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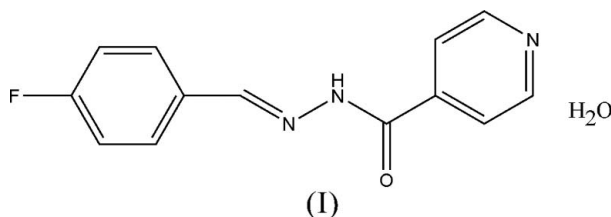
Key indicators

Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.037
 wR factor = 0.094
Data-to-parameter ratio = 8.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**(E)-N'-(4-Fluorobenzylidene)isonicotinohydra-
zide monohydrate**In the title molecule, $\text{C}_{13}\text{H}_{10}\text{FN}_3\text{O}\cdot\text{H}_2\text{O}$, the hydrazone group adopts a *trans* configuration with respect to the $\text{C}=\text{N}$ double bond. In the crystal structure, a two-dimensional network is formed *via* intermolecular $\text{O}-\text{H}\cdots\text{O}$, $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds.

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Comment

Schiff base compounds have been of great interest for many years. These compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions (Brunner *et al.*, 1983), magnetism and molecular architectures (Miller & Epstein, 2000).The molecular structure of the title compound, (I), is shown in Fig. 1. The hydrazone group adopts a *trans* configuration with respect to the $\text{C}=\text{N}$ double bond. All bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The dihedral angle between the benzene and pyridine rings is $11.5(2)^\circ$.In the crystal structure, a two-dimensional network, in the *ab* plane, is formed *via* intermolecular $\text{O}-\text{H}\cdots\text{O}$, $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds (Table 2 and Fig. 2).

Experimental

4-Fluorobenzaldehyde (0.2 mmol, 24.8 mg) and isonicotinohydra-
zide (0.2 mmol, 27.4 mg) were dissolved in methanol (15 ml). The mixture was stirred at room temperature for about 30 min and the resulting solution was set aside for 10 d to allow slow evaporation of the solvent. Large colourless block-shaped crystals of (I) separated from the solution; these were collected and washed three times with methanol.

Crystal data

 $\text{C}_{13}\text{H}_{10}\text{FN}_3\text{O}\cdot\text{H}_2\text{O}$
 $M_r = 261.26$
Orthorhombic, $P2_12_12_1$
 $a = 6.469(2)$ Å
 $b = 7.021(2)$ Å
 $c = 27.351(9)$ Å
 $V = 1242.3(7)$ Å³ $Z = 4$
 $D_x = 1.397$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 0.11$ mm⁻¹
 $T = 292(2)$ K
Block, colourless
 $0.30 \times 0.30 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	5749 measured reflections
φ and ω scans	1562 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1163 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.969$, $T_{\max} = 0.979$	$R_{\text{int}} = 0.029$
	$\theta_{\text{max}} = 27.0^\circ$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.037$	$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2]$
$wR(F^2) = 0.094$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1562 reflections	$\Delta\rho_{\text{max}} = 0.16 \text{ e } \text{\AA}^{-3}$
184 parameters	$\Delta\rho_{\text{min}} = -0.13 \text{ e } \text{\AA}^{-3}$

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N2-H1N\cdots O1W^i$	0.91 (2)	1.95 (2)	2.832 (3)	164 (2)
$O1W-H1WB\cdots O1^{ii}$	0.834 (10)	2.28 (2)	2.949 (2)	138 (3)
$O1W-H1WB\cdots N3^{ii}$	0.834 (10)	2.54 (2)	3.264 (3)	146 (3)
$O1W-H1WA\cdots N1^{iii}$	0.844 (10)	2.048 (13)	2.863 (3)	162 (2)

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

In the absence of significant anomalous dispersion effects, Friedel pairs were merged. The H atoms of the water molecules and imine group were located in a difference Fourier map and refined isotropically, with water H atoms refined with the O—H and H \cdots H distances restrained to 0.84 (1) and 1.37 (2) \AA , respectively. The other H atoms were placed in geometrically idealized positions, with C—H = 0.93 \AA , and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b) and PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97.

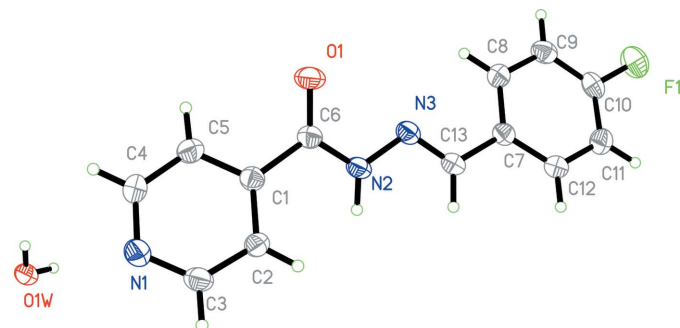


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

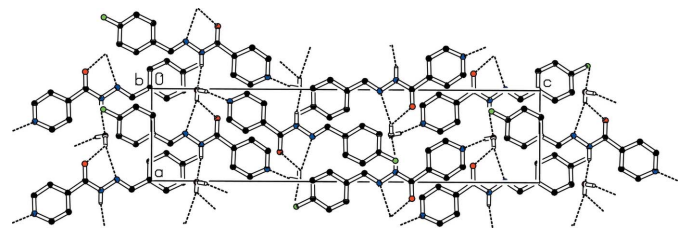


Figure 2
Part of the crystal structure of (I). Dashed lines indicate hydrogen bonds.

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