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6-Bromopyridine-2-carbaldehyde

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Key indicators

Single-crystal X-ray study
T = 290 K
Mean σ(C–C) = 0.007 Å
R factor = 0.038
wR factor = 0.099
Data-to-parameter ratio = 12.1

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

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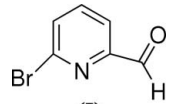
The molecule of the title compound, C_6H_4BrNO, is essentially planar. In the crystal structure, C—H···N hydrogen bonds link the molecules into a chain along the *b* axis.

Comment

6-Bromopyridine-2-carbaldehyde derivatives have received much attention as building blocks for supramolecules and ligands for transition metal catalysts and luminescent complexes (Li *et al.*, 2001; Orita *et al.*, 2004). We here report the crystal structure of the title compound, (I).



(I)

Bond lengths and angles in (I) are normal (Table 1). The molecule is essentially planar, with an r.m.s. deviation of 0.006 (4) Å for fitted non-H atoms (Fig. 1). The crystal packing reveals that the molecules translated by one unit cell along the *b*-axis direction are linked into a chain by intermolecular C—H···N hydrogen-bonding interactions (Fig. 2).

Experimental

Compound (I) was prepared according to the reported precedure of Parks *et al.* (1971). Yellow single crystals suitable for X-ray diffraction were obtained by recrystallization from ethyl acetate.

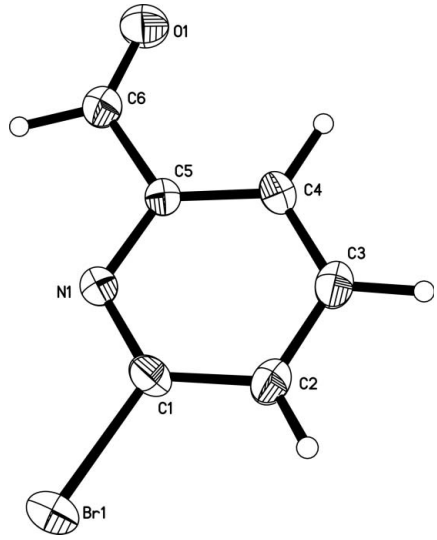


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering.

Crystal data

C_6H_4BrNO
M_r = 186.00
Monoclinic, $P2_1/a$
a = 6.908 (2) Å
b = 6.290 (4) Å
c = 15.060 (6) Å
β = 95.57 (3)°
V = 651.3 (5) Å^3
Z = 4
D_x = 1.897 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 6.22 mm^{-1}
T = 290 (2) K
Block, yellow
0.24 × 0.22 × 0.22 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
1335 measured reflections
1202 independent reflections
750 reflections with $I > 2\sigma(I)$
R_{int} = 0.012
θ_{max} = 25.4°
3 standard reflections
every 200 reflections
intensity decay: 1.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.099
S = 0.99
1202 reflections
99 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.056P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.037 (4)

Table 1
Selected geometric parameters (Å, °).

Br1—C1	1.901 (5)	C2—C3	1.368 (7)
O1—C6	1.207 (6)	C3—C4	1.364 (7)
N1—C1	1.296 (6)	C4—C5	1.376 (7)
N1—C5	1.341 (6)	C5—C6	1.481 (7)
C1—C2	1.390 (8)		
C1—N1—C5	117.1 (4)	N1—C5—C6	114.8 (4)
N1—C1—C2	124.6 (4)	C4—C5—C6	122.5 (4)
N1—C1—Br1	116.4 (4)	O1—C6—C5	123.6 (5)
N1—C5—C4	122.7 (4)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···N1^{i}	1.03 (6)	2.52 (6)	3.534 (7)	167 (4)

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

H atoms were located in a difference Fourier map and refined isotropically. The C—H bond lengths lie in the range 0.91 (5)–1.05 (6) Å.

Data collection: *DIFRAC* (Gabe *et al.*, 1993); cell refinement: *DIFRAC*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

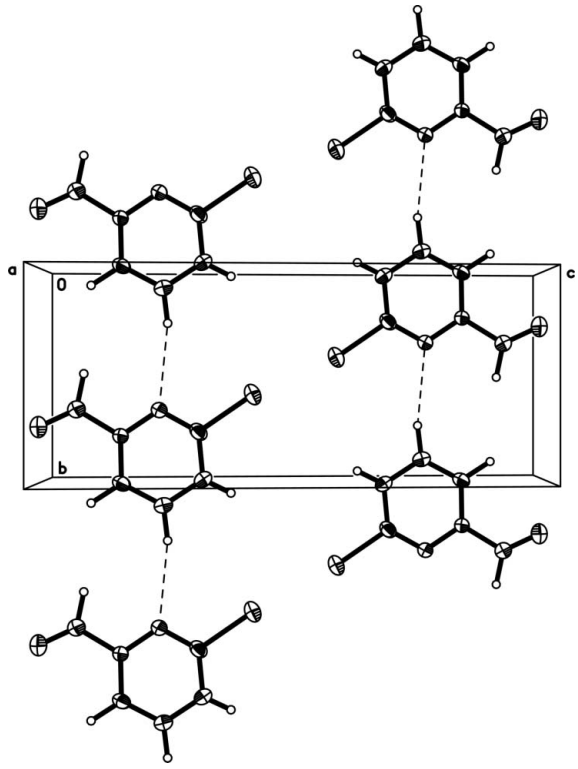


Figure 2
The crystal packing of (I), showing C—H···N hydrogen-bonded (dashed lines) chains.

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References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* **22**, 384–387.
Gabe, E. J., White, P. S. & Enright, G. D. (1993). *DIFRAC*. National Research Council Canada, Ottawa.
Li, X., Gibb, C. L. D., Kuebel, M. E. & Gibbp, B. C. (2001). *Tetrahedron*, **57**, 1175–1182.
Orita, A., Nakano, T., Yokoyama, T., Babu, G. & Otera, J. (2004). *Chem. Lett.* **33**, 1298–1299.
Parks, J. E., Wagner, B. E. & Holm, R. H. (1971). *Inorg. Chem.* **10**, 2472–2478.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.