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5-Bromo-2-chloropyrimidin-4-amine

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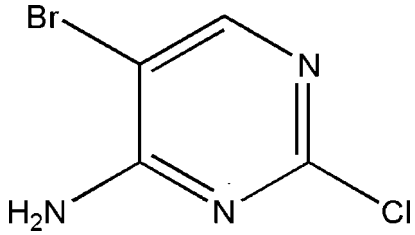
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.024; wR factor = 0.058; data-to-parameter ratio = 14.4.

In the title compound, $C_4H_3BrClN_3$, the pyrimidine ring is essentially planar (r.m.s. deviation from the plane = 0.087 Å). In the crystal, pairs of N—H···N hydrogen bonds connect the molecules into inversion dimers; these are connected by further N—H···N hydrogen bonds into a two-dimensional framework parallel to the *bc* plane.

Related literature

For background to pyrimidine derivatives, see: Yu *et al.* (2007). For related structures, see: van Albada *et al.* (2012); Yang *et al.* (2012).



Experimental

Crystal data

$C_4H_3BrClN_3$
M_r = 208.45
Monoclinic, $P2_1/c$
a = 6.0297 (1) Å
b = 8.1542 (2) Å
c = 13.4163 (3) Å
β = 90.491 (2)°
V = 659.62 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 6.54 mm^{-1}
T = 293 K
0.3 × 0.2 × 0.1 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.306, T_{max} = 1.000
43395 measured reflections
1297 independent reflections
1164 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.058
S = 1.10
1297 reflections
90 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N7—H71···N1^{i}	0.78 (3)	2.38 (3)	3.087 (3)	153 (3)
N7—H72···N3^{ii}	0.91 (4)	2.19 (4)	3.088 (3)	171 (3)

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); 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, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

MK acknowledges the help of Bahubali College of Engineering, Shravanabelagola for his research work. RK acknowledges the Department of Science & Technology for the single-crystal X-ray diffractometer sanctioned as a National Facility under project No. SR/S2/CMP-47/2003.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2560).

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supporting information

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5-Bromo-2-chloropyrimidin-4-amine

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S1. Comment

Some derivatives of pyrimidine are important chemical materials (Yu *et al.*, 2007). Here in this article, the preparation and crystal structure of the title compound is presented. Bond lengths and angles in the title compound (Fig. 1) are comparable with the similar crystal structures (van Albada *et al.*, 2012; Yang *et al.*, 2012). The pyrimidine ring is essentially planar (r.m.s. deviation from the plane 0.087 Å). The atoms Br,Cl and N7 are coplanar with the pyrimidine ring. In the crystal, molecules are linked into dimers by N7—H72···N3 hydrogen bonds and these dimers are further connected by N7—H71···N1 hydrogen bonds, forming two dimensional supramolecular network in the *bc* plane (Fig.2, (Table 2).

S2. Experimental

To a solution of stannous chloride dihydrate (2.8 ml, 0.012 mole) in hydrochloric acid (30 ml) cooled to 273K, 5-bromo-2-chloro-4-nitropyrimidine (2 g, 0.0083 mole) was added in portions while the suspension was vigorously stirred for 6 hrs. The mixture was then poured onto crushed ice, made alkaline with solid sodium hydroxide, and extracted three times with ethyl acetate (100 ml). The combined organic phase was dried over anhydrous sodium sulfate and the filtrate was evaporated to dryness. The compound was purified by successive recrystallization from acetonitrile (yield 90%, m. p. 460–461 K).

S3. Refinement

The N-bound H atoms were located in a difference Fourier map and freely refined. All other H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H distances of 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C).

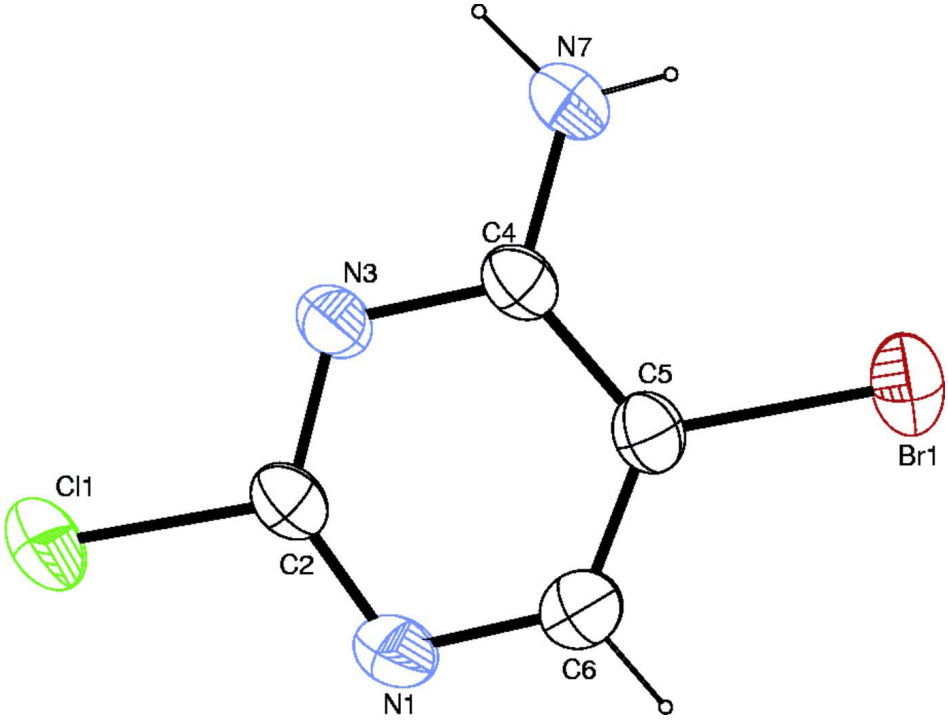

Figure 1

ORTEP view of the molecule with the atom-labeling scheme. The displacement ellipsoids are drawn at the 40% probability level. H atoms are shown as small spheres of arbitrary radii.

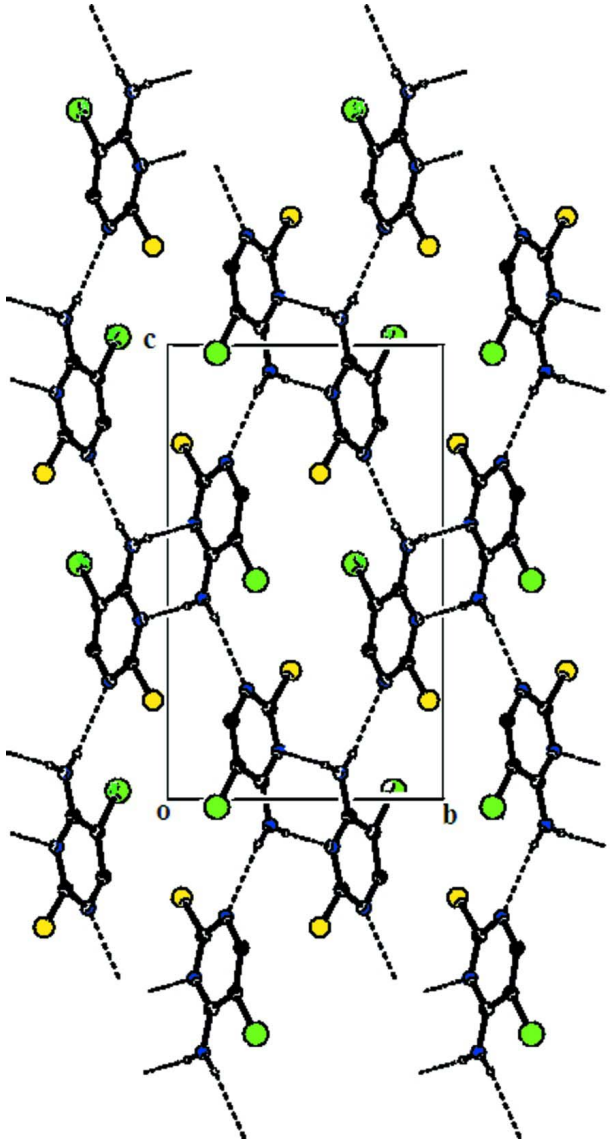

Figure 2

A molecular packing view of the title compound down the *a* axis, showing intermolecular interactions. The dotted lines show intermolecular N—H···N hydrogen bonds.

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Crystal data

$C_4H_3BrClN_3$
$M_r = 208.45$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 6.0297$ (1) Å
$b = 8.1542$ (2) Å
$c = 13.4163$ (3) Å
$\beta = 90.491$ (2)°
$V = 659.62$ (2) Å^3
$Z = 4$

$F(000) = 400$
$D_x = 2.099$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 20319 reflections
$\theta = 3.7$–29.0°
$\mu = 6.54$ mm^{-1}
$T = 293$ K
Block, white
0.3 × 0.2 × 0.1 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.1049 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.306, T_{max} = 1.000
43395 measured reflections
1297 independent reflections
1164 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 26.0°, θ_{min} = 3.9°
h = −7→7
k = −10→10
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.058
S = 1.10
1297 reflections
90 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0275P)^2 + 0.4995P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Special details

Experimental. *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27–08-2010 CrysAlis171. NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Br1	0.69350 (4)	0.17972 (4)	0.48221 (2)	0.04520 (12)
Cl1	−0.00058 (12)	0.44749 (10)	0.78250 (5)	0.04662 (19)
N1	0.3588 (4)	0.2880 (3)	0.74005 (15)	0.0397 (5)
C2	0.1934 (4)	0.3694 (3)	0.69923 (17)	0.0302 (5)
N3	0.1489 (3)	0.4025 (3)	0.60525 (14)	0.0310 (4)
C4	0.2921 (4)	0.3417 (3)	0.53797 (17)	0.0293 (5)
C5	0.4802 (4)	0.2544 (3)	0.57261 (17)	0.0308 (5)
C6	0.5050 (4)	0.2317 (4)	0.67197 (19)	0.0400 (6)
H6	0.6288	0.1744	0.6947	0.048*
N7	0.2498 (5)	0.3721 (3)	0.44228 (16)	0.0413 (6)
H71	0.317 (5)	0.329 (3)	0.401 (2)	0.037 (8)*
H72	0.125 (6)	0.428 (4)	0.425 (3)	0.063 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03877 (18)	0.05169 (19)	0.04536 (18)	0.00220 (12)	0.01297 (12)	−0.00698 (12)
Cl1	0.0474 (4)	0.0627 (5)	0.0300 (3)	0.0046 (3)	0.0130 (3)	−0.0023 (3)
N1	0.0393 (12)	0.0544 (14)	0.0254 (10)	0.0025 (10)	0.0014 (9)	0.0059 (9)
C2	0.0323 (13)	0.0332 (12)	0.0251 (11)	−0.0060 (10)	0.0038 (9)	−0.0011 (9)
N3	0.0335 (11)	0.0357 (11)	0.0238 (9)	−0.0003 (9)	0.0024 (8)	−0.0001 (8)
C4	0.0300 (12)	0.0331 (13)	0.0247 (11)	−0.0069 (10)	0.0022 (9)	−0.0016 (9)
C5	0.0303 (13)	0.0312 (12)	0.0309 (12)	−0.0037 (10)	0.0048 (10)	−0.0016 (10)
C6	0.0347 (14)	0.0483 (16)	0.0371 (13)	0.0052 (12)	−0.0010 (11)	0.0049 (12)
N7	0.0448 (14)	0.0569 (15)	0.0221 (11)	0.0080 (12)	0.0027 (10)	−0.0018 (10)

Geometric parameters (Å, º)

Br1—C5	1.877 (2)	C4—N7	1.330 (3)
Cl1—C2	1.744 (2)	C4—C5	1.415 (3)
N1—C2	1.314 (3)	C5—C6	1.353 (3)
N1—C6	1.355 (3)	C6—H6	0.9300
C2—N3	1.315 (3)	N7—H71	0.78 (3)
N3—C4	1.349 (3)	N7—H72	0.91 (4)
C2—N1—C6	112.7 (2)	C6—C5—Br1	121.5 (2)
N1—C2—N3	130.6 (2)	C4—C5—Br1	120.20 (17)
N1—C2—Cl1	115.35 (18)	C5—C6—N1	123.4 (2)
N3—C2—Cl1	114.02 (18)	C5—C6—H6	118.3
C2—N3—C4	116.1 (2)	N1—C6—H6	118.3
N7—C4—N3	117.3 (2)	C4—N7—H71	121 (2)
N7—C4—C5	123.9 (2)	C4—N7—H72	119 (2)
N3—C4—C5	118.8 (2)	H71—N7—H72	119 (3)
C6—C5—C4	118.3 (2)		
C6—N1—C2—N3	0.5 (4)	N3—C4—C5—C6	1.9 (4)
C6—N1—C2—Cl1	−179.43 (19)	N7—C4—C5—Br1	2.1 (3)
N1—C2—N3—C4	1.4 (4)	N3—C4—C5—Br1	−175.96 (17)
Cl1—C2—N3—C4	−178.71 (17)	C4—C5—C6—N1	0.1 (4)
C2—N3—C4—N7	179.4 (2)	Br1—C5—C6—N1	177.9 (2)
C2—N3—C4—C5	−2.5 (3)	C2—N1—C6—C5	−1.2 (4)
N7—C4—C5—C6	179.9 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N7—H71···N1^{i}	0.78 (3)	2.38 (3)	3.087 (3)	153 (3)
N7—H72···N3^{ii}	0.91 (4)	2.19 (4)	3.088 (3)	171 (3)

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) −*x*, −*y*+1, −*z*+1.