

(E)-N'-(3-Chlorobenzylidene)isonicotinohydrazide

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Key indicators

Single-crystal X-ray study

$T = 298$ K

Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å

R factor = 0.061

wR factor = 0.169

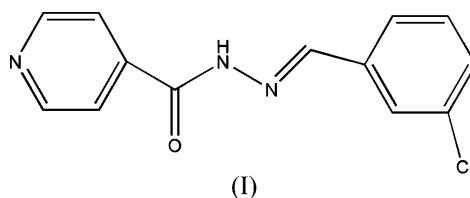
Data-to-parameter ratio = 15.2

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

The molecule of the title compound, $\text{C}_{13}\text{H}_9\text{ClN}_3\text{O}$, is roughly planar and displays a *trans* configuration with respect to the $\text{C}=\text{N}$ double bond. The dihedral angle between the benzene and pyridine rings is $4.8(3)^\circ$. The crystal structure is stabilized by intermolecular $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds.

Comment

Recently, we have reported the structures of a few Schiff base complexes (Qiu *et al.*, 2004; Zhu *et al.*, 2003). 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.



In (I), the bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The $\text{C}7=\text{N}3$ bond length of $1.277(4)$ Å conforms to the value for a double bond. The bond length of $1.359(4)$ Å between $\text{N}2$ and $\text{C}8$ 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 $4.8(3)^\circ$.

The crystal structure is stabilized by intermolecular $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds (Table 1 and Fig. 2).

Experimental

The reagents were commercial products and were used without further purification. 3-Chlorobenzaldehyde (0.1 mmol, 14.1 mg) and isonicotinohydrazide (0.1 mmol, 13.4 mg) were dissolved in ethanol (10 ml). The reaction mixture was stirred for 20 min to give a clear solution. After allowing the resulting clear solution to stand at room temperature in air for 8 d, large colourless 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

$\text{C}_{13}\text{H}_9\text{ClN}_3\text{O}$

$M_r = 259.69$

Monoclinic, $P2_1/n$

$a = 7.6299(3)$ Å

$b = 11.3388(5)$ Å

$c = 14.4189(6)$ Å

$\beta = 102.979(2)^\circ$

$V = 1215.57(9)$ Å³

$Z = 4$

$D_x = 1.419$ Mg m⁻³

Mo $K\alpha$ radiation

$\mu = 0.30$ mm⁻¹

$T = 298(2)$ K

Needle, colourless

$0.46 \times 0.08 \times 0.06$ mm

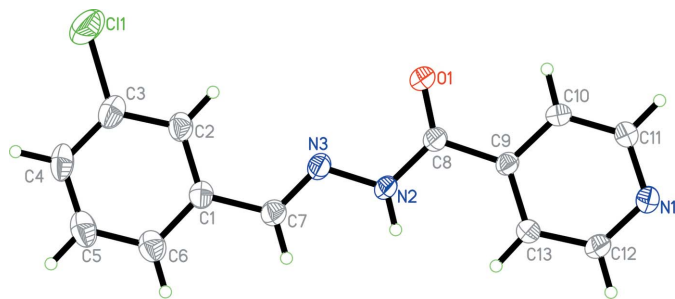


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Data collection

Bruker SMART APEX area-detector diffractometer ω scans Absorption correction: multi-scan (SADABS; Sheldrick, 1996) $T_{\min} = 0.954$, $T_{\max} = 0.975$	6893 measured reflections 2475 independent reflections 1336 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.042$ $\theta_{\text{max}} = 26.4^\circ$
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Refinement

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.061$ $wR(F^2) = 0.169$ $S = 1.03$ 2475 reflections 163 parameters H-atom parameters constrained	$w = 1/[\sigma^2(F_o^2) + (0.0682P)^2 + 0.2543P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} < 0.001$ $\Delta\rho_{\text{max}} = 0.34 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.29 \text{ e } \text{\AA}^{-3}$
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Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N2-H2A\cdots N1^i$	0.86	2.33	3.131 (3)	156

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

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

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

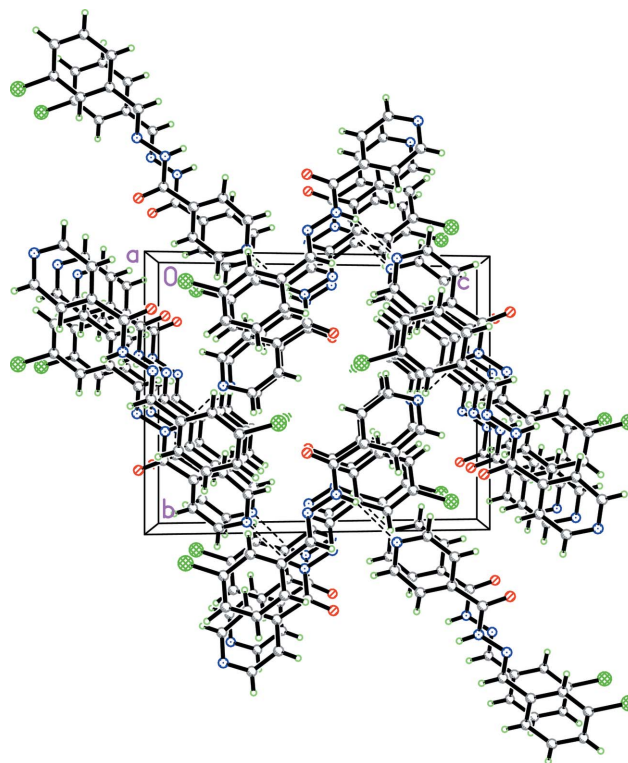


Figure 2
The crystal packing of (I), viewed along the a axis. Dashed lines show intermolecular hydrogen bonds.

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