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3-[(4-Fluorophenyl)methylenehydrazinocarbonyl]-1*H*-1,2,4-triazole monohydrate

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.007 Å
R factor = 0.057
wR factor = 0.189
Data-to-parameter ratio = 12.1

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

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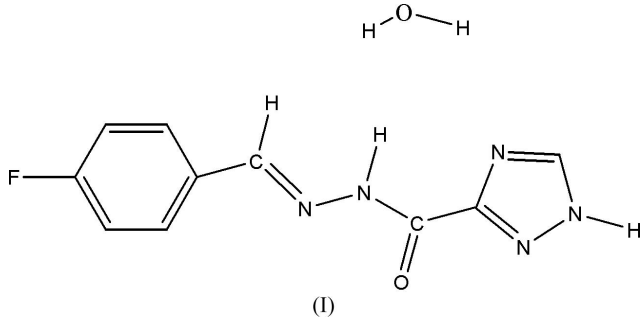
The title compound, $C_{10}H_8FN_5O\cdot H_2O$, was synthesized by the reaction of (1*H*-1,2,4-triazol-3-yl)hydrazine with 4-fluorobenzaldehyde in ethanol. The molecule is almost planar and in the crystal structure screw-related molecules are linked by N—H···O and N—H···N hydrogen bonds to form chains along the *b* axis. The chains are interlinked by the water molecules *via* O—H···N hydrogen bonds.

Comment

Azole derivatives, such as derivatives of pyrazole, imidazole, triazole (including benzotriazole), tetrazole, indole, *etc*., exhibit extensive biological activities. They have become a central focus in the study of agricultural chemicals, medicine, adjustment reagents for plant growth, and so on (Haddock & Hopwood, 1982). A Schiff base is a good type of biologically active substructure and one study of a triazole Schiff base has been reported (Sauter *et al.*, 1991). The hydrazonecarbonyl group has also been shown to be bioactive (Zhi *et al.*, 2003). Some structures of triazole compounds containing the hydrazonecarbonyl group have been reported (Pan & Yang, 2005; Yang & Pan, 2004). In a search for more effective antibacterial medicines, we have synthesized the title compound, (I).



(I)

The title molecule (Fig. 1) is almost planar. The dihedral angle between the two aromatic rings is 12.8 (2)°. As a result of conjugation, the C=O distance [1.229 (5) Å] is longer than the normal value of 1.20 Å. The C8—N2 bond distance [1.328 (5) Å], however, is essentially the same as for a standard C=N double bond (1.32 Å; Dean, 1998).

In the asymmetric unit, the water molecule is linked to the triazole derivative through an N2—H2···O2 hydrogen bond. In the crystal packing, screw-related molecules are linked by N5—H5···O1^{i} and N5—H5···N3^{i} [symmetry code: (i) $1-x$, $-\frac{1}{2}+y$, $\frac{1}{2}-z$] hydrogen bonds to form chains along the *b* axis (Table 1). The chains are interlinked by the water molecules *via* O—H···N hydrogen bonds (Fig. 2).

Experimental

(1*H*-1,2,4-Triazol-3-yl)hydrazine (0.02 mol, 2.54 g) was dissolved in anhydrous ethanol (50 ml) at room temperature. 4-Fluorobenzaldehyde (0.02 mol, 3.08 g) was added and the mixture was refluxed for 2 h, yielding a precipitate which was collected by filtration and washed with ethanol. The product was recrystallized from ethanol and dried under reduced pressure to give the title compound. The latter compound, of which 2.0 mmol (0.47 g) was dissolved in dimethylformamide (30 ml) and kept at room temperature for 30 d, yielded colourless block-shaped single crystals which were washed with distilled water.

Crystal data

$C_{10}H_8FN_5O\cdot H_2O$
$M_r = 251.23$
Monoclinic, $P2_1/c$
$a = 21.394$ (2) Å
$b = 7.796$ (2) Å
$c = 6.918$ (2) Å
$\beta = 93.70$ (2)°
$V = 1151.4$ (5) Å^3
$Z = 4$
$D_x = 1.449$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 8.4$–12.5°
$\mu = 0.12$ mm^{-1}
$T = 295$ (2) K
Block, colourless
0.20 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
2623 measured reflections
2072 independent reflections
786 reflections with $I > 2\sigma(I)$
$R_{int} = 0.064$
$\theta_{max} = 25.2°$
$h = -25 \rightarrow 25$
$k = -9 \rightarrow 1$
$l = 0 \rightarrow 8$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.189$
$S = 1.01$
2072 reflections
171 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0903P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.006$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···N3^{i}	0.86	2.34	2.934 (5)	127
N5—H5···O1^{i}	0.86	2.11	2.913 (5)	155
N2—H2···O2	0.86	2.26	2.880 (5)	129
O2—H22···N1^{ii}	0.85 (1)	2.16 (2)	2.971 (5)	161 (6)
O2—H21···N4^{iii}	0.85 (1)	2.11 (2)	2.948 (5)	169 (6)

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

The water H atoms were located in a difference map and their parameters were refined with the O—H and H···H distances restrained to 0.85 (1) and 1.35 (2) Å, respectively. All other H atoms were placed in calculated positions and included in the refinement in the riding-model approximation [N—H = 0.86 Å, C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C,N)$].

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CAD-4 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

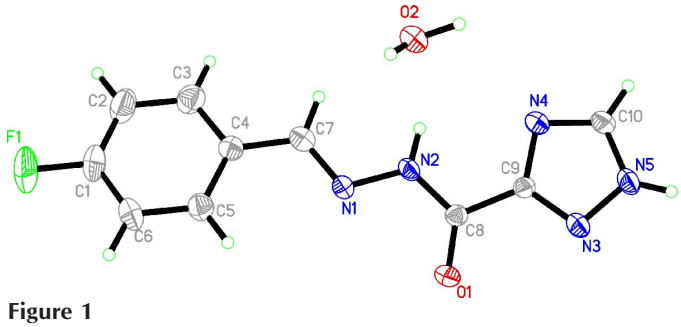


Figure 1
The structure of (I), showing the atomic numbering. Displacement ellipsoids are drawn at the 30% probability level.

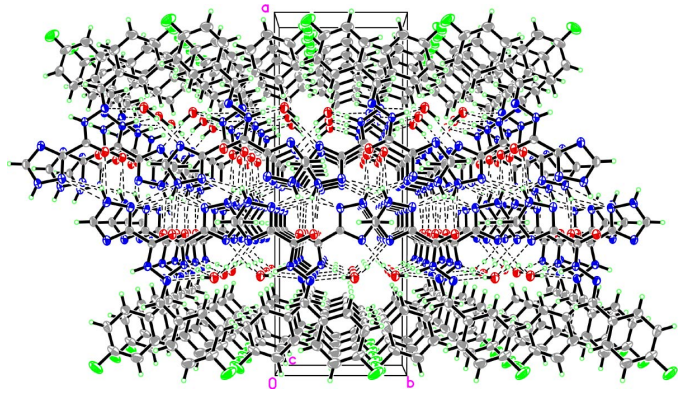


Figure 2
The packing of (I), viewed down the *c* axis, showing the intermolecular hydrogen bonds as dashed lines.

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References

Bruker (2002). *SMART* (Version 5.62), *SAINT* (Version 6.02), *SADABS* (Version 2.03) and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dean, J. A. (1998). *Lang's Handbook of Chemistry*, Vol. 4, pp. 39–41. New York: McGraw–Hill.
Enraf–Nonius (1989). *CAD-4 Software*. Enraf–Nonius, Delft, The Netherlands.
Haddock, E. & Hopwood, W. A.(1982). GB Patent No. 2 078 212.
Pan, F. Y. & Yang, J. G. (2005). *Acta Cryst.* E**61**, o63–o64.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sauter, H., Zierke, T., Reuther, W., Baus, U., Lorenz, G. & Ammermann, E. (1991). Eur. Patent No. 421 227.
Yang, J. G. & Pan, F. Y. (2004). *Acta Cryst.* E**60**, o2342–o2344.
Zhi, J. F., Bin, Z., Su, H. W. & Zheng, M. L. (2003). *Chin. J. App. Chem.* **20**, 365–367.