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2-(2-Fluoro-5-methylphenyl)-2-oxo-1-(1*H*-1,2,4-triazol-1-yl)ethyl morpholine-4-carbodithioate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.054
wR factor = 0.138
Data-to-parameter ratio = 15.0

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

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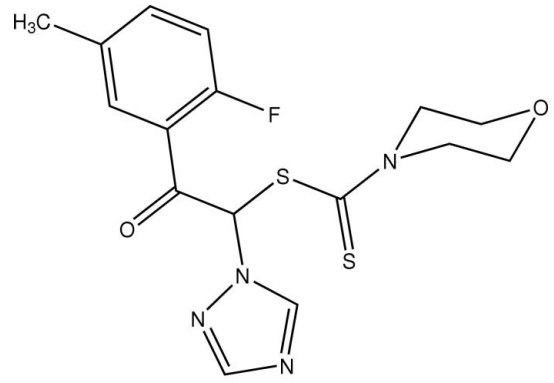
In the title compound, $C_{16}H_{17}FN_4O_2S_2$, molecules are linked into ribbons parallel to the *b* axis by C—H···O and C—H···N hydrogen bonds. The packing is further stabilized by π–π interactions involving the fluoromethylphenyl rings into two-dimensional layers in the *bc* plane.

Comment

We have recently reported the structure of 2-(4-chlorophenyl)-2-oxo-1-(1*H*-1,2,4-triazol-1-ylmethyl)ethyl morpholine-4-carbodithioate, (II) (Wang *et al.*, 2005). As part of our ongoing studies of triazole compounds, the title compound, (I), has been synthesized and its structure is reported here (Fig. 1 and Table 1).



(I)

The bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987), and are comparable to the corresponding

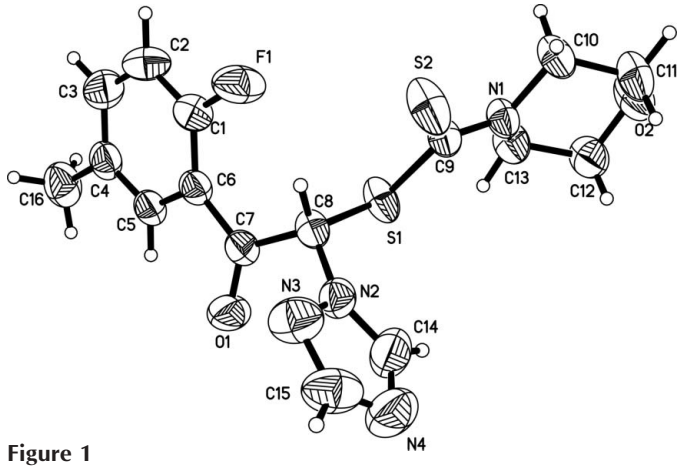


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

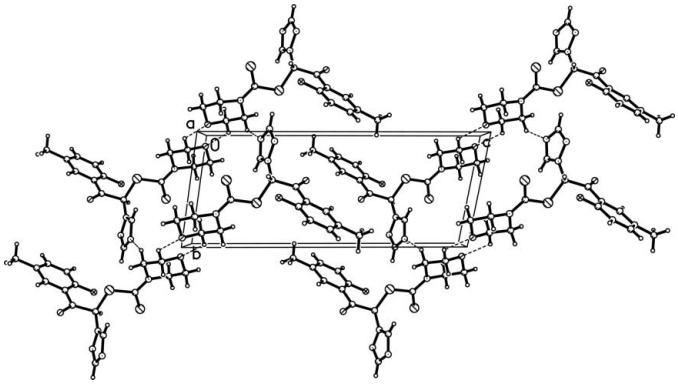


Figure 2
A view down the *a* axis, showing the ribbons along the *b* axis and π–π interactions. Hydrogen bonds are indicated by dashed lines.

values in (II). The dihedral angle between the C1–C6 and N2–N4/C14/C15 rings is 79.0 (2)°. The morpholine ring adopts a chair conformation, and atom S2 is synperiplanar with respect to C8, the C8—S1—C9—S2 torsion angle being −7.4 (2)°. In the crystal structure, molecules are linked into ribbons parallel to the *b* axis (Fig. 2) by C12—H12*B*···O2 and C13—H13*A*···N4 hydrogen bonds (Table 2). π–π stacking interactions involving the C1–C6 benzene rings [centroid *Cg*; $Cg\cdots Cg(1-x, 1-y, 1-z)$ = 3.652 Å] further stabilize the packing, forming two-dimensional layers in the *bc* plane.

Experimental

The title compound was prepared by the method of Wan *et al.* (2005). Single crystals suitable for an X-ray diffraction study were obtained by slow evaporation of an ethyl acetate–alcohol (1:1 *v*/*v*) solution over a period of one week.

Crystal data

$C_{16}H_{17}FN_4O_2S_2$
M_r = 380.46
Triclinic, $P\overline{1}$
a = 6.7311 (13) Å
b = 7.7910 (15) Å
c = 18.107 (4) Å
α = 98.200 (3)°
β = 92.649 (4)°
γ = 109.900 (3)°
V = 879.1 (3) Å^3
Z = 2
D_x = 1.437 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1446 reflections
θ = 2.3–25.9°
μ = 0.33 mm^{-1}
T = 293 (2) K
Plate, colourless
0.29 × 0.21 × 0.09 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.910, T_{max} = 0.971
4955 measured reflections
3385 independent reflections
2534 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 26.0°
$h = -8 \rightarrow 7$
$k = -9 \rightarrow 9$
$l = -16 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.138
S = 1.06
3385 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.3536P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C9	1.797 (3)	F1—C1	1.361 (3)
S1—C8	1.799 (3)	O1—C7	1.208 (3)
S2—C9	1.660 (3)		
N2—C8—C7	110.2 (2)	C7—C8—S1	105.23 (18)
N2—C8—S1	112.22 (18)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12*B*···O2^{i}	0.97	2.53	3.207 (4)	127
C13—H13*A*···N4^{ii}	0.97	2.50	3.267 (5)	135

Symmetry codes: (i) $-x, -y+2, -z$; (ii) $x+1, y+1, z$.

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å and with U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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