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2-Hydroxy-*N*-(2-pyridyl)benzamide

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.046
wR factor = 0.135
Data-to-parameter ratio = 7.4

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

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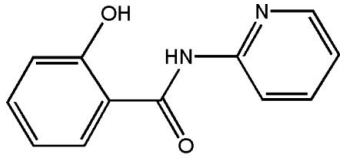
The molecule of the title compound, $C_{12}H_{10}N_2O_2$, is nearly planar, with a dihedral angle of 3.7 (2)° between the planes of the benzene and pyridine rings. Molecules are linked by intermolecular O—H···N and C—H···O hydrogen bonds, as well as possible C—H···π interactions, forming a two-dimensional zigzag hydrogen-bonded network.

Comment

Molecular self-assembly by hydrogen bonds, *e.g.* C—H···O, N—H···O and C—H···π interactions, has emerged as an attractive approach in crystal engineering (Lü *et al.*, 2005). The study of antimycobacterial properties of salicylanilides is of great interest, as salicylanilides can inhibit bacterial two-component systems, which can also be important in mycobacteria. Salicylanilide and its derivatives exhibit biological and pharmacological activities (Waisser *et al.*, 2004). The title compound, (I), was synthesized as a route to synthetic intermediates. We present here its crystal structure.



(I)

In the molecule of the title compound, (I), bond lengths and angles (Table 1) are in normal ranges (Allen *et al.*, 1987). The strong intramolecular N—H···O hydrogen bond (Table 2) causes the formation of a pseudo-six-membered ring (C1–C3/O2/H1/N1) (Fig. 1). The dihedral angle between the two planar rings [*A* (atoms C2–C7) and *B* (N2/C8–C12)] is 3.7 (2)°.

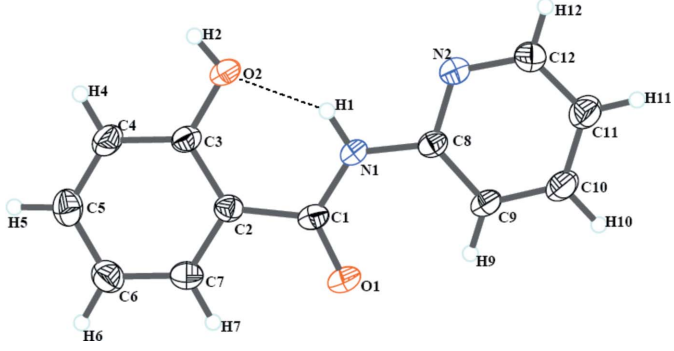


Figure 1
A drawing of the molecular structure, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The hydrogen bond is shown as a dashed line.

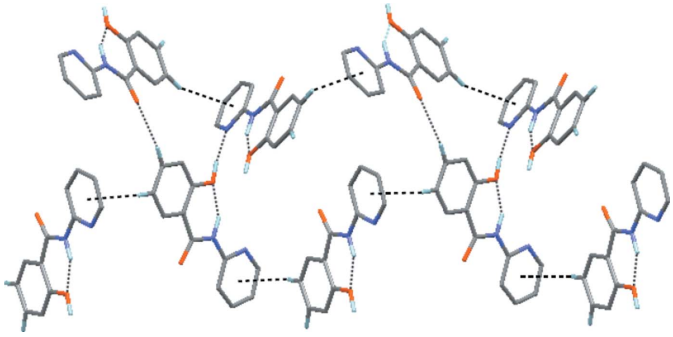


Figure 2
A packing diagram of (I). Hydrogen bonds and C—H···π interactions are shown as dashed lines. H atoms not involved in these interactions have been omitted.

The crystal structure of (I) is stabilized by intermolecular O—H···N and C—H···O hydrogen bonds (Table 2), as well as possible T-shaped C—H···π interactions with a distance of 2.88 Å between the centroid of ring *B* and atom H6(C6) at ($\frac{3}{2} - x$, $-y$, $z - \frac{1}{2}$), which result in the formation of a two-dimensional zigzag hydrogen-bonded network (Fig. 2).

Experimental

A mixture of pyridin-2-amine (0.94 g, 10.0 mmol) and 2-(methoxycarbonyl)phenol (1.52 g, 10.0 mmol) was melted at 463–483 K for 2 h with an air condenser under an argon atmosphere. The reaction mixture was then heated under reflux in ethanol (10 ml) for 10 min, filtered and the product crystallized from the same solvent (yield 1.16 g, 54%; m.p. 484–485 K).

Crystal data

$C_{12}H_{10}N_2O_2$
M_r = 214.22
Orthorhombic, $P2_12_12_1$
a = 6.1216 (16) Å
b = 12.535 (3) Å
c = 13.321 (4) Å
V = 1022.2 (5) Å^3
Z = 4
D_x = 1.392 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
Needle, colourless
0.48 × 0.19 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.955, T_{max} = 0.984
5265 measured reflections
1074 independent reflections
671 reflections with $I > 2\sigma(I)$
R_{int} = 0.106
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.135
S = 1.03
1074 reflections
145 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.1271P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.353 (5)	N2—C8	1.342 (5)
N1—C8	1.382 (5)	O1—C1	1.217 (5)
N2—C12	1.340 (6)	O2—C3	1.358 (5)
C1—N1—C8	128.4 (4)	O2—C3—C2	118.5 (4)
C12—N2—C8	118.1 (4)	N2—C8—C9	121.5 (4)
O1—C1—N1	122.5 (5)	N2—C8—N1	113.4 (4)
O1—C1—C2	121.0 (4)	C9—C8—N1	125.2 (4)
N1—C1—C2	116.4 (4)	N2—C12—C11	123.5 (5)
O2—C3—C4	121.5 (4)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.86	1.90	2.627 (5)	142
O2—H2···N2^{i}	0.82	1.88	2.676 (5)	164
C5—H5···O1^{ii}	0.93	2.50	3.384 (6)	159

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

H atoms were positioned geometrically, with O—H = 0.82 Å, N—H = 0.86 Å and C—H = 0.93 Å, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,N,O), with x = 1.5 for the hydroxyl H atom and x = 1.2 for all other H atoms. In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXTL* (Bruker, 2000).

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References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Brandenburg, K. (2005). *DIAMOND*. Release 3.1a. Crystal Impact GbR, Bonn, Germany.
Bruker (2000). *SMART* (Version 5.0), *SAINT-Plus* (Version 6) and *SHELXTL* (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Lü, X.-Q., Jiang, J.-J., zur Loye, H.-C., Kang, B.-S. & Su, C.-Y. (2005). *Inorg. Chem.* **44**, 1810–1817.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Waisser, K., Dražková, K., Kuneš, J., Klimešová, V. & Kaustová, J. (2004). *Il Farmaco*, **59**, 615–625.