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(4-Fluorobenzoyl)(1*H*-1,2,4-triazol-1-yl)methyl morpholine-4-carbodithioate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.053
wR factor = 0.112
Data-to-parameter ratio = 15.9

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

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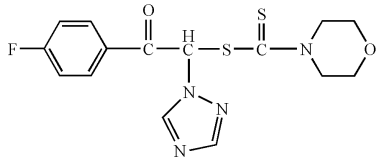
In the title compound, $C_{15}H_{15}FN_4O_2S_2$, the morpholine ring adopts a chair conformation. The dihedral angle between the benzene and triazole rings is 77.1 (7)°. There are some weak intermolecular and intramolecular interactions in the crystal structure, providing stabilization.

Comment

As an important type of fungicide, triazole compounds are highly efficient and of low toxicity (Shi *et al.*, 1995; Xu *et al.*, 2002). At present, studies on triazole derivatives are mainly concentrated on compounds with triazole as the only active group. Morpholine, a heterocyclic xenobiotic compound, is used for various industrial purposes. Some compounds containing the morpholine group possess highly fungicidal and insecticidal activity. However, reports of compounds that contain both the triazole and morpholine groups in a single molecule have rarely been found. Considering that triazole compounds have a different fungicidal mechanism from that of morpholine compounds, it is possible that the two kinds of *N*-heterocyclic groups increase the fungicidal activity. We report here the crystal structure of the title compound, (I).



(I)

In (I), the bond lengths and angles in the 1,2,4-triazole and benzene rings are generally normal (Ji *et al.*, 2002). The bond lengths and angles in the morpholine ring are also in good agreement with an earlier report (Fridman *et al.*, 2003). The C—F bond length is similar to that found by Lynch & McClenaghan (2004) [1.340 (3)–1.345 (3) Å]. The morpholine ring adopts a chair conformation. The dihedral angles formed by the benzene and triazole rings with the S1/S2/N4/C11 plane are 68.3 (1) and 70.0 (2)°, respectively. The dihedral angle between the benzene and triazole rings is 77.1 (7)°.

There are weak intermolecular and intramolecular hydrogen-bond interactions stabilizing the structure (Table 2).

Experimental

The title compound was prepared by reaction of β-(1*H*-1,2,4-triazol-1-yl)-4-fluoroacetophenone (20.5 g, 0.1 mol), CS_2 (7.6 g, 0.1 mol), $NH_3{\cdot}H_2O$ (25%, 17 g, 0.25 mol) and morpholine (8.7 g, 0.1 mol) in chloroform at room temperature. Single crystals of the title compound suitable for X-ray measurements was obtained by recrystallization from chloroform at room temperature.

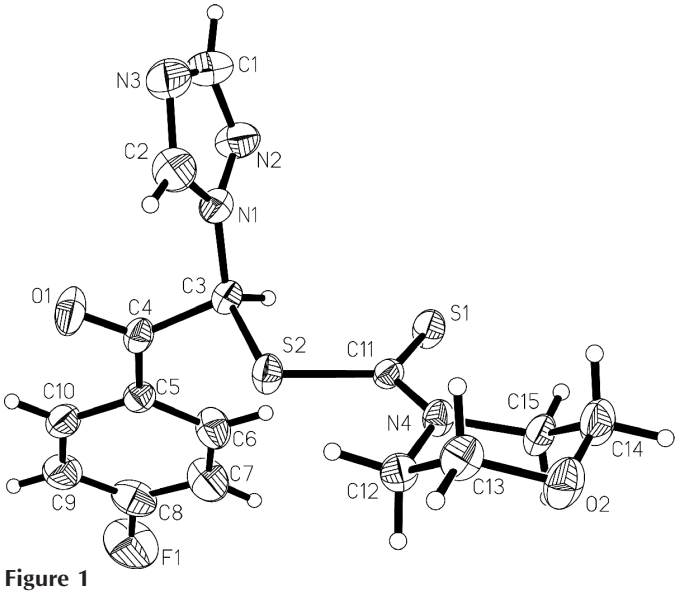


Figure 1
The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Table 1
Selected geometric parameters (Å, °).

F1—C8	1.350 (4)	O2—C14	1.411 (3)
S1—C11	1.654 (3)	O2—C13	1.417 (3)
S2—C11	1.794 (3)	N4—C11	1.325 (3)
S2—C3	1.805 (3)	N4—C12	1.469 (3)
O1—C4	1.211 (3)	N4—C15	1.476 (3)
C14—O2—C13	109.5 (2)	C11—N4—C15	121.8 (2)
C11—N4—C12	125.1 (2)	C12—N4—C15	112.2 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*A*···S1	0.98	2.53	3.127 (3)	119
C12—H12*A*···S2	0.97	2.35	2.881 (3)	114
C12—H12*A*···N2^{i}	0.97	2.60	3.283 (4)	128
C15—H15*B*···S1	0.97	2.59	3.062 (3)	110

Symmetry code: (i) $1+x, y, z$.

Crystal data

$C_{15}H_{15}FN_4O_2S_2$	$Z = 2$
$M_r = 366.45$	$D_x = 1.435$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.508$ (2) Å	Cell parameters from 20 reflections
$b = 7.605$ (2) Å	$\theta = 2$–11°
$c = 16.271$ (3) Å	$\mu = 0.34$ mm^{-1}
$\alpha = 79.23$ (3)°	$T = 293$ (2) K
$\beta = 81.42$ (3)°	Block, yellow
$\gamma = 68.91$ (3)°	0.20 × 0.20 × 0.18 mm
$V = 848.1$ (4) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	2060 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.029$
ω scans	$\theta_{max} = 26.4°$
Absorption correction: none	$h = -9 \rightarrow 9$
4932 measured reflections	$k = -9 \rightarrow 8$
3441 independent reflections	$l = -11 \rightarrow 20$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.053$	$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.112$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.31$ e Å^{-3}
3441 reflections	$\Delta\rho_{min} = -0.20$ e Å^{-3}
217 parameters	

H atoms were positioned geometrically and treated as riding on their parent C atoms, with C—H distances in the range 0.93–0.97 Å and with $U_{iso} = 1.2U_{eq}$(C).

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 (Sheldrick, 1997); molecular graphics: *SHELXTL/>PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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