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2-Chloro-4-methylpyridin-3-amine

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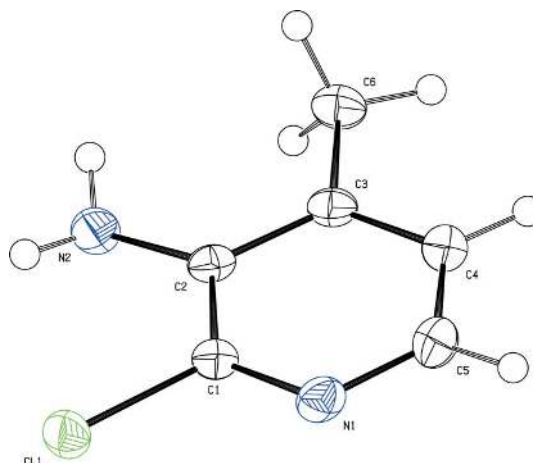
Key indicators

Single-crystal X-ray study
T = 173 K
Mean $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$
R factor = 0.034
wR factor = 0.093
Data-to-parameter ratio = 13.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Geometric parameters of the title compound, C₆H₇ClN₂, are in the usual ranges. The molecular structure shows one intramolecular N—H···Cl contact and the crystal packing is stabilized by an intermolecular N—H···N hydrogen bond.Received 10 January 2007
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Comment

Pyridine is an important structural unit found in many known therapeutic agents (Proudfoot *et al.*, 1995). Pyridine and its derivatives are important in industrial organic chemistry as fundamental building blocks (Sherman, 2004). Many pyridinyl thiazoles have proved to possess a wide range of biological activities such as cardiotoxic, anti-asthmatic, anti-inflammatory and also shown to be selective inhibitors of cytochrome P-450 2A6 (Denton *et al.*, 2005). Pyridine derivatives are known for their cardiac effects (Schoepke & Shideman, 1962). In view of the importance of pyridine derivatives, the crystal structure of the title compound, (I), is reported.

A perspective view of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.27, November 2005 update, August 2006;

**Figure 1**
The molecular structure of the title compound with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

MOGUL Version 1.1; Allen, 2002; Bruno *et al.*, 2004). As expected the molecule is planar (r.m.s. deviation for all non-H atoms 0.012 Å). The molecular conformation is characterized by an N—H···Cl contact and the crystal packing is stabilized by an N—H···N hydrogen bond, forming chains along the *c* axis (Table 1).

Experimental

A pure sample of the title compound was obtained from Srides Arco Laboratory, Mangalore, India. The sample was crystallized from acetone by slow evaporation (m.p. 333–335 K).

Crystal data

$C_6H_7ClN_2$	$Z = 4$
$M_r = 142.59$	$D_x = 1.440 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 3.9877(8) \text{ \AA}$	$\mu = 0.48 \text{ mm}^{-1}$
$b = 12.8468(15) \text{ \AA}$	$T = 173(2) \text{ K}$
$c = 12.8408(19) \text{ \AA}$	Rod, colourless
$\beta = 90.872(14)^\circ$	$0.48 \times 0.21 \times 0.20 \text{ mm}$
$V = 657.75(18) \text{ \AA}^3$	

Data collection

Stoe IPDS-II two-circle diffractometer	3879 measured reflections
ω scans	1226 independent reflections
Absorption correction: multi-scan (<i>MULABS</i> ; Spek, 2003; Blessing, 1995)	1109 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.802$, $T_{\max} = 0.910$	$R_{\text{int}} = 0.050$
	$\theta_{\max} = 25.6^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0536P)^2 + 0.1927P]$
$R[F^2 > 2\sigma(F^2)] = 0.034$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.093$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.08$	$\Delta\rho_{\max} = 0.33 \text{ e \AA}^{-3}$
1226 reflections	$\Delta\rho_{\min} = -0.24 \text{ e \AA}^{-3}$
92 parameters	Extinction correction: <i>SHELXL97</i>
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.034 (8)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2A···Cl1	0.86 (3)	2.55 (3)	2.9796 (17)	111.9 (19)
N2—H2B···N1 ¹	0.84 (2)	2.28 (2)	3.089 (2)	162 (2)

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

H atoms were found in a difference map, but those bonded to C were refined using a riding model, with C—H = 0.95 Å for aromatic or C—H = 0.98 Å for methyl H atoms. $U_{\text{iso}}(\text{H})$ values were set at $1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$. The methyl group was allowed to rotate but not to tip. H atoms bonded to nitrogen were refined freely.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON* and *SHELXL97*.

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References

- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.
 Blessing, R. H. (1995). *Acta Cryst.* **A51**, 33–38.
 Bruno, I. J., Cole, J. C., Kessler, M., Luo Jie, Motherwell, W. D. S., Purkis, L. H., Smith, B. R., Taylor, R., Cooper, R. I., Harris, S. E. & Orpen, A. G. (2004). *J. Chem. Inf. Comput. Sci.* **44**, 2133–2144.
 Denton, T. T., Zhang, X. & Cashman, J. R. (2005). *J. Med. Chem.* **48**, 224–239.
 Proudfoot, J. R., Patel, U. R., Kapadia, S. R. & Hargrave, K. D. (1995). *J. Med. Chem.* **38**, 1406–1410.
 Schoepke, H. G. & Shideman, F. E. (1962). *J. Pharmacol. Exptl Ther.* **135**, 358–366.
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. Univ. of Göttingen, Germany.
 Sherman, A. R. (2004). *Encyclopedia of Reagents for Organic Synthesis*, edited by L. Paquette. New York: J. Wiley & Sons.
 Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
 Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.