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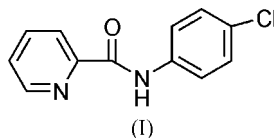
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Key indicators

Single-crystal X-ray study

T = 291 KMean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$ *R* factor = 0.043*wR* factor = 0.125

Data-to-parameter ratio = 13.4

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.The title molecule, $\text{C}_{12}\text{H}_9\text{ClN}_2\text{O}$, is almost planar. Inter-
molecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules into
chains along the *a* axis.**Comment**Picoloylhydrazide compounds exhibit antitubercular and
antineoplastic activities. However, owing to the existence of an
imino group, these compounds are toxic to some extent (Wu &
Liu, 2004). Hydrazone and hydrazide compounds have been
synthesized by the condensation reaction of amino and
carbonyl groups and their toxicity has been studied (Wu &
Liu, 2001, 2003*a,b,c*, 2004). As we are interested in pico-
loylhydrazide compounds, the crystal structure of the title
compound, (I), is reported.The title molecule is almost planar (Fig. 1); the dihedral
angle between the pyridine and benzene rings is $2.9 (1)^\circ$. The
 $\text{C}7-\text{N}1-\text{C}6-\text{C}5$ torsion angle is $-178.50 (17)^\circ$. The bond
lengths and angles in (I) are normal. Intermolecular $\text{C}-\text{H}\cdots\text{O}$
hydrogen bonds (Table 1) link the molecules into
chains along the *a* axis.**Experimental**A benzene solution (5 ml) of thionyl chloride (5 mmol) was added
slowly to a vigorously stirred benzene solution (10 ml) of picolinic
acid (2 mmol). The mixture was heated at 365 K for 2 h and then
cooled. An ethanol solution (10 ml) of 4-chloroaniline (2 mmol) was
added to the mixture and stirred for 1 h, and then the solution was
filtered. After allowing the resulting solution to stand in air for 10 d,
colourless block-shaped crystals were formed on slow evaporation of
the solvent. The crystals were isolated, washed with ethanol and
dried.**Crystal data** $\text{C}_{12}\text{H}_9\text{ClN}_2\text{O}$ $M_r = 232.66$ Triclinic, $P\bar{1}$ $a = 6.308 (3) \text{ \AA}$ $b = 8.251 (3) \text{ \AA}$ $c = 10.766 (4) \text{ \AA}$ $\alpha = 87.358 (4)^\circ$ $\beta = 86.463 (4)^\circ$ $\gamma = 77.518 (4)^\circ$ $V = 545.8 (4) \text{ \AA}^3$ $Z = 2$ $D_x = 1.416 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation $\mu = 0.33 \text{ mm}^{-1}$ $T = 291 (2) \text{ K}$

Block, colourless

 $0.50 \times 0.40 \times 0.26 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.853$, $T_{\max} = 0.921$

3842 measured reflections
 1940 independent reflections
 1294 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$
 $\theta_{\text{max}} = 25.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.126$
 $S = 1.08$
 1940 reflections
 145 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0698P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.25 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\text{min}} = -0.27 \text{ e } \text{Å}^{-3}$

Table 1

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1N\cdots N2$	0.86	2.22	2.664 (3)	112
$C8-H8\cdots O1^i$	0.93	2.46	3.276 (3)	147

Symmetry code: (i) $x - 1, y, z$.

All H atoms were placed in calculated positions ($N-H = 0.86 \text{ Å}$ and $C-H = 0.93 \text{ Å}$) and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); 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: SHELXL97.

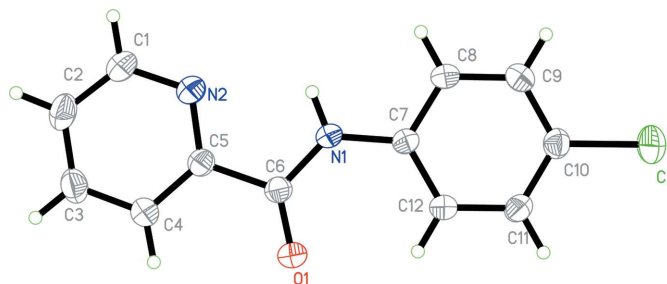


Figure 1

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

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References

- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (1997a). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
 Sheldrick, G. M. (1997b). *SHELXTL*. Version. 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
 Siemens (1996). *SMART* and *SAINTE*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
 Wu, W. S. & Liu, S. X. (2001). *Chin. J. Struct. Chem.* **20**, 226–228.
 Wu, W. S. & Liu, S. X. (2003a). *Chem. J. Chin. Univ.* **24**, 2137–2142.
 Wu, W. S. & Liu, S. X. (2003b). *Chin. J. Inorg. Chem.* **19**, 1065–1072.
 Wu, W. S. & Liu, S. X. (2003c). *Acta Chem. Sin.* **61**, 1014–1019.
 Wu, W. S. & Liu, S. X. (2004). *Chin. J. Struct. Chem.* **23**, 105–111.