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# 2′-(2-Fluorobenzylidene)-2-hydroxybenzohydrazide

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**Key indicators**

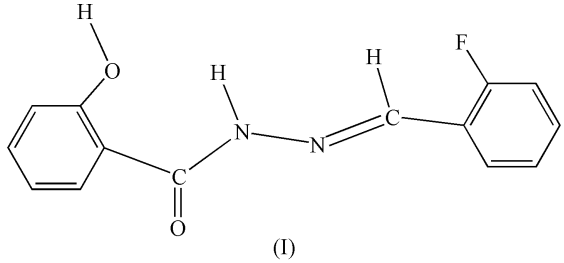
Single-crystal X-ray study
*T* = 298 K
Mean σ(C–C) = 0.003 Å
*R* factor = 0.054
*wR* factor = 0.142
Data-to-parameter ratio = 10.0

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

The title compound, $C_{14}H_{11}FN_2O_2$, was synthesized by the reaction of 2-hydroxybenzoylhydrazine with 2-fluorobenzaldehyde in ethanol. The molecule is planar and an intramolecular N—H···O hydrogen bond is observed. In the crystal packing, symmetry-related molecules form O—H···O hydrogen-bonded chains along the [201] direction.

## Comment

Some benzoylhydrazone compounds possess bacteriostatic activity. This type of compound has wide application in tuberculosis treatment and also exhibits fungicidal activity (Edwards *et al.*, 1975). Incorporation of an F atom in benzoylhydrazones has been found to enhance the above activities (Yang *et al.*, 1999). 2-Fluorobenzaldehyde is an effective intermediate in producing fever-allaying, pain-relieving and tumor-preventing medicines (Donnell & Bennett, 1984). In order to explore more effective antibacterial medicines and promote basic research on them, we have synthesized the title compound, (I).




(I)

The title molecule (Fig. 1) is essentially planar, with an r.m.s. deviation of 0.08 Å. As a result of conjugation, the C═O distance [1.230 (2) Å] is longer than the normal value of 1.20 Å, and the C1—N1 bond distance [1.339 (2) Å] is longer than the C═N double-bond distance (1.32 Å; John, 1998) and shorter than the C—N single-bond distance (1.475 Å; John, 1998).

An intramolecular N—H···O hydrogen bond is observed between the NH group and the hydroxy O atom (Table 2). The

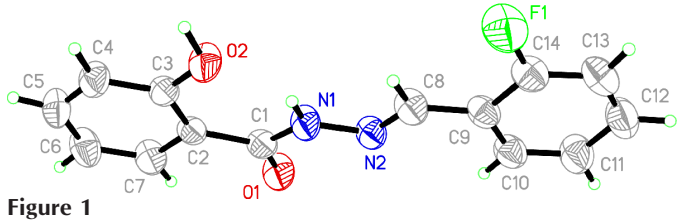



**Figure 1**
The structure of (I), showing the atomic numbering. Displacement ellipsoids are drawn at the 50% probability level.

crystal packing reveals that symmetry-related molecules are linked along the [201] direction *via* O—H···O hydrogen bonds (Fig. 2) to form chains.

## Experimental

2-Fluorobenzaldehyde (0.02 mol, 3.08 g) was dissolved in an ethanol solution (50 ml) of 2-hydroxybenzoylhydrazine (0.02 mol, 3.04 g). The mixture was refluxed for 2 h and the precipitate formed was collected by filtration and recrystallized from ethanol to give the title compound. The title compound (2 mmol, 0.58 g) was dissolved in DMF (30 ml) and kept at room temperature for 30 d to obtain colourless single crystals, which were collected and washed with distilled water.

*Crystal data*

$C_{14}H_{11}FN_2O_2$
$M_r$ = 258.25
Monoclinic, $P2_1/c$
$a$ = 4.9184 (8) Å
$b$ = 23.655 (4) Å
$c$ = 10.6092 (17) Å
$\beta$ = 101.556 (3)°
$V$ = 1209.3 (3) Å$^3$
$Z$ = 4
$D_x$ = 1.418 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 1820 reflections
$\theta$ = 5.2–51.7°
$\mu$ = 0.11 mm$^{-1}$
$T$ = 298 (2) K
Block, colourless
0.49 × 0.35 × 0.11 mm

*Data collection*

Bruker SMART APEX area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min}$ = 0.949, $T_{max}$ = 0.988
6145 measured reflections
2164 independent reflections
1639 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.117
$\theta_{max}$ = 25.2°
$h = -5 \rightarrow 5$
$k = -28 \rightarrow 25$
$l = -12 \rightarrow 12$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.142
$S$ = 1.01
2164 reflections
216 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0729P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| O1—C1 | 1.230 (2) | N2—C8 | 1.263 (2) |
| O2—C3 | 1.357 (2) | F1—C14 | 1.353 (2) |
| N1—C1 | 1.339 (2) | C1—C2 | 1.488 (2) |
| N1—N2 | 1.371 (2) | C8—C9 | 1.457 (3) |
| | | | |
| O1—C1—N1 | 122.05 (16) | C3—C2—C1 | 125.88 (16) |
| N1—C1—C2 | 117.05 (15) | C10—C9—C14 | 116.52 (18) |
| C7—C2—C1 | 116.37 (15) | C10—C9—C8 | 123.54 (17) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O2 | 0.88 (2) | 1.93 (2) | 2.632 (2) | 136 (2) |
| O2—H2···O1$^{i}$ | 0.89 (3) | 1.77 (3) | 2.638 (2) | 162 (3) |

Symmetry code: (i) $1+x, \frac{1}{2}-y, \frac{1}{2}+z$.

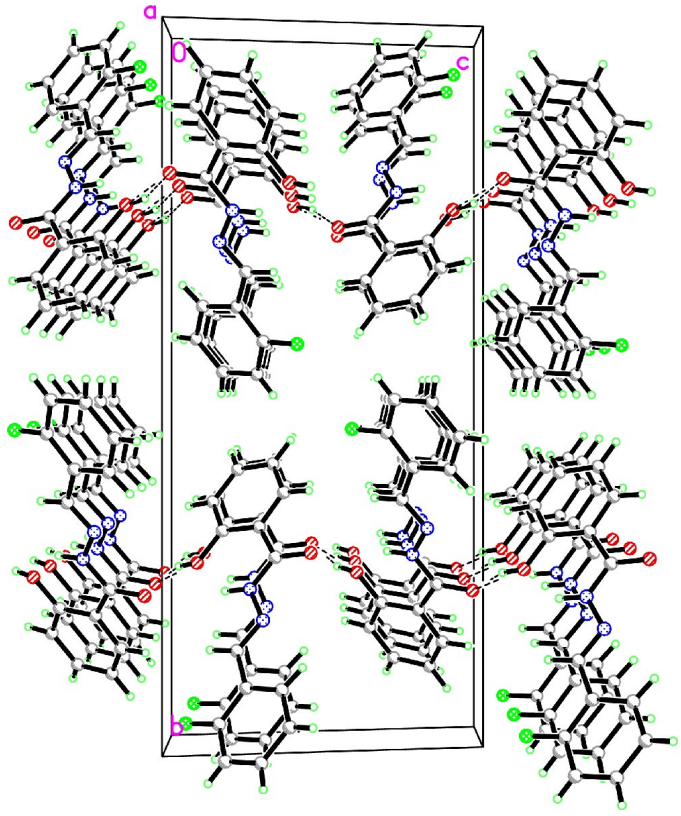



**Figure 2**
Packing of (I), viewed down the *a* axis, showing hydrogen-bonded chains. Hydrogen bonds are indicated by dashed lines.

All H atoms were located in a difference map and their parameters were refined. The N—H distance is 0.88 (2) Å and the C—H distances lie in the range 0.85 (3)–0.99 (2) Å.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2002); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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