

3-Chloro-6-[2-(cyclopentylidene)-hydrazin-1-yl]pyridazine

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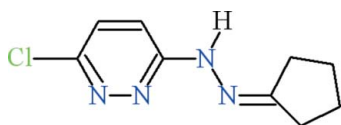
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.050; wR factor = 0.120; data-to-parameter ratio = 13.2.

The asymmetric unit of the title compound, $\text{C}_9\text{H}_{11}\text{ClN}_4$, contains two virtually planar molecules that differ in conformation about the bond connecting the hydrazine and pyridazine units. The 3-chloro-6-hydrazinylpyridazine and cyclopentane groups are oriented at dihedral angles of 4.5 (3) and 8.8 (4)° in the two molecules. In the crystal, the molecules form a one dimensional polymeric structure extending along the a axis via $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds. The crystal structure was an inversion twin [ratio of the twin domains = 0.73 (9):0.27 (9)].

Related literature

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



Experimental

Crystal data

$\text{C}_9\text{H}_{11}\text{ClN}_4$
 $M_r = 210.67$
 Orthorhombic, $Pca2_1$
 $a = 10.180$ (5) Å
 $b = 9.870$ (5) Å
 $c = 20.049$ (3) Å
 $V = 2014.5$ (15) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.34$ mm⁻¹
 $T = 296$ K
 $0.30 \times 0.15 \times 0.14$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2005)
 $T_{\min} = 0.942$, $T_{\max} = 0.950$
 7740 measured reflections
 3355 independent reflections
 2130 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$
 $wR(F^2) = 0.120$
 $S = 1.00$
 3355 reflections
 254 parameters
 1 restraint
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.18$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.17$ e Å⁻³
 Absolute structure: Flack (1983), 1307 Friedel pairs
 Flack parameter: 0.73 (9)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N3}-\text{H3A}\cdots\text{N5}^i$	0.86	2.52	3.295 (5)	150
$\text{N3}-\text{H3A}\cdots\text{N6}^i$	0.86	2.27	3.088 (5)	159
$\text{N7}-\text{H7}\cdots\text{N1}^i$	0.86	2.19	3.041 (5)	170

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

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); 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.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2360).

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supplementary materials

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3-Chloro-6-[2-(cyclopentylidene)hydrazin-1-yl]pyridazine

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Comment

In continuation to our studies on 3-chloro-6-hydrazinylpyridazine derivatives (Ather *et al.*, 2010*a,b,c*), the title compound (Fig. 1) is being reported here.

There are two symmetry independent molecule in the asymmetric unit of title compound that differ in conformation. In one molecule 3-chloro-6-hydrazinylpyridazine moiety A (C1—C4/N1—N4/CL1) and cyclopentane group B (C5—C9) are planar with r. m. s. deviations of 0.0104 and 0.0354 Å. The dihedral angle between A/B is 8.5 (4)°. In the second symmetry independent molecule 3-chloro-6-hydrazinylpyridazine moiety C (C10—C13/N5—N8/CL2) and cyclopentane group D (C14—C18) are also planar with r. m. s. deviations of 0.0068 and 0.0046 Å. The dihedral angle between C/D is 4.5 (3)°. The title compound consists of one dimensional polymeric chains via N—H···N hydrogen bonds extending along the crystallographic *a*-axis (Table 1, Fig. 2).

Experimental

3-Chloro-6-hydrazinylpyridazine (0.5 g, 3.46 mmol), dissolved in ethanol (10 ml) and refluxed for 15 min. Cyclopentanone (0.291 g, 3.459 mmol) was added to the former solution and refluxed about 3 h, till the completion of reaction monitored through TLC. On completion of the reaction mixture was concentrated under vacuum. The crude product was recrystallized in ethanol which yielded the light yellow needles of the title compound.

Refinement

The structure was refined as an inversion twin with 0.73 (9):0.27(9) ratio of the twin domains. The H-atoms were positioned geometrically (N—H = 0.86, C—H = 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C, N})$, where $x = 1.2$ for all H-atoms.

Figures

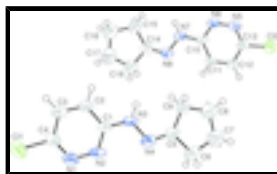


Fig. 1. View of the title compound with the atom numbering scheme. The thermal ellipsoids are drawn at the 50% probability level. H-atoms are shown as small spheres of arbitrary radii.

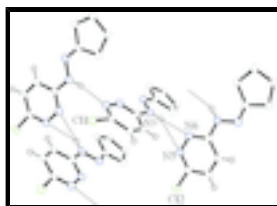


Fig. 2. The partial packing diagram (PLATON; Spek, 2009) showing polymeric chains extending along the *a*-axis. The H-atoms of cyclopentane are omitted for clarity.

3-Chloro-6-{2-[cyclopentylidene]hydrazin-1-yl}pyridazine

Crystal data

$C_9H_{11}ClN_4$	$F(000) = 880$
$M_r = 210.67$	$D_x = 1.389 \text{ Mg m}^{-3}$
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: P 2c -2ac	Cell parameters from 1374 reflections
$a = 10.180 (5) \text{ \AA}$	$\theta = 2.9\text{--}28.3^\circ$
$b = 9.870 (5) \text{ \AA}$	$\mu = 0.34 \text{ mm}^{-1}$
$c = 20.049 (3) \text{ \AA}$	$T = 296 \text{ K}$
$V = 2014.5 (15) \text{ \AA}^3$	Needle, light yellow
$Z = 8$	$0.30 \times 0.15 \times 0.14 \text{ mm}$

Data collection

Bruker Kappa APEXII CCD diffractometer	3355 independent reflections
Radiation source: fine-focus sealed tube graphite	2130 reflections with $I > 2\sigma(I)$
Detector resolution: $7.60 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.044$
ω scans	$\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 2.9^\circ$
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2005)	$h = -12 \rightarrow 12$
$T_{\text{min}} = 0.942$, $T_{\text{max}} = 0.950$	$k = -12 \rightarrow 11$
7740 measured reflections	$l = -24 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.050$	H-atom parameters constrained
$wR(F^2) = 0.120$	$w = 1/[\sigma^2(F_o^2) + (0.053P)^2]$
$S = 1.00$	where $P = (F_o^2 + 2F_c^2)/3$
3355 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
254 parameters	$\Delta\rho_{\text{max}} = 0.18 \text{ e \AA}^{-3}$
1 restraint	$\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1307 Friedel pairs
	Flack parameter: 0.73 (9)

Special details

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.05268 (12)	-0.05719 (13)	0.64742 (7)	0.0730 (4)
N1	0.2266 (4)	-0.1211 (3)	0.5585 (2)	0.0563 (10)
N2	0.3221 (4)	-0.1007 (3)	0.5124 (2)	0.0540 (10)
N3	0.4576 (4)	0.0479 (3)	0.4564 (2)	0.0564 (10)
H3A	0.4848	0.1290	0.4488	0.068*
N4	0.5125 (4)	-0.0589 (3)	0.4229 (2)	0.0576 (10)
C1	0.3608 (4)	0.0263 (4)	0.5012 (2)	0.0403 (10)
C2	0.3031 (4)	0.1383 (4)	0.5338 (2)	0.0495 (11)
H2	0.3302	0.2261	0.5240	0.059*
C3	0.2085 (4)	0.1165 (4)	0.5791 (2)	0.0489 (12)
H3	0.1686	0.1871	0.6022	0.059*
C4	0.1736 (4)	-0.0193 (4)	0.5896 (2)	0.0490 (12)
C5	0.5972 (5)	-0.0292 (4)	0.3777 (3)	0.0553 (12)
C6	0.6610 (5)	-0.1391 (5)	0.3385 (3)	0.0860 (17)
H6A	0.7147	-0.1958	0.3671	0.103*
H6B	0.5955	-0.1954	0.3169	0.103*
C7	0.7435 (8)	-0.0690 (6)	0.2881 (4)	0.112 (3)
H7A	0.8349	-0.0934	0.2945	0.134*
H7B	0.7175	-0.0972	0.2436	0.134*
C8	0.7283 (7)	0.0760 (6)	0.2945 (4)	0.101 (2)
H8A	0.6859	0.1125	0.2551	0.121*
H8B	0.8137	0.1187	0.2991	0.121*
C9	0.6450 (4)	0.1042 (4)	0.3559 (2)	0.0574 (12)
H9A	0.6972	0.1466	0.3906	0.069*
H9B	0.5720	0.1634	0.3449	0.069*
C12	0.72267 (11)	0.48307 (11)	-0.15057 (7)	0.0678 (4)
N5	0.5643 (3)	0.6264 (3)	-0.07810 (19)	0.0544 (10)
N6	0.4710 (3)	0.6489 (3)	-0.03214 (19)	0.0512 (9)
N7	0.3193 (3)	0.5761 (3)	0.04280 (19)	0.0527 (10)
H7	0.2969	0.6590	0.0495	0.063*
N8	0.2597 (4)	0.4729 (3)	0.0777 (2)	0.0555 (11)
C10	0.4144 (4)	0.5451 (4)	-0.0025 (2)	0.0444 (11)
C11	0.4524 (4)	0.4099 (4)	-0.0162 (2)	0.0471 (11)
H11	0.4124	0.3377	0.0057	0.056*
C12	0.5459 (4)	0.3885 (4)	-0.0607 (2)	0.0466 (11)
H12	0.5744	0.3014	-0.0710	0.056*
C13	0.6001 (4)	0.5023 (4)	-0.0916 (2)	0.0464 (11)
C14	0.1787 (4)	0.5052 (4)	0.1230 (3)	0.0533 (12)

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C15	0.1343 (4)	0.6416 (4)	0.1458 (3)	0.0658 (12)
H15A	0.0928	0.6908	0.1096	0.079*
H15B	0.2080	0.6943	0.1622	0.079*
C16	0.0371 (6)	0.6142 (7)	0.2012 (3)	0.105 (2)
H16A	0.0666	0.6569	0.2421	0.125*
H16B	-0.0480	0.6515	0.1896	0.125*
C17	0.0264 (7)	0.4674 (7)	0.2109 (4)	0.095 (2)
H17A	0.0509	0.4442	0.2562	0.114*
H17B	-0.0637	0.4389	0.2038	0.114*
C18	0.1122 (5)	0.3979 (5)	0.1643 (3)	0.0870 (19)
H18A	0.0617	0.3377	0.1359	0.104*
H18B	0.1770	0.3446	0.1882	0.104*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0700 (7)	0.0779 (9)	0.0711 (9)	-0.0235 (6)	0.0072 (8)	0.0036 (8)
N1	0.068 (3)	0.0344 (19)	0.067 (3)	-0.0143 (19)	0.000 (2)	-0.0021 (19)
N2	0.069 (2)	0.0250 (17)	0.068 (3)	-0.0104 (17)	-0.008 (2)	-0.0068 (17)
N3	0.077 (3)	0.0236 (18)	0.068 (3)	-0.0011 (16)	0.011 (2)	-0.0014 (18)
N4	0.070 (3)	0.034 (2)	0.068 (3)	0.0026 (17)	0.005 (2)	-0.0077 (19)
C1	0.050 (3)	0.029 (2)	0.042 (3)	-0.0022 (17)	-0.005 (2)	-0.0016 (18)
C2	0.065 (3)	0.026 (2)	0.057 (3)	0.000 (2)	0.003 (3)	0.0006 (19)
C3	0.057 (3)	0.032 (2)	0.058 (3)	0.005 (2)	-0.006 (3)	-0.0003 (19)
C4	0.050 (3)	0.046 (3)	0.052 (3)	-0.014 (2)	-0.010 (2)	0.005 (2)
C5	0.065 (3)	0.039 (3)	0.062 (3)	0.008 (2)	0.003 (3)	-0.002 (2)
C6	0.100 (4)	0.048 (3)	0.110 (5)	0.008 (3)	0.035 (4)	-0.016 (3)
C7	0.149 (7)	0.072 (4)	0.114 (6)	0.012 (4)	0.069 (5)	-0.006 (4)
C8	0.117 (6)	0.069 (4)	0.119 (6)	0.008 (3)	0.056 (5)	0.010 (4)
C9	0.069 (3)	0.051 (3)	0.053 (3)	-0.003 (2)	0.007 (3)	0.000 (2)
C12	0.0699 (7)	0.0664 (8)	0.0672 (8)	-0.0042 (6)	0.0083 (7)	-0.0049 (7)
N5	0.066 (3)	0.035 (2)	0.063 (3)	-0.0066 (17)	-0.002 (2)	0.0023 (17)
N6	0.061 (2)	0.0271 (18)	0.066 (2)	-0.0021 (16)	0.001 (2)	-0.0045 (17)
N7	0.061 (2)	0.0283 (18)	0.069 (3)	0.0018 (17)	0.006 (2)	-0.0037 (18)
N8	0.063 (2)	0.033 (2)	0.070 (3)	-0.0065 (18)	0.010 (2)	0.0003 (18)
C10	0.053 (3)	0.028 (2)	0.052 (3)	0.0021 (18)	-0.005 (2)	-0.001 (2)
C11	0.055 (3)	0.025 (2)	0.062 (3)	-0.0033 (18)	0.001 (3)	0.003 (2)
C12	0.055 (3)	0.026 (2)	0.058 (3)	-0.0014 (19)	-0.004 (3)	-0.0035 (19)
C13	0.052 (2)	0.039 (2)	0.048 (3)	-0.002 (2)	-0.008 (2)	-0.002 (2)
C14	0.056 (3)	0.045 (3)	0.059 (3)	-0.001 (2)	0.002 (3)	-0.004 (2)
C15	0.071 (3)	0.056 (3)	0.071 (3)	0.005 (2)	0.001 (3)	-0.015 (3)
C16	0.121 (5)	0.075 (5)	0.117 (6)	0.010 (4)	0.041 (5)	-0.012 (4)
C17	0.108 (5)	0.097 (5)	0.079 (5)	0.003 (4)	0.017 (4)	-0.008 (4)
C18	0.105 (4)	0.057 (3)	0.098 (5)	-0.006 (3)	0.044 (4)	0.006 (3)

Geometric parameters (\AA , $^\circ$)

C11—C4	1.732 (5)	C12—C13	1.730 (5)
N1—C4	1.299 (5)	N5—C13	1.306 (5)

N1—N2	1.357 (5)	N5—N6	1.342 (5)
N2—C1	1.333 (5)	N6—C10	1.317 (5)
N3—C1	1.351 (5)	N7—C10	1.362 (5)
N3—N4	1.370 (5)	N7—N8	1.377 (5)
N3—H3A	0.8600	N7—H7	0.8600
N4—C5	1.285 (6)	N8—C14	1.268 (5)
C1—C2	1.413 (5)	C10—C11	1.416 (5)
C2—C3	1.341 (6)	C11—C12	1.322 (6)
C2—H2	0.9300	C11—H11	0.9300
C3—C4	1.402 (6)	C12—C13	1.397 (6)
C3—H3	0.9300	C12—H12	0.9300
C5—C9	1.470 (6)	C14—C15	1.492 (6)
C5—C6	1.489 (6)	C14—C18	1.504 (7)
C6—C7	1.485 (8)	C15—C16	1.511 (7)
C6—H6A	0.9700	C15—H15A	0.9700
C6—H6B	0.9700	C15—H15B	0.9700
C7—C8	1.445 (7)	C16—C17	1.466 (9)
C7—H7A	0.9700	C16—H16A	0.9700
C7—H7B	0.9700	C16—H16B	0.9700
C8—C9	1.522 (8)	C17—C18	1.452 (8)
C8—H8A	0.9700	C17—H17A	0.9700
C8—H8B	0.9700	C17—H17B	0.9700
C9—H9A	0.9700	C18—H18A	0.9700
C9—H9B	0.9700	C18—H18B	0.9700
C4—N1—N2	120.7 (4)	C13—N5—N6	119.6 (3)
C1—N2—N1	117.7 (3)	C10—N6—N5	119.4 (3)
C1—N3—N4	120.1 (3)	C10—N7—N8	119.1 (3)
C1—N3—H3A	119.9	C10—N7—H7	120.5
N4—N3—H3A	119.9	N8—N7—H7	120.5
C5—N4—N3	116.3 (4)	C14—N8—N7	117.7 (4)
N2—C1—N3	118.4 (3)	N6—C10—N7	115.9 (4)
N2—C1—C2	122.4 (4)	N6—C10—C11	121.7 (4)
N3—C1—C2	119.2 (4)	N7—C10—C11	122.3 (4)
C3—C2—C1	119.1 (4)	C12—C11—C10	118.6 (4)
C3—C2—H2	120.5	C12—C11—H11	120.7
C1—C2—H2	120.5	C10—C11—H11	120.7
C2—C3—C4	115.9 (4)	C11—C12—C13	117.1 (4)
C2—C3—H3	122.0	C11—C12—H12	121.5
C4—C3—H3	122.0	C13—C12—H12	121.5
N1—C4—C3	124.2 (4)	N5—C13—C12	123.5 (4)
N1—C4—C11	116.7 (3)	N5—C13—C12	116.5 (3)
C3—C4—C11	119.1 (4)	C12—C13—C12	120.0 (3)
N4—C5—C9	129.5 (4)	N8—C14—C15	130.1 (4)
N4—C5—C6	119.9 (4)	N8—C14—C18	120.6 (4)
C9—C5—C6	110.6 (4)	C15—C14—C18	109.3 (4)
C7—C6—C5	105.4 (4)	C14—C15—C16	105.2 (4)
C7—C6—H6A	110.7	C14—C15—H15A	110.7
C5—C6—H6A	110.7	C16—C15—H15A	110.7
C7—C6—H6B	110.7	C14—C15—H15B	110.7

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C5—C6—H6B	110.7	C16—C15—H15B	110.7
H6A—C6—H6B	108.8	H15A—C15—H15B	108.8
C8—C7—C6	109.9 (5)	C17—C16—C15	108.9 (5)
C8—C7—H7A	109.7	C17—C16—H16A	109.9
C6—C7—H7A	109.7	C15—C16—H16A	109.9
C8—C7—H7B	109.7	C17—C16—H16B	109.9
C6—C7—H7B	109.7	C15—C16—H16B	109.9
H7A—C7—H7B	108.2	H16A—C16—H16B	108.3
C7—C8—C9	108.2 (5)	C18—C17—C16	109.7 (5)
C7—C8—H8A	110.1	C18—C17—H17A	109.7
C9—C8—H8A	110.1	C16—C17—H17A	109.7
C7—C8—H8B	110.1	C18—C17—H17B	109.7
C9—C8—H8B	110.1	C16—C17—H17B	109.7
H8A—C8—H8B	108.4	H17A—C17—H17B	108.2
C5—C9—C8	105.1 (4)	C17—C18—C14	107.0 (5)
C5—C9—H9A	110.7	C17—C18—H18A	110.3
C8—C9—H9A	110.7	C14—C18—H18A	110.3
C5—C9—H9B	110.7	C17—C18—H18B	110.3
C8—C9—H9B	110.7	C14—C18—H18B	110.3
H9A—C9—H9B	108.8	H18A—C18—H18B	108.6
C4—N1—N2—C1	1.3 (6)	C13—N5—N6—C10	-1.8 (6)
C1—N3—N4—C5	175.2 (4)	C10—N7—N8—C14	174.9 (4)
N1—N2—C1—N3	178.8 (4)	N5—N6—C10—N7	-179.1 (3)
N1—N2—C1—C2	-2.2 (6)	N5—N6—C10—C11	2.2 (6)
N4—N3—C1—N2	0.8 (6)	N8—N7—C10—N6	-177.4 (4)
N4—N3—C1—C2	-178.2 (4)	N8—N7—C10—C11	1.4 (6)
N2—C1—C2—C3	2.1 (6)	N6—C10—C11—C12	-1.0 (6)
N3—C1—C2—C3	-178.9 (4)	N7—C10—C11—C12	-179.7 (4)
C1—C2—C3—C4	-0.9 (6)	C10—C11—C12—C13	-0.4 (6)
N2—N1—C4—C3	-0.1 (6)	N6—N5—C13—C12	0.2 (6)
N2—N1—C4—C11	-180.0 (3)	N6—N5—C13—C12	-179.1 (3)
C2—C3—C4—N1	0.0 (6)	C11—C12—C13—N5	0.9 (6)
C2—C3—C4—C11	179.8 (3)	C11—C12—C13—C12	-179.8 (3)
N3—N4—C5—C9	-0.2 (7)	N7—N8—C14—C15	0.4 (7)
N3—N4—C5—C6	-179.5 (4)	N7—N8—C14—C18	-178.5 (4)
N4—C5—C6—C7	175.6 (6)	N8—C14—C15—C16	179.9 (5)
C9—C5—C6—C7	-3.9 (7)	C18—C14—C15—C16	-1.1 (6)
C5—C6—C7—C8	-1.7 (8)	C14—C15—C16—C17	0.7 (6)
C6—C7—C8—C9	6.3 (9)	C15—C16—C17—C18	0.0 (8)
N4—C5—C9—C8	-171.9 (6)	C16—C17—C18—C14	-0.6 (7)
C6—C5—C9—C8	7.5 (6)	N8—C14—C18—C17	-179.8 (5)
C7—C8—C9—C5	-8.4 (7)	C15—C14—C18—C17	1.1 (6)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 \cdots N5 ⁱ	0.93	2.73	3.500 (6)	141
N3—H3A \cdots N5 ⁱ	0.86	2.52	3.295 (5)	150

N3—H3A···N6 ⁱ	0.86	2.27	3.088 (5)	159
N7—H7···N1 ⁱⁱ	0.86	2.19	3.041 (5)	170
C12—H12···N4 ⁱⁱⁱ	0.93	2.55	3.323 (5)	140

Symmetry codes: (i) $-x+1, -y+1, z+1/2$; (ii) $-x+1/2, y+1, z-1/2$; (iii) $-x+1, -y, z-1/2$.

Fig. 1

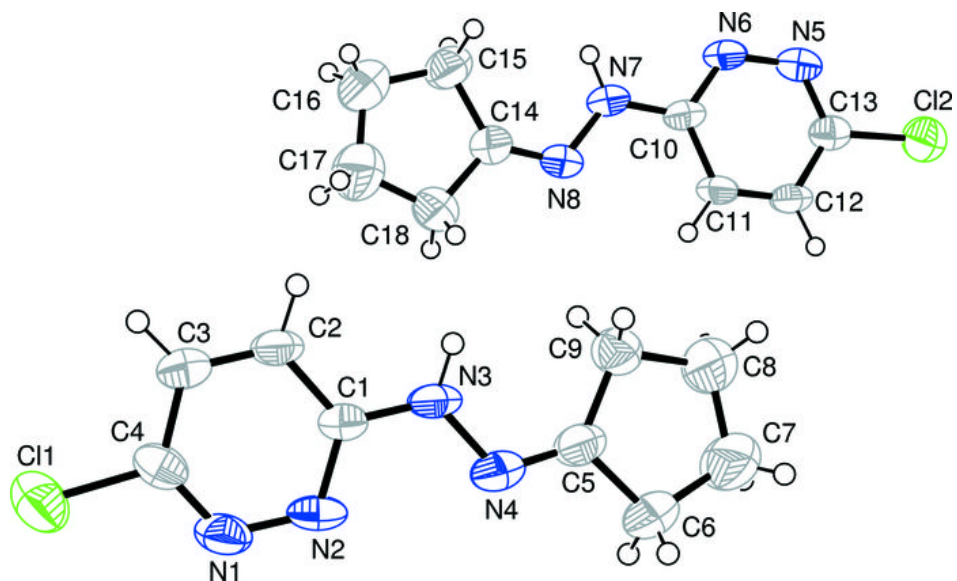


Fig. 2

