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3-Bromopyridin-2-amine

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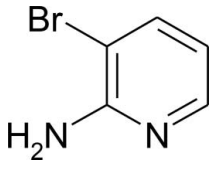
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.082; data-to-parameter ratio = 17.6.

In the crystal structure of the title compound, $C_5H_5BrN_2$, molecules assemble *via* pairs of N—H···N hydrogen bonds into inversion dimers using only the *syn* H atom on the amine group. These dimers then assemble further into two-dimensional layers *via* type I C—Br···Br [Br···Br = 3.693 (s6) Å] halogen bonding along the (102) plane.

Related literature

For halogen bonding, see: Metrangelo *et al.* (2005). For a related structure, see: Hu *et al.* (2011).



Experimental

Crystal data

$C_5H_5BrN_2$
M_r = 173.02
Monoclinic, $P2_1/c$
a = 12.2179 (6) Å
b = 4.0007 (2) Å
c = 12.8451 (6) Å
β = 109.731 (3)°
V = 591.01 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 6.84 mm^{-1}
T = 173 K
0.5 × 0.4 × 0.09 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: integration (*XPREP*; Bruker, 2004)
T_{min} = 0.131, T_{max} = 0.578
5622 measured reflections
1428 independent reflections
1200 reflections with $I > 2\sigma(I)$
R_{int} = 0.093

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.082
S = 0.99
1428 reflections
81 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.04 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*S*···N1^{i}	0.81 (4)	2.21 (4)	3.019 (4)	173 (3)

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* and *XPREP* (Bruker 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2050).

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supporting information

Acta Cryst. (2012). E**68**, o385 [doi:10.1107/S1600536811055541]

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S1. Comment

The title compound is being used as a co-crystal former for potential co-crystal with the molecule 2-chloro-4-nitro-benzoic acid. As its structure has not been determined previously, and for screening purposes, it is now reported (Fig. 1). The title molecule forms centrosymmetric dimers using the *syn* H2S atom on the amine group. The *anti* H atom H2A is not involved in any intermolecular interactions. The dimers are joined by type II C—Br···Br halogen bonding (Metrangelo *et al.*, 2005) to form 2-D layers (Fig. 2). The related compound, 3-chloropyridin-2-amine (Hu *et al.*, 2011), has the same hydrogen bonded dimers, but forms instead chains of dimers through C—Cl···Cl halogen bonding of type I.

S2. Experimental

Crystals were grown by slow evaporation of a methanol solution of the title compound, 0.200 g (1.16 mmol) in 8 ml of methanol, and afforded light brown plates after three days of slow evaporation at ambient conditions.

S3. Refinement

The aromatic C-bound H atoms were geometrically placed, C—H bond length of 0.95 Å and refined as riding with U_{iso}(H) = 1.2U_{eq}(C). The N-bound H atoms were located in the difference map and coordinates as well as isotropic displacement parameters refined freely.

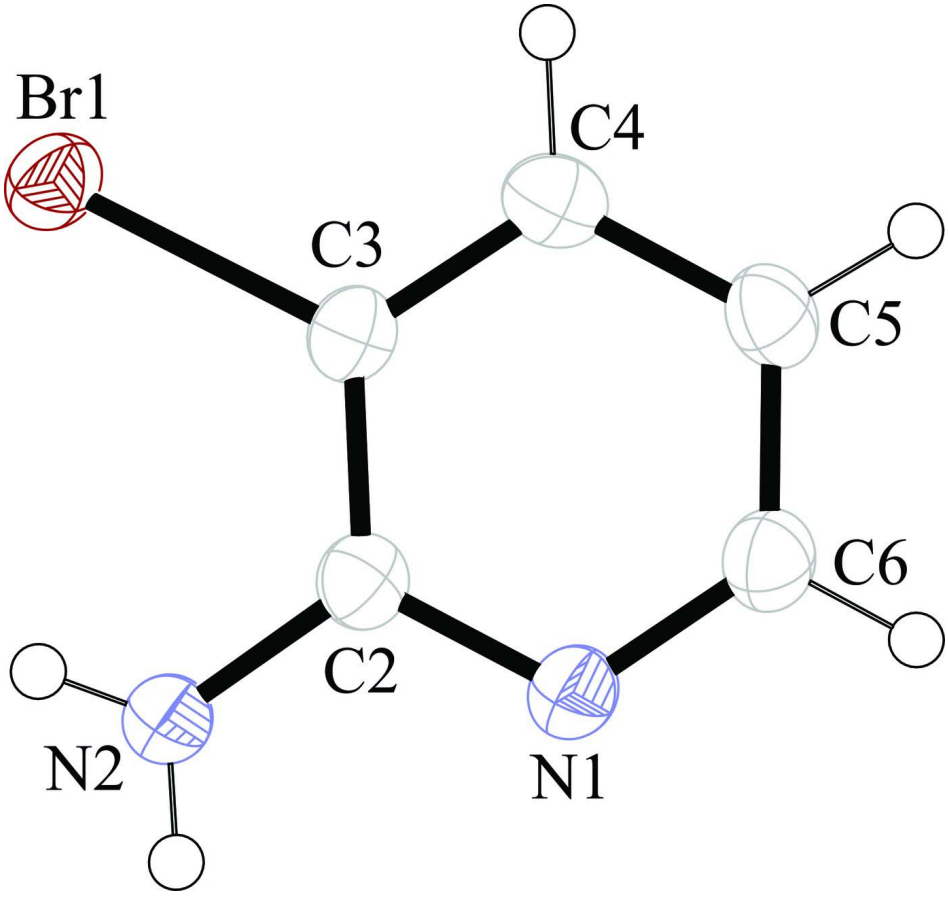

Figure 1

The asymmetric unit of (I) showing the atomic numbering scheme. Displacement ellipsoids are shown at the 50% probability level.

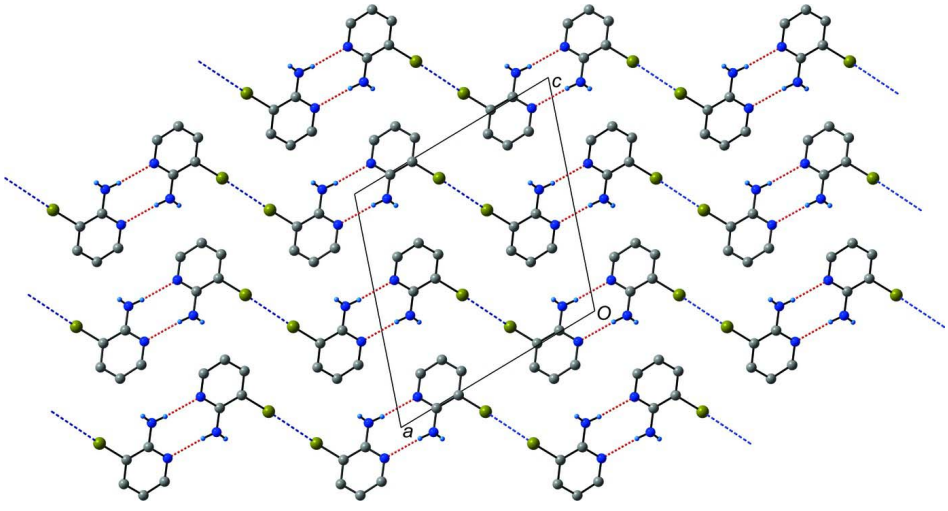

Figure 2

Packing diagram of (I). Intermolecular N—H···N hydrogen bonds are shown as dashed red lines forming dimers. Note that the *anti* H is not used in any hydrogen bonding interactions. The C—Br···Br halogen bonds are shown as dashed blue lines.

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$M_r = 173.02$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.2179$ (6) Å
$b = 4.0007$ (2) Å
$c = 12.8451$ (6) Å
$\beta = 109.731$ (3)°
$V = 591.01$ (5) Å^3
$Z = 4$
$F(000) = 336$
$D_x = 1.945$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2888 reflections
$\theta = 3.2$–$28.3°$
$\mu = 6.84$ mm^{-1}
$T = 173$ K
Plate, brown
0.5 × 0.4 × 0.09 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
ω scans
Absorption correction: integration (*XPREP*; Bruker, 2004)
$T_{min} = 0.131$, $T_{max} = 0.578$
5622 measured reflections
1428 independent reflections
1200 reflections with $I > 2\sigma(I)$
$R_{int} = 0.093$
$\theta_{max} = 28.0°$, $\theta_{min} = 1.8°$
$h = -16 \rightarrow 15$
$k = -5 \rightarrow 5$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.082$
$S = 0.99$
1428 reflections
81 parameters
0 restraints
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.04$ e Å^{-3}
$\Delta\rho_{min} = -0.77$ e Å^{-3}

Special details

Experimental. Numerical integration absorption corrections based on indexed crystal faces were applied using the *XPREP* routine (Bruker, 2004)

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C2	0.8182 (2)	0.4235 (7)	0.4926 (2)	0.0288 (6)
C3	0.7048 (2)	0.3668 (6)	0.4912 (2)	0.0267 (5)
C4	0.6702 (2)	0.4704 (7)	0.5771 (2)	0.0309 (6)
H4	0.5934	0.4287	0.5763	0.037*
C5	0.7499 (3)	0.6374 (7)	0.6653 (2)	0.0327 (6)
H5	0.729	0.7168	0.7258	0.039*
C6	0.8602 (3)	0.6833 (7)	0.6615 (2)	0.0334 (6)
H6	0.915	0.7976	0.7215	0.04*
N1	0.8956 (2)	0.5781 (6)	0.5793 (2)	0.0325 (5)

N2	0.8547 (3)	0.3359 (7)	0.4077 (2)	0.0386 (6)
Br1	0.59557 (2)	0.15619 (6)	0.36599 (2)	0.03201 (13)
H2S	0.923 (3)	0.345 (7)	0.415 (3)	0.030 (9)*
H2A	0.820 (4)	0.210 (8)	0.362 (4)	0.043 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0309 (14)	0.0294 (12)	0.0253 (12)	0.0002 (11)	0.0084 (11)	0.0031 (10)
C3	0.0271 (14)	0.0256 (12)	0.0238 (12)	0.0031 (9)	0.0039 (11)	0.0034 (9)
C4	0.0282 (14)	0.0331 (13)	0.0319 (13)	0.0070 (11)	0.0107 (11)	0.0076 (12)
C5	0.0359 (16)	0.0376 (15)	0.0250 (13)	0.0059 (11)	0.0109 (12)	0.0036 (10)
C6	0.0343 (16)	0.0367 (15)	0.0273 (13)	−0.0010 (12)	0.0079 (12)	0.0002 (11)
N1	0.0286 (13)	0.0408 (12)	0.0266 (11)	−0.0041 (10)	0.0073 (10)	−0.0022 (10)
N2	0.0303 (15)	0.0568 (18)	0.0309 (13)	−0.0112 (12)	0.0134 (12)	−0.0120 (12)
Br1	0.02548 (18)	0.03463 (19)	0.03161 (18)	0.00029 (10)	0.00396 (12)	−0.00178 (10)

Geometric parameters (Å, º)

C2—N1	1.344 (4)	C5—C6	1.378 (5)
C2—N2	1.357 (4)	C5—H5	0.95
C2—C3	1.398 (4)	C6—N1	1.336 (4)
C3—C4	1.372 (4)	C6—H6	0.95
C3—Br1	1.904 (3)	N2—H2S	0.81 (4)
C4—C5	1.390 (4)	N2—H2A	0.78 (4)
C4—H4	0.95		
N1—C2—N2	117.1 (3)	C6—C5—H5	121.3
N1—C2—C3	120.2 (2)	C4—C5—H5	121.3
N2—C2—C3	122.7 (3)	N1—C6—C5	124.6 (3)
C4—C3—C2	120.8 (3)	N1—C6—H6	117.7
C4—C3—Br1	119.7 (2)	C5—C6—H6	117.7
C2—C3—Br1	119.5 (2)	C6—N1—C2	118.4 (2)
C3—C4—C5	118.7 (3)	C2—N2—H2S	120 (3)
C3—C4—H4	120.6	C2—N2—H2A	122 (3)
C5—C4—H4	120.6	H2S—N2—H2A	113 (4)
C6—C5—C4	117.3 (3)		
N1—C2—C3—C4	0.7 (4)	C3—C4—C5—C6	−1.1 (4)
N2—C2—C3—C4	−177.6 (3)	C4—C5—C6—N1	−0.1 (4)
N1—C2—C3—Br1	178.6 (2)	C5—C6—N1—C2	1.7 (4)
N2—C2—C3—Br1	0.3 (4)	N2—C2—N1—C6	176.5 (3)
C2—C3—C4—C5	0.9 (4)	C3—C2—N1—C6	−1.9 (4)
Br1—C3—C4—C5	−177.04 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*S*···N1^{i}	0.81 (4)	2.21 (4)	3.019 (4)	173 (3)

Symmetry code: (i) −*x*+2, −*y*+1, −*z*+1.