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Key indicators

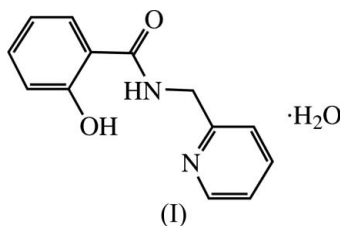
Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.051
 wR factor = 0.162
Data-to-parameter ratio = 14.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.2-Hydroxy-*N*-(2-pyridylmethyl)benzamide
monohydrate

In the title compound, $\text{C}_{13}\text{H}_{12}\text{N}_2\text{O}_2 \cdot \text{H}_2\text{O}$, all bond lengths and angles are normal. The hydroxy group is involved in hydrogen bonding, which links the molecules into centrosymmetric dimers. The solvent water molecules, acting as donors and acceptors of hydrogen bonds, link the dimers into two-dimensional sheets. The crystal packing is further stabilized by weak intermolecular $\text{C}-\text{H} \cdots \text{O}$ interactions.

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Comment

Salicylamide and its derivatives have attracted much attention because many of these derivatives show biological activity and can be used as bactericides, weedicides, insecticides and regulators of plant growth (Silverman *et al.*, 2005). 2-Aminomethylpyridine, an asymmetrical *N,N'*-bidentate ligand, can form many novel structural complexes (Paraschiv *et al.*, 2003). We report here the crystal structure of the title compound, (I).



The molecule of (I) shows a wing-like conformation, with a dihedral angle of $76.2(1)^\circ$ between the mean planes of the $\text{O1/O2/N1/C1}-\text{C8}$ and pyridine moieties. All bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The intramolecular hydrogen bonds, *viz.* $\text{N1}-\text{H1A} \cdots \text{O1}$ and $\text{C5}-\text{H5A} \cdots \text{O2}$ (Table 1), contribute to the planarity of the $\text{O1/O2/N1/C1}-\text{C8}$ fragment (Fig. 1). In the crystal structure, the hydroxy group O1/H1B and atom N2 are involved in hydrogen bonds (Table 1), which link the molecules of (I) into centrosymmetric dimers. The water molecules, acting as donors and acceptors of hydrogen bonds (Table 1), link the dimers into two-dimensional sheets. The crystal packing (Fig. 2) is further stabilized by weak intermolecular $\text{C}-\text{H} \cdots \text{O}$ interactions (Table 1).

Experimental

To a solution of ethyl salicylate (16.6 g, 0.1 mol) in *N,N*-dimethylformamide (10 ml) was added 2-aminomethylpyridine (10.8 g, 0.1 mol), and the resulting mixture was stirred at 413 K for 6 h. After cooling to room temperature, the mixture was dissolved in chloroform (20 ml) and then washed three times with water. The isolated chloroform layer was evaporated to dryness. The crude product was

recrystallized from ethanol to give the title compound. Colourless single crystals suitable for an X-ray diffraction study were obtained by slow evaporation of an ethyl acetate solution over a period of 6 d.

Crystal data

$C_{13}H_{12}N_2O_2 \cdot H_2O$
 $M_r = 246.26$
 Monoclinic, $P2_1/c$
 $a = 10.849$ (3) Å
 $b = 4.6324$ (13) Å
 $c = 25.094$ (6) Å
 $\beta = 102.484$ (9)°
 $V = 1231.3$ (6) Å³

$Z = 4$
 $D_x = 1.328$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 293$ (2) K
 Needle, colourless
 $0.50 \times 0.14 \times 0.07$ mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.954$, $T_{\max} = 0.993$

6488 measured reflections
 2434 independent reflections
 1321 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.046$
 $\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.162$
 $S = 0.89$
 2434 reflections
 171 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0862P)^2 + 0.05P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.14$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.13$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N1-H1A \cdots O1$	0.86	1.97	2.659 (3)	136
$C5-H5A \cdots O2$	0.93	2.42	2.758 (3)	101
$O1-H1B \cdots N2^i$	0.82	1.88	2.680 (3)	165
$O1W-H1W \cdots O1W^{ii}$	0.85 (3)	1.87 (3)	2.728 (3)	177 (4)
$O1W-H2W \cdots O2^{iii}$	0.85 (2)	1.98 (2)	2.827 (3)	175 (3)
$C12-H12A \cdots O1W^{iv}$	0.93	2.49	3.300 (4)	146

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

All H atoms were located in a difference Fourier map. Water H atoms were refined with O–H distance restraints of 0.85 (1) Å. The remaining H atoms were placed in idealized positions (C–H = 0.93–0.97 Å, N–H = 0.86 Å and O–H = 0.82 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ and $1.5U_{\text{eq}}(\text{O})$.

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); software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

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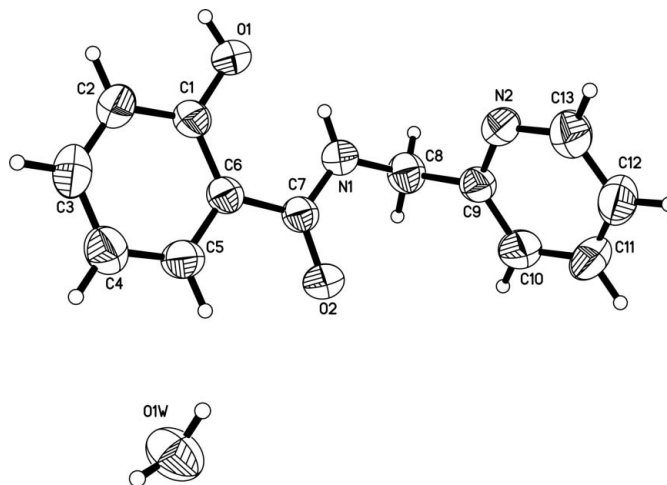


Figure 1

The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

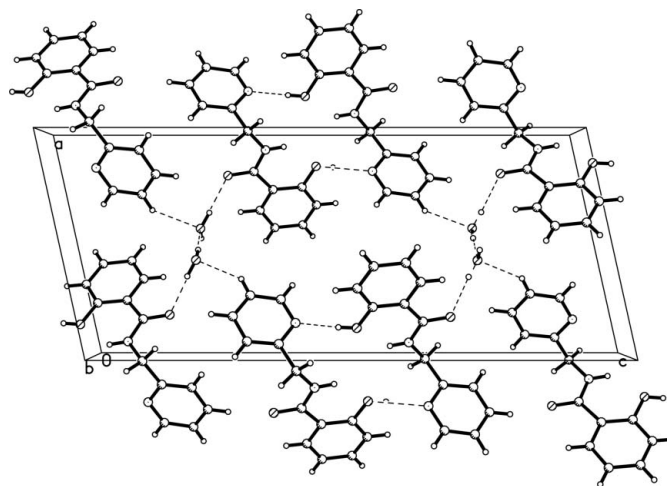


Figure 2

The packing diagram, viewed down the b axis. The intermolecular hydrogen bonds are shown as dashed lines.

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