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(*E*)-*N*′-(3-Bromobenzylidene)isonicotinohydrazide

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.116
Data-to-parameter ratio = 17.3

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

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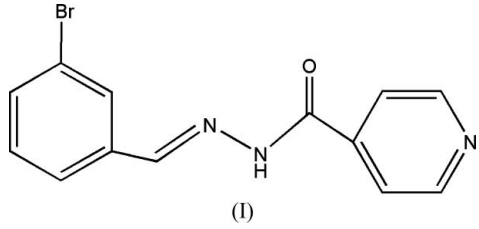
The title compound, $C_{13}H_{10}BrN_3O$, is roughly planar and displays a *trans* configuration with respect to the C=N double bond. The dihedral angle between the benzene and pyridine rings is 4.2 (3)°. The crystal structure is stabilized by intermolecular N—H···N hydrogen bonds.

Comment

Recently, we have reported the structures of a few Schiff base complexes (Qiu *et al.*, 2004; Zhu *et al.*, 2003), including the isostructural chloro analogue of the title compound (Qiu *et al.*, 2006). As an extension of our work on the structural characterization of Schiff base compounds, the crystal structure of the title compound, (I), is reported here.



(I)

In (I), the bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The C7=N1 bond length of 1.271 (4) Å conforms to the value for a double bond. The bond length of 1.357 (4) Å between N2 and C8 is greater than the value for a double bond, and less than the value for a single bond, because of conjugation effects in the molecule. The dihedral angle between the benzene and pyridine rings is 4.2 (3)°.

The crystal structure is stabilized by intermolecular N—H···N hydrogen bonds (Table 1 and Fig. 2).

Experimental

The reagents were commercial products and were used without further purification. 3-Bromobenzaldehyde (0.1 mmol, 18.5 mg) and

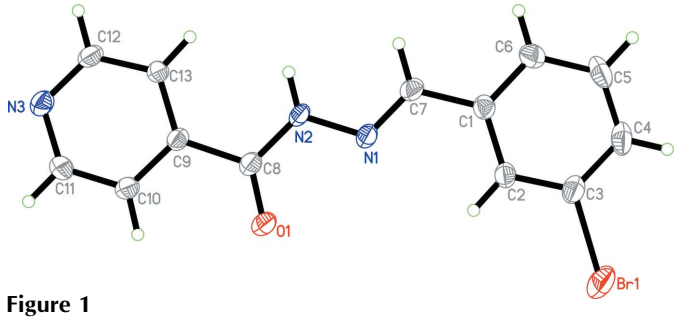


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

isonicotinohydrazide (0.1 mmol, 13.4 mg) were dissolved in ethanol (15 ml). The reaction mixture was stirred for 10 min to give a clear yellow solution. After allowing the solution to stand at room temperature in air for 11 d, large yellow crystals were formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed three times with ethanol and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 58%).

Crystal data

$C_{13}H_{10}BrN_3O$
M_r = 304.15
Monoclinic, $P2_1/n$
a = 7.6462 (2) Å
b = 11.3780 (3) Å
c = 14.4193 (4) Å
β = 101.898 (1)°
V = 1227.51 (6) Å^3
Z = 4
D_x = 1.646 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.34 mm^{-1}
T = 298 (2) K
Block, yellow
0.48 × 0.24 × 0.12 mm

Data collection

Bruker SMART APEX area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.395, T_{max} = 0.668
7494 measured reflections
2817 independent reflections
1656 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 27.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.116
S = 1.04
2817 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 0.3476P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N3^{i}	0.86	2.36	3.160 (3)	155

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

All H atoms were placed in geometrically idealized positions (C—H = 0.93 Å and N—H = 0.86 Å) and constrained to ride on their parent atoms. They were treated as riding atoms, with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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: *SHELXTL*.

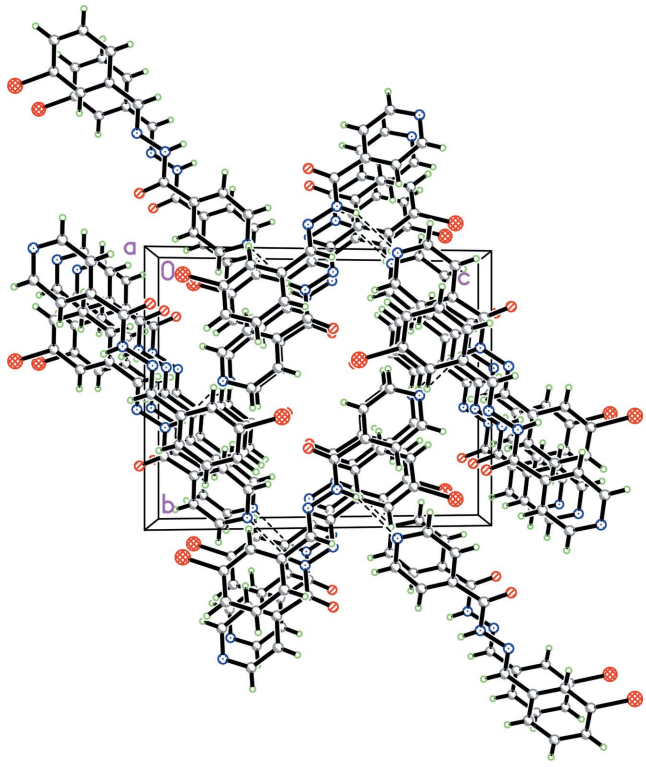


Figure 2
The crystal packing of (I), viewed along the *a* axis. Dashed lines show intermolecular hydrogen bonds.

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