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N′-[1-(5-Bromo-2-hydroxyphenyl)methylidene]-isonicotinohydrazide

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The molecule of the title compound, $C_{13}H_{10}BrN_3O_2$, is approximately planar and displays a *trans* configuration with respect to the C=N double bond. The crystal structure is stabilized by intermolecular N—H···N hydrogen bonds, forming layers parallel to the *ab* plane.

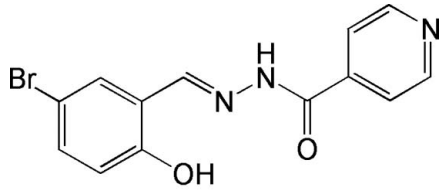
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.096
Data-to-parameter ratio = 16.2

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

Comment

The background to this investigation is set out in the preceding paper (Yang, 2006). The structure of the title compound, (I), is reported here.



(I)

In (I) (Fig. 1), all bond lengths are within normal ranges (Allen *et al.*, 1987) and comparable with those of similar compounds (Qian *et al.*, 2006; Qiu, Xu *et al.*, 2006; Qiu, Fang, Liu & Zhu, 2006; Qiu, Fang, Yang *et al.*, 2006). The C7—N1 bond length of 1.269 (4) Å conforms to the value for a double bond. The bond length of 1.354 (4) Å between atoms C8 and N2 is intermediate between a C—N single bond and a C=N double bond. The dihedral angle between the benzene ring and the pyridine ring is 11.2 (3)°.

The molecular structure is stablized by an intramolecular O—H···N hydrogen bond (Table 1). In the crystal structure, molecules are linked through intermolecular N—H···N hydrogen bonds (Table 1), forming layers parallel to the *ab* plane (Fig. 2).

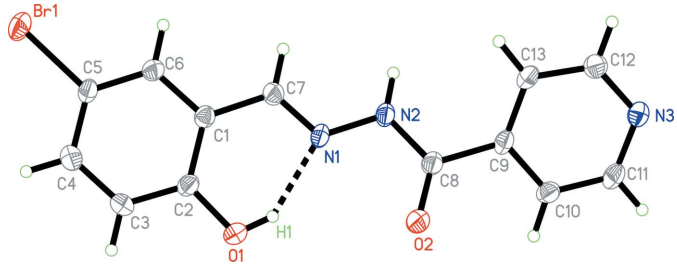


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular hydrogen bond is shown as a dashed line.

Experimental

5-Bromosalicylaldehyde (0.1 mmol, 20.2 mg) and pyridine-4-carboxylic acid hydrazide (0.1 mmol, 13.7 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature to give a clear yellow solution. Crystals of (I) were formed by gradual evaporation of the solvent over 3 d at room temperature. Analysis found: C 48.86, H 3.07, N 13.23%; calculated for $C_{13}H_{10}BrN_3O_2$: C 48.77, H 3.15, N 13.13%.

Crystal data

$C_{13}H_{10}BrN_3O_2$
M_r = 320.15
Monoclinic, $P2_1/n$
a = 8.563 (1) Å
b = 15.875 (2) Å
c = 9.368 (2) Å
β = 100.448 (2)°
V = 1252.4 (3) Å^3
Z = 4
D_x = 1.698 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.28 mm^{-1}
T = 298 (2) K
Block, yellow
0.27 × 0.23 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.471, T_{max} = 0.590
(expected range = 0.442–0.554)
10587 measured reflections
2857 independent reflections
1872 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.096
S = 1.02
2857 reflections
176 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0213P)^2 + 0.3987P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.86	2.581 (4)	146
N2—H2···N3^{i}	0.895 (10)	2.14 (3)	3.029 (4)	169 (4)

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

Atom H2 was located in a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) Å. The other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with O—H = 0.82 Å, C—H = 0.93 Å, and U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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*.

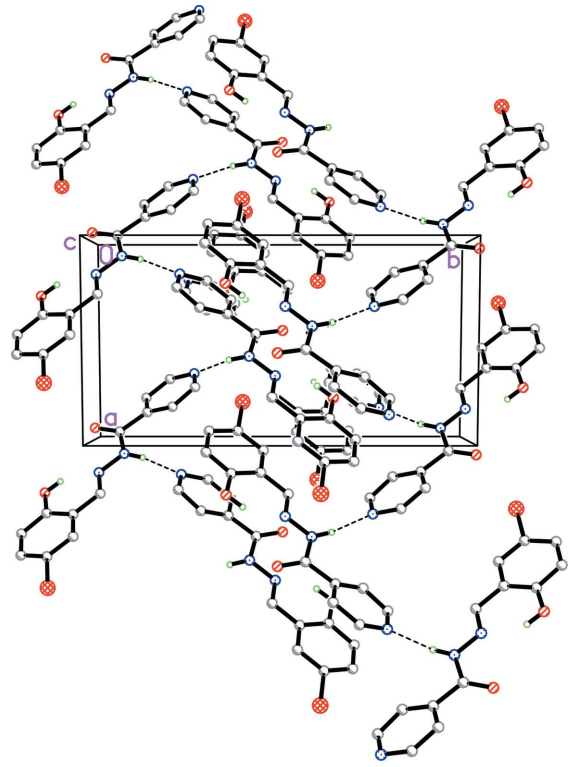


Figure 2
The packing of (I), viewed along the c axis. Dashed lines indicate intermolecular hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

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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.
Bruker (2002). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Qian, H.-Y., Yin, Z.-G., Jia, J., Liu, S.-M. & Feng, L.-Q. (2006). *Acta Cryst.* E**62**, o3623–o3624.
Qiu, X.-Y., Fang, X.-N., Liu, W.-S. & Zhu, H.-L. (2006). *Acta Cryst.* E**62**, o2685–o2686.
Qiu, X.-Y., Fang, X.-N., Yang, S.-L., Liu, W.-S. & Zhu, H.-L. (2006). *Acta Cryst.* E**62**, o2687–o2688.
Qiu, X.-Y., Xu, H.-J., Liu, W.-S. & Zhu, H.-L. (2006). *Acta Cryst.* E**62**, o2304–o2305.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Yang, D.-S. (2006). *Acta Cryst.* E**62**, o3755–o3756.