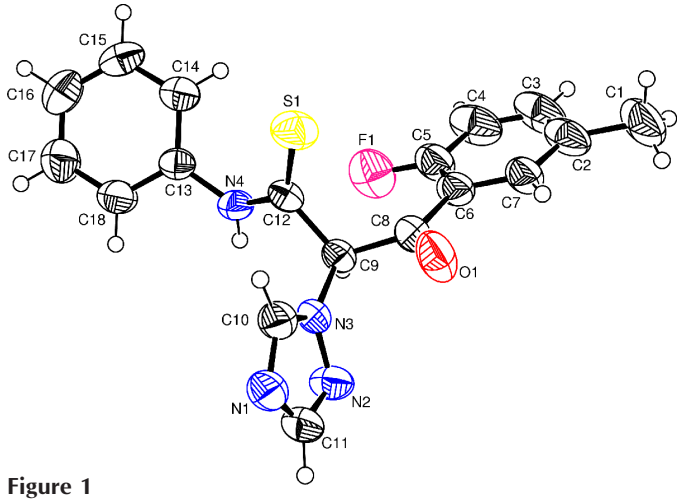


Figure 1
A molecular view (*ORTEP*-3; Farrugia, 1997) of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

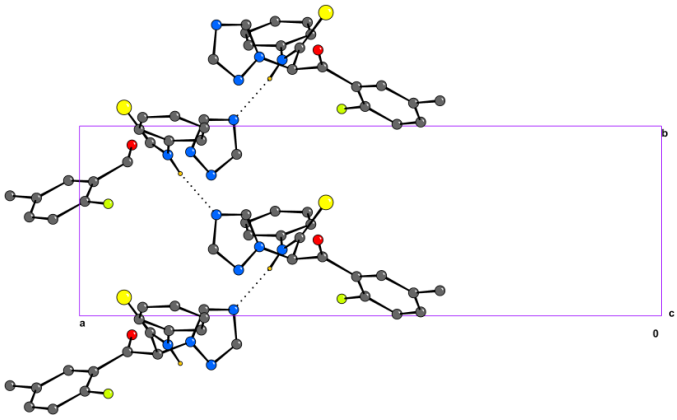


Figure 2
Part of the packing in (I) (*CAMERON*; Watkin *et al.*, 1993), showing the N—H···N hydrogen-bonding interactions as dashed lines.

[1.363 (7) Å and 1.355 (6) Å in $C_{13}H_{13}F_2IO_3$ (Mark *et al.*, 2001)]. The carbonyl group is coplanar with the C2—C7 benzene ring (*p*1). The five atoms S1/C9/C12/C13/N4 lie in a plane (*p*2). The dihedral angles formed by the C13—C18 benzene ring and triazole ring with *p*1 and *p*2 are 57.4 (3)/89.8 (6) and 42.1 (3)/83.9 (0)°, respectively.

The most interesting structural feature of (I) is the occurrence of an N—H···N interaction between the NH group and one of the triazole N atoms of a symmetry-related molecule, resulting in the formation of chains parallel to the *b* axis (Table 2 and Fig. 2).

Experimental

The title compound was prepared by reaction of 1-(2-fluoro-5-methylphenyl)-2-(1*H*-1,2,4-triazol-1-yl)ethanone (4.14 g, 0.02 mol), phenyl isothiocyanate (2.24 g, 0.02 mol) and potassium hydroxide (2.24 g, 0.04 mol) in dimethyl sulfoxide solution (30 ml) at room temperature. Single crystals of the title compound suitable for X-ray measurements were obtained by recrystallization from chloroform/ethyl acetate (1:3 *v*/*v*) at room temperature.

Crystal data

$C_{18}H_{15}FN_4OS$
M_r = 354.40
Monoclinic, $C2/c$
a = 23.939 (5) Å
b = 7.1430 (14) Å
c = 22.029 (4) Å
β = 113.73 (3)°
V = 3448.4 (14) Å^3
Z = 8
D_x = 1.365 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 20 reflections
θ = 2–11°
μ = 0.21 mm^{-1}
T = 293 (2) K
Block, yellow
0.25 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.951, T_{max} = 0.963
9580 measured reflections
3518 independent reflections
1620 reflections with $I > 2\sigma(I)$
R_{int} = 0.078
θ_{max} = 26.4°
$h = -29 \rightarrow 29$
$k = -8 \rightarrow 7$
$l = -26 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.110
S = 1.00
3518 reflections
227 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C12	1.650 (3)	N2—N3	1.362 (3)
F1—C5	1.361 (4)	N3—C10	1.316 (3)
O1—C8	1.203 (3)	N3—C9	1.456 (3)
N1—C10	1.323 (3)	N4—C12	1.325 (3)
N1—C11	1.341 (3)	N4—C13	1.427 (3)
N2—C11	1.311 (3)		
C10—N1—C11	101.8 (3)	N2—N3—C9	119.7 (2)
C11—N2—N3	101.7 (2)	C12—N4—C13	128.7 (2)
C10—N3—N2	109.5 (2)	C12—N4—H4	115.7
C10—N3—C9	130.6 (3)	C13—N4—H4	115.7
C14—C13—N4—C12	44.3 (4)	N2—N3—C9—C8	−87.1 (3)
N2—N3—C9—C12	149.4 (2)	N3—C9—C8—C6	163.4 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···N1^{i}	0.86	2.07	2.922 (3)	172

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

The H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H distances in the range 0.93–0.98 Å and U_{iso}(H) = 1.2 and 1.5 times U_{eq} of the parent atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97; molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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