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#### Key indicators

Single-crystal X-ray study

$T = 298$  K

Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å

$R$  factor = 0.054

$wR$  factor = 0.148

Data-to-parameter ratio = 12.6

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

## 4-Fluorobenzaldehyde salicylhydrazone

The title compound,  $\text{C}_{14}\text{H}_{11}\text{FN}_2\text{O}_2$ , crystallizes with two molecules in the asymmetric unit. Both molecules are roughly planar and adopts a *trans* configuration with respect to the  $\text{C}=\text{N}$  double bond. In the crystal structure, intermolecular  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds result in the formation of sheets parallel to the *ac* plane.

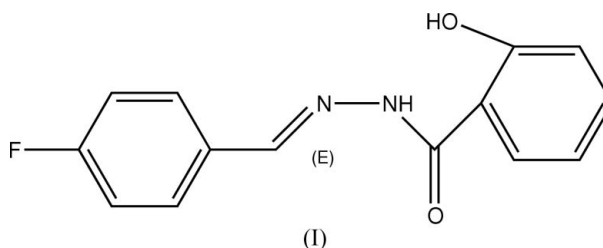
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#### Comment

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 deprotonated hydroxyl group of the salicylhydrazone will sometimes cause the N atom of the hydrazone to become more electron-rich as a result of conjugation effects, and the N atom can thus coordinate more strongly (Bansse *et al.*, 1998). As an extension of work on the structural characterization of salicylhydrazone Schiff base compounds (Ma *et al.*, 2005), we report here the crystal structure of (I), a new salicylhydrazone with 4-fluorobenzaldehyde.

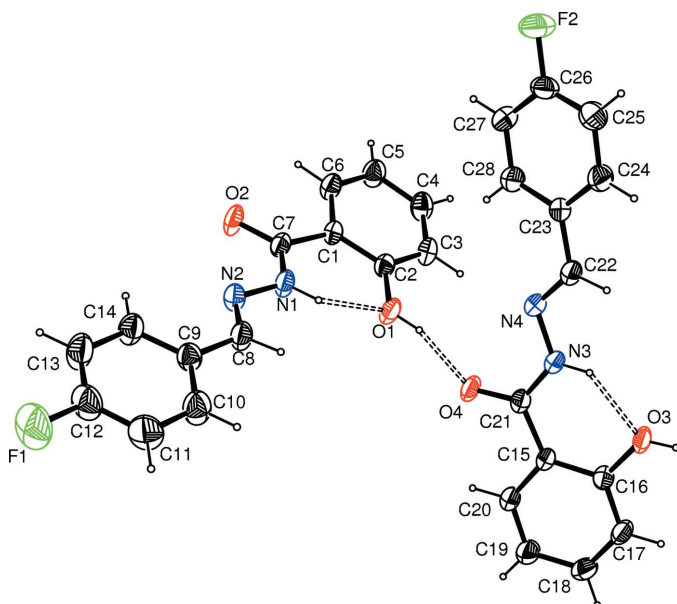


In the title compound, (I), which crystallizes with two molecules in the asymmetric unit (Fig. 1),  $\text{C}-\text{N}$  bonds in the hydrazone units are rather short (Table 1) owing to conjugation effects (Ma *et al.*, 2005). All other bond lengths are within normal ranges (Cambridge Structural Database, Version 5.26; Allen, 2002). The dihedral angles between the two benzene rings are  $7.3(2)^\circ$  and  $18.7(1)^\circ$  in the two molecules.

The occurrence of  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds results in the formation of infinite chains which are linked by  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, forming sheets parallel to the *ac* plane (Table 2 and Fig. 2).

#### Experimental

The reagents were commercial products and were used without further purification. 4-Fluorobenzaldehyde (0.2 mmol, 28 mg) and 2-hydroxybenzhydrazide (0.2 mmol, 30.4 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for



**Figure 1**  
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Hydrogen bonds are represented by dashed lines.

about 10 min to give a clear yellow solution. The solution was set aside for 8 d to allow slow evaporation of the solvent. Large colourless prism-shaped crystals separated; these were collected and washed three times with water.

#### Crystal data

$C_{14}H_{11}FN_2O_2$   
 $M_r = 258.25$   
 Monoclinic,  $P2_1/n$   
 $a = 4.9532$  (4) Å  
 $b = 47.867$  (4) Å  
 $c = 10.7392$  (9) Å  
 $\beta = 102.953$  (2)°  
 $V = 2481.4$  (4) Å<sup>3</sup>  
 $Z = 8$

$D_x = 1.383$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 3063 reflections  
 $\theta = 4.7$ – $41.4$ °  
 $\mu = 0.10$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 Prism, colourless  
 $0.35 \times 0.18 \times 0.12$  mm

#### Data collection

Bruker SMART APEX area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 2002)  
 $T_{\min} = 0.964$ ,  $T_{\max} = 0.988$   
 23870 measured reflections

4358 independent reflections  
 2137 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.078$   
 $\theta_{\text{max}} = 25.0$ °  
 $h = -5 \rightarrow 5$   
 $k = -56 \rightarrow 56$   
 $l = -12 \rightarrow 12$

#### Refinement

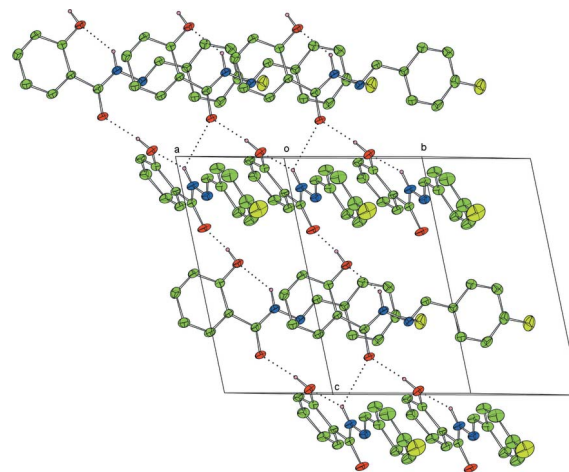
Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.054$   
 $wR(F^2) = 0.148$   
 $S = 0.87$   
 4358 reflections  
 345 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.086P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.23$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.22$  e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

N1—C7	1.338 (3)	N3—C21	1.340 (3)
N1—N2	1.370 (3)	N3—N4	1.383 (3)
N2—C8	1.263 (3)	N4—C22	1.273 (3)



**Figure 2**

The crystal packing of (I), showing the formation of sheets. O—H...O and N—H...O hydrogen bonds are represented by dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H1...O4	0.82	1.86	2.662 (2)	165
O3—H3...O2 <sup>i</sup>	0.82	1.86	2.643 (2)	159
N1—H1A...O1	0.86	2.00	2.653 (3)	132
N1—H1A...O4 <sup>ii</sup>	0.86	2.53	3.109 (3)	126
N3—H3A...O3	0.86	1.94	2.638 (3)	137

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

All H atoms were placed in geometrically idealized positions (N—H 0.86, O—H 0.82 and C—H 0.93 Å) and treated as riding on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{O}, \text{N})$ .

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPIII (Burnett & Johnson, 1996), ORTEP-3 for Windows (Farrugia, 1997) and CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: SHELXL97.

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#### References

- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.  
 Banske, W., Fliegner, J., Sawusch, S., Schilde, U. & Uhlemann, E. (1998). *Z. Naturforsch. Teil B*, **53**, 689–695.  
 Bruker (2002). SADABS, SAINT and SMART. Bruker AXS Inc., Madison, Wisconsin.  
 Brunner, H., Riepl, G., Weitzer, H. (1983). *Angew. Chem. Int. Ed. Engl.* **22**, 331–332.  
 Burnett, M. N. & Johnson, C. K. (1996). ORTEPIII. Report ORNL-6895. Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.  
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.  
 Ma, J., Zhang, S. P., Sheng, L. Q., Fan, M., Yang, Y. L., Shao S. C. (2005). *Acta Cryst.* **E61**, o1747–o1748.  
 Miller, J. S. & Epstein, A. J. (2000). *Coord. Chem. Rev.* **206–207**, 651–660.  
 Sheldrick G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.  
 Watkin, D. M., Pearce, L. & Prout, C. K. (1993). CAMERON. Chemical Crystallography Laboratory, University of Oxford, England.