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## Structure Reports

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### 3-Chloro-6-(1*H*-pyrazol-1-yl)pyridazine

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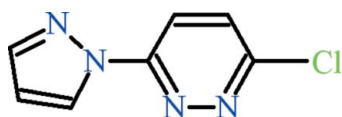
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å;  $R$  factor = 0.062;  $wR$  factor = 0.154; data-to-parameter ratio = 13.0.

The title compound,  $\text{C}_7\text{H}_5\text{ClN}_4$ , is almost planar (r.m.s. deviation = 0.022 Å). The dihedral angle between the aromatic rings is 2.82 (5)°. The packing results in polymeric chains extending along the  $a$  axis. In the crystal, molecules are connected to each other through intermolecular  $\text{C}-\text{H}\cdots\text{N}$  hydrogen bonds, resulting in  $R_2^2(10)$  ring motifs.

#### Related literature

For related structures, see: Ather *et al.* (2009, 2010*a,b*). For graph-set notation, see: Bernstein *et al.* (1995).



#### Experimental

##### Crystal data

$\text{C}_7\text{H}_5\text{ClN}_4$   
 $M_r = 180.60$   
 Triclinic,  $P\bar{1}$   
 $a = 5.684$  (3) Å  
 $b = 6.526$  (3) Å  
 $c = 11.130$  (6) Å  
 $\alpha = 83.00$  (3)°  
 $\beta = 77.64$  (2)°

$\gamma = 88.04$  (3)°  
 $V = 400.2$  (4) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.42$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.30 \times 0.14 \times 0.14$  mm

##### Data collection

Bruker Kappa APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2005)  
 $T_{\min} = 0.982$ ,  $T_{\max} = 0.988$

5550 measured reflections  
 1422 independent reflections  
 774 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.071$

##### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.062$   
 $wR(F^2) = 0.154$   
 $S = 1.08$   
 1422 reflections

109 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.22$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.22$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C3}-\text{H3}\cdots\text{N2}^i$	0.93	2.46	3.321 (6)	154
$\text{C5}-\text{H5}\cdots\text{N4}^{ii}$	0.93	2.55	3.468 (7)	169

Symmetry codes: (i)  $x + 1, y, z$ ; (ii)  $x - 1, y, z$ .

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; 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 PLATON (Spek, 2009); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON.

The authors acknowledge the provision of funds for the purchase of diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2034).

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**supplementary materials**

*Acta Cryst.* (2010). E66, o2016 [ doi:10.1107/S1600536810027121 ]

### 3-Chloro-6-(1*H*-pyrazol-1-yl)pyridazine

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#### Comment

The title compound (I, Fig. 1) has been prepared as nucleus to synthesize a series of pyrazolylpyridazine derivatives. In this context, we have already reported some compounds (Ather *et al.*, 2009, 2010*a*, 2010*b*).

The title compound is essentially planar. The r. m. s. deviation of all heavy atoms from the mean square plane is 0.0223 Å. The angle between the heterocyclic aromatic rings is 2.82 (5)°. Each molecule is connected to the adjacent molecules through C—H···N intermolecular H-bonds (Table 1, Fig. 2) and  $R_2^2(10)$  ring motifs (Bernstein *et al.*, 1995) are formed. In this way the packing forms one dimensional polymeric chains extending along the crystallographic *a* axis.

#### Experimental

3-Chloro-6-hydrazinylpyridazine (0.5 g, 3.46 mmol) was dissolved in ethanol (15 ml) and malon dialdehyde bis-(diethylacetal) (0.327 g, 3.46 mmol) was added dropwise under continuous stirring. Few drops of acetic acid were also added in the reaction mixture as catalyst and the solution was refluxed for 2 h. The reaction was monitored by TLC. After completion, the reaction mixture was precipitated by adding water. The filtered precipitate was dried and colorless needles of (I) appeared on the walls of the beaker due to evaporation.

#### Refinement

Although all H-atoms appear in the difference Fourier map they were positioned geometrically (C—H = 0.93 Å) and refined as riding atoms with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

#### Figures

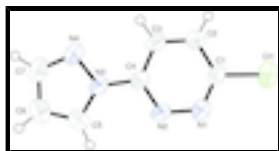


Fig. 1. View of the title compound with the atom numbering scheme. The thermal ellipsoids are drawn at the 50% probability level. H-atoms are shown as small spheres of arbitrary radii.

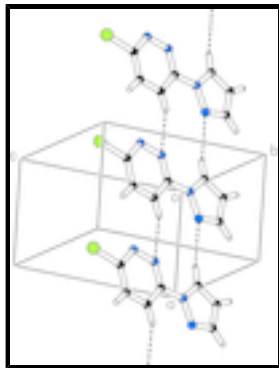


Fig. 2. Packing diagram of the title compound (*PLATON*: Spek, 2009) showing that the molecules form polymeric chains extending along the *a* axis.

### 3-Chloro-6-(1*H*-pyrazol-1-yl)pyridazine

#### Crystal data

$C_7H_5ClN_4$

$M_r = 180.60$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 5.684$  (3) Å

$b = 6.526$  (3) Å

$c = 11.130$  (6) Å

$\alpha = 83.00$  (3)°

$\beta = 77.64$  (2)°

$\gamma = 88.04$  (3)°

$V = 400.2$  (4) Å<sup>3</sup>

$Z = 2$

$F(000) = 184$

$D_x = 1.499$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 774 reflections

$\theta = 3.2$ – $25.1$ °

$\mu = 0.42$  mm<sup>-1</sup>

$T = 296$  K

Needle, colourless

$0.30 \times 0.14 \times 0.14$  mm

#### Data collection

Bruker Kappa APEXII CCD  
diffractometer

Radiation source: fine-focus sealed tube  
graphite

Detector resolution: 8.20 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2005)

$T_{\min} = 0.982$ ,  $T_{\max} = 0.988$

5550 measured reflections

1422 independent reflections

774 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.071$

$\theta_{\max} = 25.1$ °,  $\theta_{\min} = 3.2$ °

$h = -6 \rightarrow 6$

$k = -7 \rightarrow 7$

$l = -13 \rightarrow 13$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.062$

Primary atom site location: structure-invariant direct  
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring  
sites

$$wR(F^2) = 0.154$$

$$S = 1.08$$

1422 reflections

109 parameters

0 restraints

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0381P)^2 + 0.276P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 0.22 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$$

### Special details

**Geometry.** Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.0311 (2)	0.6902 (2)	0.86426 (11)	0.0772 (6)
N1	-0.0066 (6)	0.7294 (6)	0.6368 (3)	0.0586 (14)
N2	0.0752 (6)	0.7486 (6)	0.5126 (3)	0.0525 (14)
N3	0.3753 (6)	0.7757 (5)	0.3384 (3)	0.0449 (14)
N4	0.6127 (6)	0.7910 (6)	0.2806 (3)	0.0576 (16)
C1	0.1521 (8)	0.7182 (7)	0.7066 (4)	0.0503 (17)
C2	0.4010 (7)	0.7237 (7)	0.6628 (4)	0.0506 (17)
C3	0.4819 (7)	0.7451 (6)	0.5399 (4)	0.0450 (16)
C4	0.3094 (7)	0.7556 (6)	0.4674 (4)	0.0417 (16)
C5	0.2316 (9)	0.7798 (8)	0.2556 (4)	0.0676 (19)
C6	0.3770 (10)	0.7966 (9)	0.1421 (5)	0.078 (2)
C7	0.6095 (9)	0.8042 (8)	0.1617 (5)	0.0701 (19)
H2	0.50643	0.71294	0.71672	0.0608*
H3	0.64564	0.75254	0.50460	0.0538*
H5	0.06440	0.77251	0.27366	0.0814*
H6	0.33112	0.80200	0.06646	0.0928*
H7	0.74672	0.81708	0.09857	0.0841*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cl1	0.0676 (9)	0.1105 (13)	0.0459 (8)	-0.0045 (8)	0.0038 (6)	-0.0068 (7)
N1	0.040 (2)	0.084 (3)	0.047 (2)	-0.002 (2)	0.0002 (19)	-0.005 (2)
N2	0.028 (2)	0.076 (3)	0.051 (2)	-0.0027 (17)	-0.0050 (16)	-0.003 (2)
N3	0.0321 (19)	0.055 (3)	0.044 (2)	-0.0020 (17)	-0.0012 (16)	-0.0033 (18)
N4	0.041 (2)	0.076 (3)	0.049 (3)	-0.0033 (19)	0.0048 (17)	-0.005 (2)

## supplementary materials

C1	0.046 (3)	0.061 (3)	0.040 (3)	-0.004 (2)	0.002 (2)	-0.009 (2)
C2	0.040 (3)	0.060 (3)	0.052 (3)	-0.001 (2)	-0.011 (2)	-0.005 (2)
C3	0.031 (2)	0.049 (3)	0.052 (3)	-0.0045 (19)	-0.004 (2)	-0.001 (2)
C4	0.039 (2)	0.038 (3)	0.046 (3)	0.0016 (19)	-0.003 (2)	-0.008 (2)
C5	0.058 (3)	0.097 (4)	0.051 (3)	-0.002 (3)	-0.021 (3)	-0.004 (3)
C6	0.079 (4)	0.104 (5)	0.050 (3)	-0.009 (3)	-0.015 (3)	-0.006 (3)
C7	0.061 (3)	0.089 (4)	0.051 (3)	-0.008 (3)	0.008 (2)	-0.005 (3)

### Geometric parameters (Å, °)

C11—C1	1.732 (5)	C2—C3	1.338 (6)
N1—N2	1.353 (5)	C3—C4	1.392 (6)
N1—C1	1.306 (6)	C5—C6	1.348 (7)
N2—C4	1.319 (5)	C6—C7	1.388 (8)
N3—N4	1.366 (5)	C2—H2	0.9300
N3—C4	1.395 (5)	C3—H3	0.9300
N3—C5	1.354 (6)	C5—H5	0.9300
N4—C7	1.320 (6)	C6—H6	0.9300
C1—C2	1.394 (6)	C7—H7	0.9300
C11...C11 <sup>i</sup>	3.632 (3)	C3...N2 <sup>vi</sup>	3.321 (6)
C11...H7 <sup>ii</sup>	2.9500	C3...C3 <sup>iv</sup>	3.411 (6)
N1...C2 <sup>iii</sup>	3.318 (6)	C3...C3 <sup>v</sup>	3.339 (6)
N1...C3 <sup>iii</sup>	3.305 (6)	C3...C4 <sup>iv</sup>	3.442 (6)
N2...C3 <sup>iii</sup>	3.321 (6)	C3...C4 <sup>v</sup>	3.491 (6)
N4...C2 <sup>iv</sup>	3.342 (6)	C4...C3 <sup>iv</sup>	3.442 (6)
N4...C2 <sup>v</sup>	3.299 (6)	C4...C3 <sup>v</sup>	3.491 (6)
N1...H2 <sup>iii</sup>	2.7200	C7...H5 <sup>vi</sup>	3.0900
N1...H3 <sup>iii</sup>	2.7000	H2...N1 <sup>vi</sup>	2.7200
N2...H3 <sup>iii</sup>	2.4600	H3...N1 <sup>vi</sup>	2.7000
N2...H5	2.6600	H3...N2 <sup>vi</sup>	2.4600
N4...H5 <sup>vi</sup>	2.5500	H3...N4	2.5200
N4...H3	2.5200	H5...N2	2.6600
C2...N1 <sup>vi</sup>	3.318 (6)	H5...N4 <sup>iii</sup>	2.5500
C2...N4 <sup>iv</sup>	3.342 (6)	H5...C7 <sup>iii</sup>	3.0900
C2...N4 <sup>v</sup>	3.299 (6)	H7...C11 <sup>vii</sup>	2.9500
C3...N1 <sup>vi</sup>	3.305 (6)		
N2—N1—C1	117.9 (4)	N3—C5—C6	106.9 (5)
N1—N2—C4	119.1 (3)	C5—C6—C7	105.7 (5)
N4—N3—C4	120.1 (3)	N4—C7—C6	112.0 (5)
N4—N3—C5	111.4 (3)	C1—C2—H2	121.00
C4—N3—C5	128.5 (4)	C3—C2—H2	121.00
N3—N4—C7	104.0 (4)	C2—C3—H3	122.00
C11—C1—N1	114.7 (3)	C4—C3—H3	122.00
C11—C1—C2	120.4 (3)	N3—C5—H5	126.00
N1—C1—C2	124.9 (4)	C6—C5—H5	127.00

C1—C2—C3	117.2 (4)	C5—C6—H6	127.00
C2—C3—C4	116.9 (4)	C7—C6—H6	127.00
N2—C4—N3	114.7 (4)	N4—C7—H7	124.00
N2—C4—C3	124.0 (4)	C6—C7—H7	124.00
N3—C4—C3	121.3 (4)		
C1—N1—N2—C4	-0.1 (6)	N4—N3—C5—C6	0.4 (6)
N2—N1—C1—C11	-179.1 (3)	C4—N3—C5—C6	-178.6 (4)
N2—N1—C1—C2	-0.3 (7)	N3—N4—C7—C6	-0.3 (6)
N1—N2—C4—N3	-180.0 (4)	C11—C1—C2—C3	179.8 (3)
N1—N2—C4—C3	-0.2 (6)	N1—C1—C2—C3	1.0 (7)
C4—N3—N4—C7	179.0 (4)	C1—C2—C3—C4	-1.3 (6)
C5—N3—N4—C7	0.0 (5)	C2—C3—C4—N2	1.0 (6)
N4—N3—C4—N2	178.0 (4)	C2—C3—C4—N3	-179.3 (4)
N4—N3—C4—C3	-1.7 (6)	N3—C5—C6—C7	-0.6 (6)
C5—N3—C4—N2	-3.1 (6)	C5—C6—C7—N4	0.6 (7)
C5—N3—C4—C3	177.2 (4)		

Symmetry codes: (i)  $-x, -y+1, -z+2$ ; (ii)  $x-1, y, z+1$ ; (iii)  $x-1, y, z$ ; (iv)  $-x+1, -y+1, -z+1$ ; (v)  $-x+1, -y+2, -z+1$ ; (vi)  $x+1, y, z$ ; (vii)  $x+1, y, z-1$ .

*Hydrogen-bond geometry* ( $\text{\AA}, ^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C3—H3 $\cdots$ N2 <sup>vi</sup>	0.9300	2.4600	3.321 (6)	154.00
C5—H5 $\cdots$ N4 <sup>iii</sup>	0.9300	2.5500	3.468 (7)	169.00

Symmetry codes: (vi)  $x+1, y, z$ ; (iii)  $x-1, y, z$ .

Fig. 1

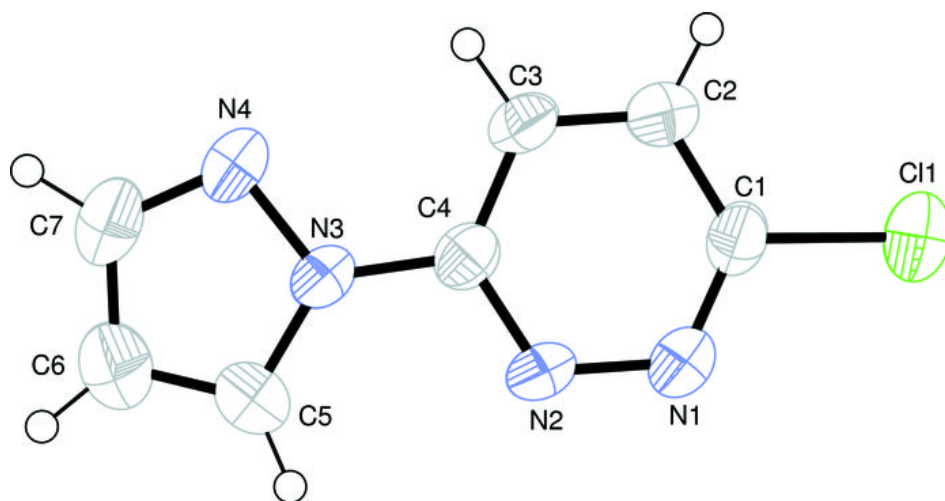




Fig. 2

