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6-Chloro-2-(dibromomethyl)pyridine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.022
wR factor = 0.054
Data-to-parameter ratio = 13.8

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

In the crystal structure of the title compound, $C_6H_4Br_2ClN$, all atoms but Br are located on a crystallographic mirror plane. The crystal packing is stabilized by offset π–π stacking.

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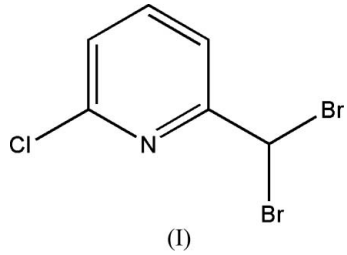
Comment

All atoms of the title compound, (I), except the two Br atoms, are located on a crystallographic mirror plane, so the molecule is perfectly planar with the two Br atoms located symmetrically on each side of the mirror plane (Fig. 1).



(I)

The packing is stabilized by offset π–π stacking, with a centroid-to-centroid distance of 3.87 Å and a plane-to-plane distance of 3.52 Å (Fig. 2)

Experimental

2-Chloro-6-methylpyridine (20 g, 0.157 mol) was dissolved in carbon tetrachloride (200 ml) and the solution was added to *N*-bromosuccinimide (56 g, 0.314 mol) and benzoyl peroxide (0.25 g). The mixture was refluxed for 24 h and then cooled to room temperature. The succinimide precipitate was filtered off and the filtrate was evaporated under reduced pressure to give a light-brown oil. Purification with flash chromatography (petroleum ether 333–363 K) gave a white solid (Gultneh *et al.*, 2003).

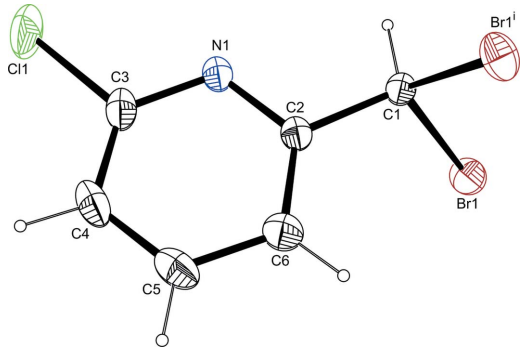


Figure 1
A molecular view of (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $-x$, $-y+\frac{1}{2}$, z.]

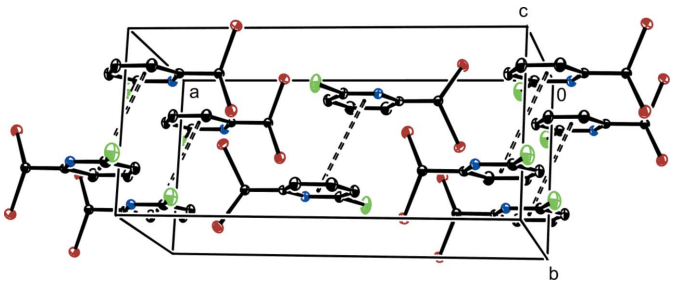


Figure 2
The packing of (I), showing the offset π–π stacking (dashed lines). Displacement ellipsoids are drawn at the 20% probability level and H atoms have been omitted for clarity.

Crystal data

$C_6H_4Br_2ClN$
M_r = 285.37
Orthorhombic, *Pnma*
a = 14.839 (3) Å
b = 7.0388 (12) Å
c = 7.9745 (14) Å
V = 832.9 (3) Å^3
Z = 4
D_x = 2.276 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2146 reflections
θ = 2.8–27.7°
μ = 9.97 mm^{-1}
T = 293 (2) K
Block, colourless
0.28 × 0.22 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.06, T_{max} = 0.16
4261 measured reflections
803 independent reflections
725 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 25.0°
$h = -15 \rightarrow 17$
$k = -8 \rightarrow 8$
$l = -9 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.055
S = 1.13
803 reflections
58 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0267P)^2 + 0.4103P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

H atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 ($C_{aromatic}$) or 0.98 Å ($C_{methine}$) and with U_{iso}(H) = 1.2U_{eq}(C)

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Bruker, 1999).

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