Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(2-Hydroxylbenzoyl)-*N*′-(picolinoyl)hydrazine

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Received 31 August 2006
Accepted 2 September 2006

The title molecule, $C_{13}H_{11}N_3O_3$, is non-planar. The dihedral angle between the pyridine and benzene rings is 80.5 (1)°. Intermolecular O—H···O and N—H···O hydrogen bonds link the molecules into columns along the *a* axis.

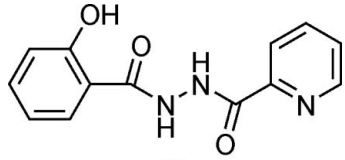
Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.004 Å
R factor = 0.039
wR factor = 0.105
Data-to-parameter ratio = 9.0

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

Comment

N-Aroyl-*N*′-picolinoyl hydrazines can be used as potential agents to treat iron-overload disease (Bernhardt *et al.*, 2005). We report here the crystal structure of the title compound, (I).



(I)

The title molecule is non-planar (Fig.1). The amide group (N2/C6/O1) attached to the pyridine ring is twisted by 15.2 (3)°, while that (N3/C7/O2) attached to the benzene ring is twisted by 10.0 (2)°. The dihedral angle between the N2/C6/O1 and N3/C7/O2 planes is 76.8 (1)°. The C6—N2—N3—C7 torsion angle is −77.6 (3)° and the O1—C6···C7—O2 pseudo-torsion angle of 89.6° indicates a +synclinal orientation for the two carbonyl groups. The dihedral angle between the pyridine and benzene rings is 80.5 (1)°.

One of the hydrazine NH groups is involved in an intramolecular N3—H3*A*···O3 hydrogen bond. Intermolecular N—H···O and O—H···O hydrogen bonds (Table 1) involving the other NH group and the OH group link symmetry-related molecules into columns along the *a* axis (Fig.2).

Experimental

The title compound was synthesized according to a literature method (Bernhardt *et al.*, 2001). Crude products were recrystallized twice from ethanol (yield 70%). Single crystals suitable for X-diffraction study were obtained by slow evaporation of an ethanol solution.

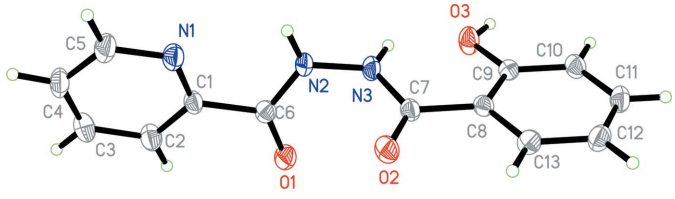


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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Crystal data

$C_{13}H_{11}N_3O_3$
M_r = 257.25
Orthorhombic, $P2_12_12_1$
a = 4.6152 (7) Å
b = 10.0698 (16) Å
c = 24.928 (4) Å
V = 1158.5 (3) Å^3
Z = 4
D_x = 1.475 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 291 (2) K
Needle, colourless
0.46 × 0.15 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
6078 measured reflections
1551 independent reflections
1260 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.105
S = 1.04
1551 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 0.0547P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2^{i}	0.86	2.29	2.988 (3)	138
N3—H3A···O3	0.86	1.95	2.636 (3)	136
O3—H3B···O1^{ii}	0.82	1.87	2.678 (3)	170

Symmetry codes: (i) $x-1, y, z$; (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+2$.

All H atoms were placed in geometrically idealized positions (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) = 1.2 or 1.5 times U_{eq}(C,N,O). In the absence of significant anomalous dispersion effects, Friedel pairs were merged before the final refinement.

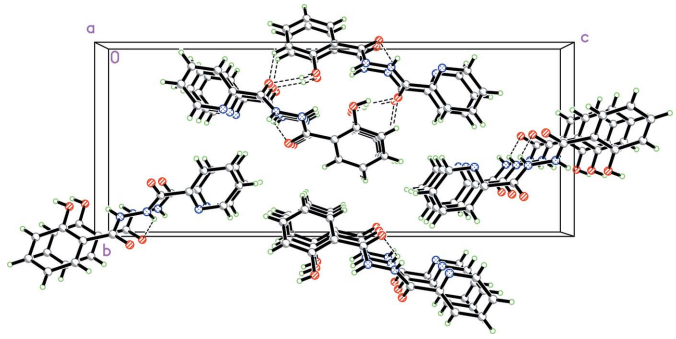

Figure 2
The crystal packing of (I), viewed along the *a* axis. Dashed lines indicate intermolecular hydrogen bonds.

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

The authors thank Fuyang Normal College, China, for research grant No. 2005LQ06.

References

Bernhardt, P. V., Chin, P. & Richardson, D. R. (2001). *J. Biol. Inorg. Chem.* **6**, 801–809.
Bernhardt, P. V., Chin, P., Sharp, P. C., Wang, J.-Y. C. & Richardson, R. (2005). *J. Biol. Inorg. Chem.* **10**, 761–777.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version. 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.