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1-(6-Chloropyridin-3-ylmethyl)-1*H*-benzimidazole

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.037
wR factor = 0.092
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.

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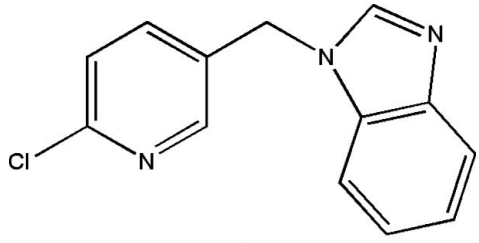
In the title compound, $C_{13}H_{10}ClN_3$, the benzimidazole and chloropyridyl groups are planar and make a dihedral angle of 68.01 (18)°. There are two weak C—H···N hydrogen bonds, producing sheets parallel to (100).

Comment

Recently, a variety of reports regarding the synthesis or modification of benzimidazole and its derivatives have appeared, as a result of their chemical and biological interest, for example their anticancer, antiviral, germicidal and cytotoxic activities (Soderlind *et al.*, 1999; Townsend *et al.*, 1995; Pedini *et al.*, 1991 and Beady *et al.*, 2000, respectively). In particular, some derivatives also show high insecticidal activity (Maki *et al.*, 1989). However, research on the serotonergic activity of these derivatives has been rarely reported. In our research, the title compound, (I), has been found to act on blood-vessel constriction associated with serotonin and to assist our research we have determined the crystal structure.



(I)

The molecular structure is shown in Fig. 1. The C7—N2 and C8—N3 bond lengths (Table 1) in the benzimidazole system confirm the delocalization of the π electrons in this system.

In the crystal structure (Fig. 2 and Table 2), a weak intermolecular hydrogen-bond contact exists between atoms C10 and N3, forming chains along the *b* axis. A second, slightly weaker, hydrogen bond involving C3 and N1 is also present, forming sheets parallel to (100).

Experimental

A mixture of 6-chloro-3-(chloromethyl)pyridine (2 mmol), 1*H*-benzimidazole (2 mmol), anhydrous potassium carbonate (2 mmol), and dry dimethylformamide (15 ml) was stirred at 323 K for 10 h. After cooling, the mixture was treated with water (50 ml) and extracted with dichloromethane (3 × 50 ml). The organic layer was washed with water, dried over anhydrous Na_2SO_4 and concentrated. The residue was chromatographed over a column of silica gel and eluted with petroleum ether–ethyl acetate (2:1 *v*/*v*) to give the desired

product (yield 73%). Single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution (m.p. 415.8–417.3 K).

Crystal data

$C_{13}H_{10}ClN_3$	$Z = 4$
$M_r = 243.69$	$D_x = 1.424$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 8.390$ (5) Å	$\mu = 0.31$ mm^{-1}
$b = 11.547$ (7) Å	$T = 298$ (2) K
$c = 11.737$ (7) Å	Plate, light yellow
$V = 1137.0$ (12) Å^3	0.50 × 0.20 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer	5749 measured reflections
	2063 independent reflections
φ and ω scans	1821 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	$R_{int} = 0.026$
	$\theta_{max} = 25.3°$
$T_{min} = 0.859$, $T_{max} = 0.975$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.037$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.092$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
$S = 1.04$	$\Delta\rho_{min} = -0.16$ e Å^{-3}
2063 reflections	Absolute structure: Flack (1983)
154 parameters	Flack parameter: 0.10 (9)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.335 (3)	C7—N2	1.353 (3)
C1—C2	1.366 (3)	C8—N3	1.378 (3)
C2—C3	1.369 (3)	C8—C13	1.383 (3)
C2—C6	1.501 (3)	C8—C9	1.387 (3)
C3—C4	1.364 (3)	C9—C10	1.360 (3)
C4—C5	1.360 (3)	C10—C11	1.379 (4)
C5—N1	1.302 (3)	C11—C12	1.366 (3)
C5—Cl1	1.736 (2)	C12—C13	1.371 (3)
C6—N2	1.452 (3)	C13—N2	1.378 (3)
C7—N3	1.291 (3)		
N1—C1—C2	124.6 (2)	C13—C8—C9	119.6 (2)
C1—C2—C3	116.3 (2)	C10—C9—C8	118.2 (2)
C1—C2—C6	121.6 (2)	C9—C10—C11	121.2 (2)
C3—C2—C6	122.1 (2)	C12—C11—C10	121.8 (2)
C4—C3—C2	120.6 (2)	C11—C12—C13	116.8 (2)
C5—C4—C3	117.4 (2)	C12—C13—N2	132.26 (19)
N1—C5—C4	124.8 (2)	C12—C13—C8	122.40 (19)
N1—C5—Cl1	115.88 (18)	N2—C13—C8	105.33 (17)
C4—C5—Cl1	119.30 (19)	C5—N1—C1	116.2 (2)
N2—C6—C2	112.03 (18)	C7—N2—C13	105.67 (18)
N3—C7—N2	114.5 (2)	C7—N2—C6	126.6 (2)
N3—C8—C13	110.15 (18)	C13—N2—C6	127.17 (18)
N3—C8—C9	130.3 (2)	C7—N3—C8	104.37 (18)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···N1^{i}	0.93	2.71	3.634 (4)	176
C10—H10···N3^{ii}	0.93	2.60	3.457 (3)	153

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

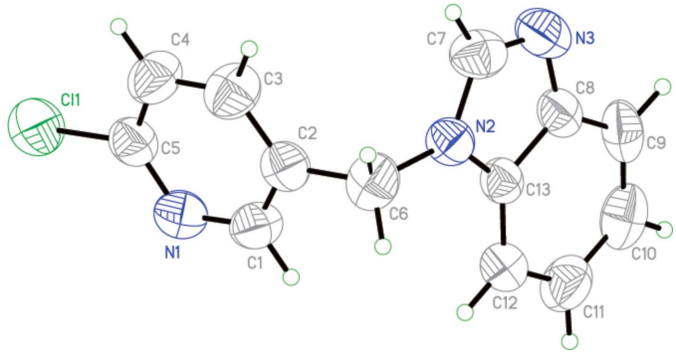


Figure 1
The molecular structure of (I), with the atom numbering, showing displacement ellipsoids drawn at the 30% probability level.

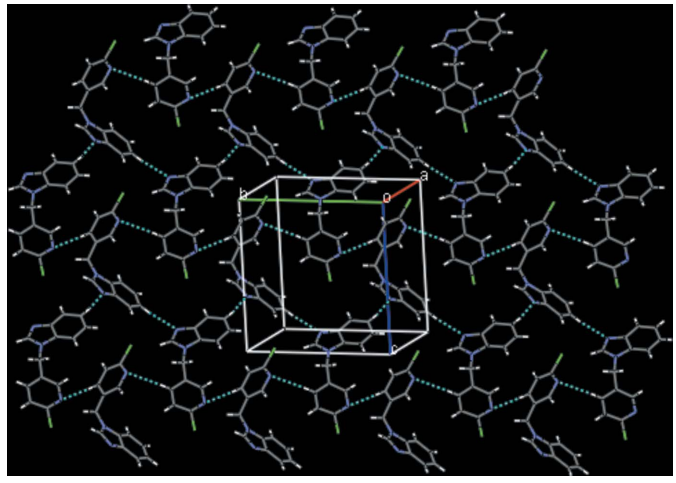


Figure 2
The two-dimensional network structure of (I) formed by intermolecular hydrogen bonding interactions (shown as dashed lines).

After their initial location in a difference Fourier map, all H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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