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5-Bromo-2-(hydroxymethyl)pyridine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.015 Å
R factor = 0.056
wR factor = 0.142
Data-to-parameter ratio = 15.8

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

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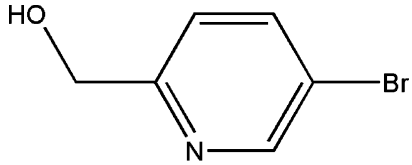
The molecule of the title compound, C_6H_6BrNO, is essentially planar. Intermolecular O—H···Br hydrogen bonds link the molecules into a chain along [101].

Comment

The title compound, (I), is an intermediate in the synthesis of a non-haem template for attaching peptides (Van den Heuvel *et al.*, 2004). The molecule of (I) (Fig. 1) is essentially planar. The hydroxyl O atom deviates from the mean plane through the remaining non-H atoms by 0.183 (10) Å.



(I)

An intramolecular C—H···O interaction is observed in the molecular structure of (I) (Table 1). Symmetry-related molecules are linked *via* O—H···Br intermolecular interactions to form infinite one-dimensional chains along [101].

Experimental

Compound (I) was prepared by the reported procedure of Van den Heuvel *et al.* (2004). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethyl acetate (25 ml) solution of (I) (1.0 g).

Crystal data

C_6H_6BrNO
M_r = 188.03
Monoclinic, $P2_1$
a = 4.039 (1) Å
b = 8.974 (2) Å
c = 9.224 (2) Å
β = 93.09 (3)°
V = 333.85 (13) Å^3
Z = 2
D_x = 1.870 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 6.07 mm^{-1}
T = 293 (2) K
Block, brown
0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.263, T_{max} = 0.377
(expected range = 0.208–0.297)
1479 measured reflections
1294 independent reflections
1093 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.142$
$S = 1.04$
1294 reflections
82 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0999P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.77$ e Å^{-3}
Absolute structure: Flack (1983), with 601 Friedel pairs
Flack parameter: −0.01 (3)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···Br1^{i}	0.82	2.47	3.272 (7)	165
C4—H4···O1	0.93	2.49	2.809 (11)	100

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

H atoms were placed in idealized positions and allowed to ride on their parent atoms, with O—H = 0.82 Å and C—H = 0.93 or 0.97 Å, and U_{iso}(H) = 1.2–1.5U_{eq}(C,O).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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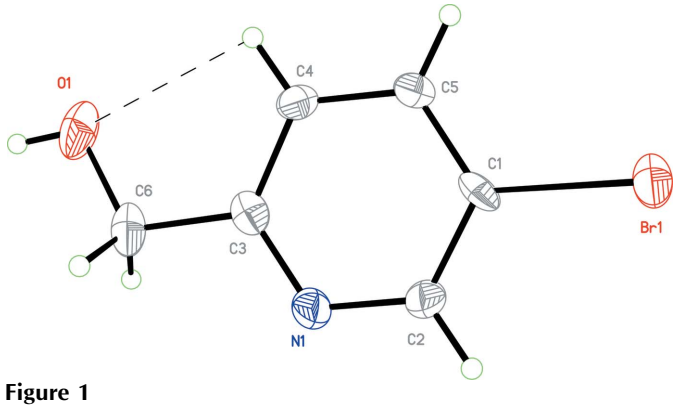

Figure 1
The structure of (I). Displacement ellipsoids are drawn at the 50% probability level. The dashed line indicates the intramolecular C—H···O hydrogen bond.

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