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Crystal structure and Hirshfeld surface analysis of 5,5-dichloro-2-(dichloromethyl)-6,6-dimethyl-5,6-dihydropyrimidin-4-amine

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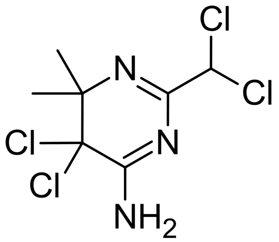
In the title compound, $C_7H_9Cl_4N_3$, the central 4,5-dihydropyrimidine ring adopts an approximate twist-boat conformation. In the crystal, molecules are connected in the $[10\overline{1}]$ direction by ribbons of N—H$\cdots$N hydrogen-bonded dimers with an $R_2^2(8)$ motif.

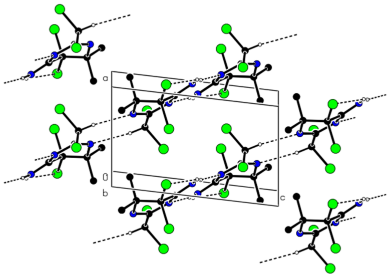
1. Chemical context

N-containing compounds have attracted much attention due to their properties in the fields of molecular recognition, crystal engineering, catalysis, coordination chemistry and organic synthesis (Gadzhieva *et al.*, 2005; Maharramov *et al.*, 2011; Gurbanov *et al.*, 2022; Polyanskii *et al.*, 2019). Depending on the main N-skeleton as well as the attached substituents, the supramolecular arrangements and catalytic activity of the corresponding metal complexes can be regulated (Aliyeva *et al.*, 2024; Gurbanov *et al.*, 2018; Huseynov *et al.*, 2018). Numerous synthetic strategies for the synthesis of new N-containing compounds have been developed including metal-mediated synthesis (Gurbanov *et al.*, 2023; Mahmudov *et al.*, 2023). Attachment of –Cl and –NH_2 groups on the N-heterocycle can alter the supramolecular mode of the corresponding organic materials. Thus, in the current work we have synthesized the title compound, which provides multiple intermolecular non-covalent interactions.



2. Structural commentary

The central 4,5-dihydropyrimidine ring exhibits an approximate twist-boat conformation. Atoms C1/C2/N1/N2 are almost coplanar (r.m.s. deviation = 0.006 Å) and C3 and C4 deviate from their best plane by 0.824 (2) and 0.317 (2) Å, respectively. The molecule features a short intramolecular N—H$\cdots$Cl contact (Fig. 1; Table 1) forming a $C(5)$ motif (Bernstein *et al.*, 1995). The C—N distances in the 4,5-dihydropyrimidine ring are consistent with single- and double-bond characteristics [C1═N2 = 1.276 (2), C4═N1 = 1.307 (2)



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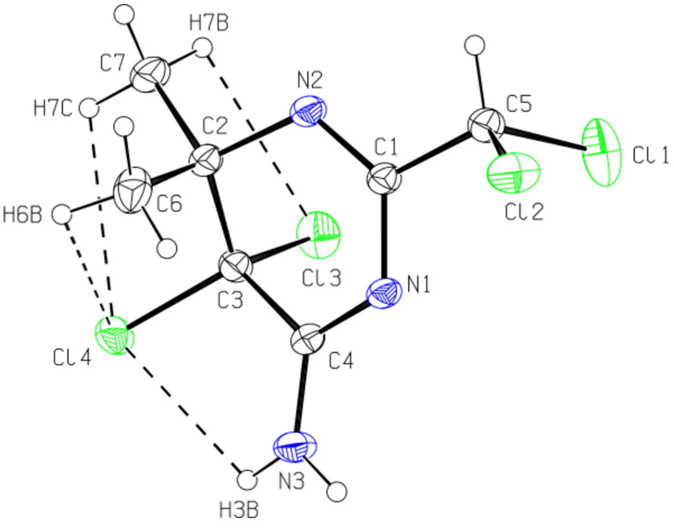


Figure 1
The title molecule with the atom-labelling scheme and displacement ellipsoids drawn at the 30% probability level. Short intramolecular H···Cl contacts are indicated by dashed lines.

C2—N2 = 1.473 (2), C1—N1 = 1.387 (2) and C4—N3 = 1.313 (2) Å]. The single C—N bond length [1.313 (2) Å] for the NH_2 group attached to the pyrimidine ring is significantly shorter than a typical C—N single bond (around 1.47 Å). The other bond lengths and angles are comparable to those in the structures discussed in the *Database survey* section.

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, molecules are linked into dimers with an $R_2^2(8)$ motif by N—H···N hydrogen bonds, forming ribbons in the [10$\overline{1}$] direction, which also feature pairwise C—H···N hydrogen bonds (Table 1; Figs. 2, 3 and 4). No C—H···π or π–π interactions are found. van der Waals interactions between the ribbons consolidate the crystal structure.

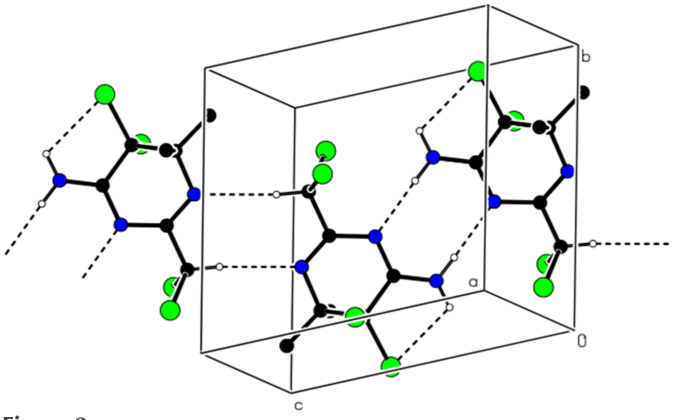


Figure 2
Partial packing of the title compound in the unit cell, showing N—H···N and C—H···N hydrogen bonds as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N1^{i}	0.90	2.08	2.978 (2)	174
C5—H5*A*···N2^{ii}	0.98	2.54	3.506 (3)	170

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

Crystal Explorer 17.5 (Spackman *et al.*, 2021) was utilized to generate Hirshfeld surfaces (Fig. 5) and two-dimensional

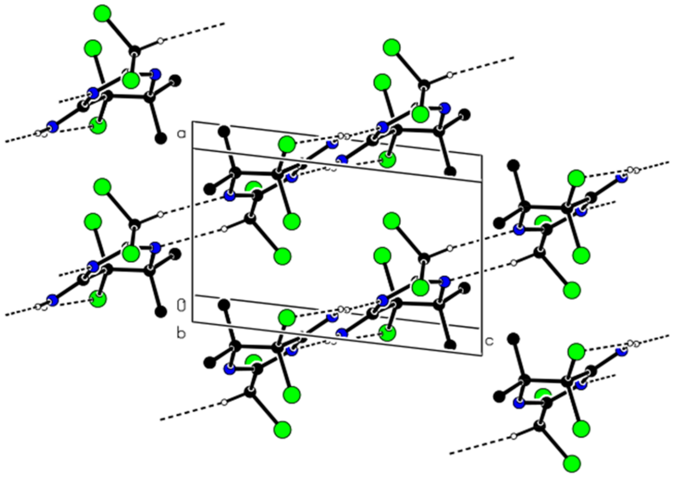


Figure 3
The view of the interactions shown in Fig. 2 from the *b*-axis.

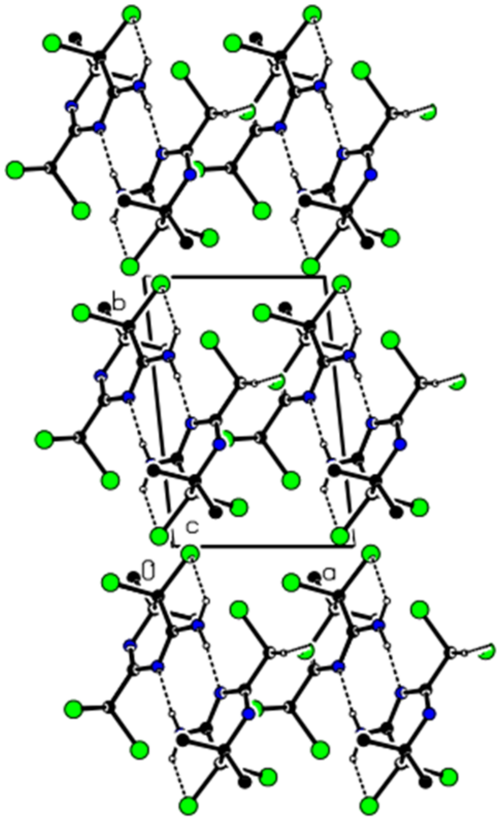


Figure 4
The view of the interactions shown in Fig. 2 from the *c*-axis.

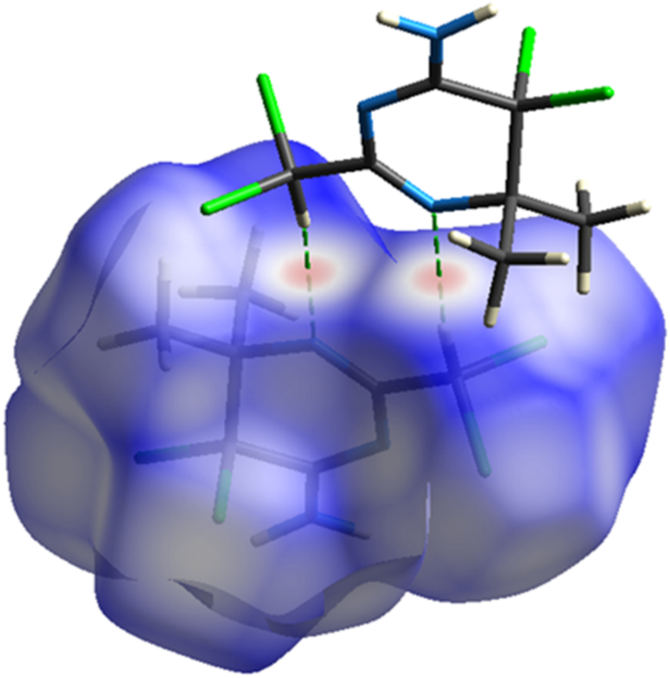
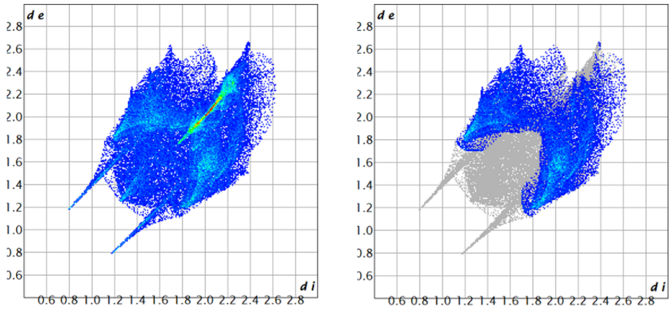
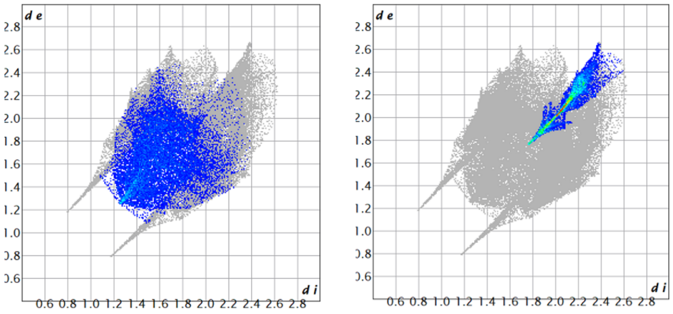


Figure 5
View of the three-dimensional Hirshfeld surface of the compound plotted over $d_{\rm norm}$.



(a) All...All (b) Cl...H/H...Cl



(c) H...H (d) Cl...Cl

Figure 6
The two-dimensional fingerprint plots, showing (*a*) all interactions, and delineated into (*b*) Cl···H/H···Cl, (*c*) H···H and (*d*) Cl···Cl interactions [d_e and d_i represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

fingerprint plots (Fig. 6) in order to quantify the intermolecular interactions in the crystal (Table 1). The most important Cl···H/H···Cl interactions appear as two symmetrical broad wings with $d_e + d_i = 2.85$ Å and contribute 42.9% to the Hirshfeld surface (Fig. 6*b*). The intermolecular H···H contacts, contributing 25.9% to the overall crystal packing, are reflected in Fig. 6*c* as widely scattered points of high density due to the large hydrogen content of the molecule, with the tip at $d_e = d_i = 1.25$ Å. The observed Cl···Cl contact distance of 3.5355 (8) Å is slightly longer than the conventional 3.50 Å van der Waals separation. The Cl···Cl contacts (16.2%) have an arrow-shaped distribution of points with the tip at $d_e = d_i = 1.75$ Å (Fig. 6*d*). The N···H/H···N interactions represent 9.5% of the total Hirshfeld surface. These interactions are manifested as two symmetrical sharp spikes at $d_e + d_i = 1.95$ Å (Fig. 6*a*). The Cl···N/N···Cl (4.4%), Cl···C/C···Cl (0.7%) and C···H/H···C (0.4%) interactions all contribute in smaller ways.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 6.00, update of April 2025; Groom *et al.*, 2016) for 4,5-dihydropyrimidine resulted in 77 hits. Entries KIMHIB (Wan *et al.*, 2023) and ZEDLOJ (Mori & Maeda, 1994) are the closest analogues of the title compound.

KIMHIB crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit of the orthorhombic space group $Pna2_1$. ZEDLOJ crystallizes in the monoclinic space group $A2/a$. In KIMHIB, the dihydropyrimidine ring of molecule *A* adopts a distorted screw-boat conformation with ring puckering parameters $Q_T = 0.433$ (6) Å, $\theta = 112.2$ (8)° and $\varphi = 328.7$ (9)°, whereas the dihydropyrimidine ring of molecule *B* exhibits a distorted twist-boat conformation [$Q_{\rm T} = 0.459$ (6) Å, $\theta = 109.2$ (7)°, $\varphi = 81.1$ (8)°]. In ZEDLOJ, the central pyrimidine ring adopts a distorted screw-boat conformation [$Q_{\rm T} = 0.462$ (2) Å, $\theta = 67.2$ (2) °, $\varphi = 216.1$ (3) °]. Idealized values for screw-boat and twist-boat conformations are: $\theta = 67.5°$ and 90°, and $\varphi = (60k + 30)°$, respectively, where *k* is an integer.

In KIMHIB, the molecular conformation may be associated with C—H···N intramolecular interactions. In the crystal, molecules form layers parallel to the (100) plane *via* C—H···π interactions with van der Waals interactions between the layers, no π–π interactions are observed. In ZEDLOJ, the molecular conformation may be supported by C—H···N hydrogen bonds. Classical intermolecular hydrogen bonds are not observed, with C—H···π and van der Waals interactions consolidating of the structure.

5. Synthesis and crystallization

To a mixture of 0.5 ml dichloroacetonitrile and 1.5 ml of NH_4OH (28–30%) solution was added 10 mg of $Pd(CH_3COO)_2$ in 5 ml acetone. The mixture was stirred for 24 h at r.t. The precipitate was filtered and dissolved in CH_2Cl_2. Light-yellow crystals of the title compound suitable for X-ray structural analysis were obtained after *ca* 2 d. Yield 60%; IR (ATR, 298 K): 3320 and 3203 ν(N—H), 1641 and

1602 ν(C═N); M_r = 276.97; elemental analysis calculated (%) for $C_7H_9Cl_4N_3$: C 30.36, H 3.28, N 15.17; found: C 30.33, H 3.27, N 15.14. ^{1}H NMR in DMSO-d_6, δ(p.p.m.): 1.98 (3H, –CH_3) and 2.07 (3H,–CH_3), 5.91 (1H, –$CHCl_2$), 8.35 (2H,–NH_2). ^{13}C NMR in DMSO-d_6, δ (p.p.m.): 18.62 and 23.65 (–CH_3), 67.02 (–CCH_3), 70.99 (–$CHCl_2$), 112.44 (–CCl_2–), 150.51 and 165.34 (C═N).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The hydrogen atoms were placed in calculated positions and refined as riding models with fixed isotropic displacement parameters [C—H = 0.96 and 0.98 Å, N—H = 0.90 Å with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(N, C)].

Acknowledgements

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_7H_9Cl_4N_3$
M_r	276.97
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	6.1069 (3), 9.1118 (4), 10.2591 (5)
α, β, γ (°)	90.981 (2), 96.700 (2), 95.980 (2)
V (Å^3)	563.63 (5)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.01
Crystal size (mm)	0.25 × 0.18 × 0.12
Data collection	
Diffractometer	Bruker D8 Quest PHOTON 100 detector
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015
$T_{\rm min}$, $T_{\rm max}$	0.793, 0.874
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8178, 2272, 1998
$R_{\rm int}$	0.037
(sin $\theta/\lambda)_{\rm max}$ (Å^{-1})	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.083, 1.07
No. of reflections	2272
No. of parameters	129
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\rm max}$, $\Delta\rho_{\rm min}$ (e Å^{-3})	0.39, −0.36

Computer programs: *APEX3* and *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

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Computing details

5,5-Dichloro-2-(dichloromethyl)-6,6-dimethyl-5,6-dihydropyrimidin-4-amine

Crystal data

$C_7H_9Cl_4N_3$
$M_r = 276.97$
Triclinic, $P\bar{1}$
$a = 6.1069\ (3)$ Å
$b = 9.1118\ (4)$ Å
$c = 10.2591\ (5)$ Å
$\alpha = 90.981\ (2)°$
$\beta = 96.700\ (2)°$
$\gamma = 95.980\ (2)°$
$V = 563.63\ (5)$ Å^3

$Z = 2$
$F(000) = 280$
$D_x = 1.632$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5453 reflections
$\theta = 3.1–26.4°$
$\mu = 1.01$ mm^{-1}
$T = 296$ K
Plate, light-yellow
0.25 × 0.18 × 0.12 mm

Data collection

Bruker D8 Quest PHOTON 100 detector diffractometer
Detector resolution: 0 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015
$T_{\min} = 0.793$, $T_{\max} = 0.874$
8178 measured reflections

2272 independent reflections
1998 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.037$
$\theta_{\max} = 26.4°$, $\theta_{\min} = 2.3°$
$h = -7 \rightarrow 7$
$k = -11 \rightarrow 11$
$l = -12 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.083$
$S = 1.07$
2272 reflections
129 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0247P)^2 + 0.3903P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.39$ e Å^{-3}
$\Delta\rho_{\min} = -0.36$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2993 (3)	0.46088 (19)	0.77624 (17)	0.0290 (4)
C2	0.1477 (3)	0.2365 (2)	0.85204 (18)	0.0327 (4)
C3	0.1199 (3)	0.18825 (19)	0.70582 (18)	0.0291 (4)
C4	0.0636 (3)	0.3194 (2)	0.62278 (17)	0.0281 (4)
C5	0.4578 (3)	0.5991 (2)	0.8006 (2)	0.0368 (4)
H5A	0.535164	0.597285	0.889662	0.044*
C6	−0.0758 (4)	0.2743 (3)	0.8909 (2)	0.0470 (5)
H6A	−0.053847	0.318689	0.977638	0.071*
H6B	−0.176096	0.185742	0.889584	0.071*
H6C	−0.136976	0.342158	0.829808	0.071*
C7	0.2421 (4)	0.1190 (2)	0.9398 (2)	0.0471 (5)
H7A	0.238776	0.146708	1.030174	0.071*
H7B	0.392426	0.110595	0.924333	0.071*
H7C	0.154603	0.025863	0.920024	0.071*
Cl1	0.65595 (12)	0.60821 (8)	0.68869 (9)	0.0749 (2)
Cl2	0.31392 (11)	0.75861 (6)	0.78797 (6)	0.05086 (18)
Cl3	0.37541 (9)	0.13811 (6)	0.65640 (6)	0.04623 (16)
Cl4	−0.08182 (8)	0.03163 (5)	0.67338 (5)	0.04116 (15)
N1	0.1654 (3)	0.45015 (16)	0.65682 (14)	0.0299 (3)
N2	0.3036 (3)	0.37185 (17)	0.87098 (15)	0.0344 (4)
N3	−0.0794 (3)	0.29820 (18)	0.51650 (16)	0.0399 (4)
H3A	−0.114976	0.373990	0.465988	0.048*
H3B	−0.140745	0.207580	0.487858	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0314 (9)	0.0258 (8)	0.0287 (9)	0.0033 (7)	−0.0013 (7)	0.0040 (7)
C2	0.0379 (10)	0.0298 (9)	0.0281 (9)	−0.0019 (8)	−0.0017 (7)	0.0068 (7)
C3	0.0288 (8)	0.0252 (8)	0.0320 (9)	0.0023 (7)	−0.0016 (7)	0.0036 (7)
C4	0.0304 (9)	0.0296 (9)	0.0243 (8)	0.0051 (7)	0.0014 (7)	0.0044 (7)
C5	0.0409 (10)	0.0280 (9)	0.0384 (10)	−0.0005 (8)	−0.0062 (8)	0.0081 (8)
C6	0.0519 (13)	0.0490 (13)	0.0421 (12)	0.0011 (10)	0.0176 (10)	0.0011 (10)
C7	0.0578 (13)	0.0369 (11)	0.0411 (12)	−0.0043 (10)	−0.0108 (10)	0.0179 (9)
Cl1	0.0567 (4)	0.0623 (4)	0.1098 (6)	−0.0065 (3)	0.0378 (4)	0.0052 (4)
Cl2	0.0716 (4)	0.0310 (3)	0.0473 (3)	0.0127 (2)	−0.0098 (3)	−0.0047 (2)
Cl3	0.0395 (3)	0.0437 (3)	0.0588 (3)	0.0141 (2)	0.0107 (2)	0.0032 (2)
Cl4	0.0436 (3)	0.0295 (2)	0.0461 (3)	−0.00512 (19)	−0.0052 (2)	0.0032 (2)
N1	0.0350 (8)	0.0266 (7)	0.0266 (7)	0.0031 (6)	−0.0034 (6)	0.0062 (6)

N2	0.0422 (9)	0.0291 (8)	0.0284 (8)	−0.0025 (7)	−0.0062 (7)	0.0064 (6)
N3	0.0512 (10)	0.0306 (8)	0.0330 (9)	0.0007 (7)	−0.0132 (7)	0.0041 (7)

Geometric parameters (Å, º)

C1—N2	1.276 (2)	C5—Cl1	1.760 (2)
C1—N1	1.387 (2)	C5—Cl2	1.774 (2)
C1—C5	1.504 (2)	C5—H5A	0.9800
C2—N2	1.473 (2)	C6—H6A	0.9600
C2—C7	1.526 (3)	C6—H6B	0.9600
C2—C6	1.536 (3)	C6—H6C	0.9600
C2—C3	1.541 (3)	C7—H7A	0.9600
C3—C4	1.525 (2)	C7—H7B	0.9600
C3—Cl4	1.7851 (18)	C7—H7C	0.9600
C3—Cl3	1.7960 (19)	N3—H3A	0.9000
C4—N1	1.307 (2)	N3—H3B	0.9001
C4—N3	1.313 (2)		

N2—C1—N1	129.26 (17)	C1—C5—H5A	108.5
N2—C1—C5	114.72 (16)	Cl1—C5—H5A	108.5
N1—C1—C5	115.98 (15)	Cl2—C5—H5A	108.5
N2—C2—C7	107.95 (15)	C2—C6—H6A	109.5
N2—C2—C6	107.44 (16)	C2—C6—H6B	109.5
C7—C2—C6	111.29 (18)	H6A—C6—H6B	109.5
N2—C2—C3	108.66 (14)	C2—C6—H6C	109.5
C7—C2—C3	111.77 (17)	H6A—C6—H6C	109.5
C6—C2—C3	109.58 (16)	H6B—C6—H6C	109.5
C4—C3—C2	108.96 (15)	C2—C7—H7A	109.5
C4—C3—Cl4	112.61 (12)	C2—C7—H7B	109.5
C2—C3—Cl4	111.15 (13)	H7A—C7—H7B	109.5
C4—C3—Cl3	105.30 (12)	C2—C7—H7C	109.5
C2—C3—Cl3	111.34 (12)	H7A—C7—H7C	109.5
Cl4—C3—Cl3	107.34 (10)	H7B—C7—H7C	109.5
N1—C4—N3	121.44 (17)	C4—N1—C1	116.08 (15)
N1—C4—C3	118.94 (15)	C1—N2—C2	116.41 (15)
N3—C4—C3	119.58 (16)	C4—N3—H3A	121.1
C1—C5—Cl1	110.83 (14)	C4—N3—H3B	122.3
C1—C5—Cl2	110.93 (14)	H3A—N3—H3B	116.6
Cl1—C5—Cl2	109.46 (11)		

N2—C2—C3—C4	−51.33 (19)	Cl3—C3—C4—N3	98.37 (18)
C7—C2—C3—C4	−170.35 (16)	N2—C1—C5—Cl1	117.03 (17)
C6—C2—C3—C4	65.79 (19)	N1—C1—C5—Cl1	−64.87 (19)
N2—C2—C3—Cl4	−176.00 (12)	N2—C1—C5—Cl2	−121.15 (17)
C7—C2—C3—Cl4	64.98 (19)	N1—C1—C5—Cl2	56.9 (2)
C6—C2—C3—Cl4	−58.88 (18)	N3—C4—N1—C1	175.14 (18)
N2—C2—C3—Cl3	64.38 (17)	C3—C4—N1—C1	−7.3 (2)
C7—C2—C3—Cl3	−54.64 (19)	N2—C1—N1—C4	−16.6 (3)

C6—C2—C3—Cl3	−178.50 (13)	C5—C1—N1—C4	165.66 (17)
C2—C3—C4—N1	40.3 (2)	N1—C1—N2—C2	1.1 (3)
Cl4—C3—C4—N1	164.11 (14)	C5—C1—N2—C2	178.85 (16)
Cl3—C3—C4—N1	−79.24 (18)	C7—C2—N2—C1	155.08 (19)
C2—C3—C4—N3	−142.10 (18)	C6—C2—N2—C1	−84.8 (2)
Cl4—C3—C4—N3	−18.3 (2)	C3—C2—N2—C1	33.7 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N1^{i}	0.90	2.08	2.978 (2)	174
N3—H3*B*···Cl4	0.90	2.53	2.9364 (17)	108
C5—H5*A*···N2^{ii}	0.98	2.54	3.506 (3)	170
C6—H6*B*···Cl4	0.96	2.75	3.109 (2)	103
C7—H7*B*···Cl3	0.96	2.76	3.112 (2)	103
C7—H7*C*···Cl4	0.96	2.77	3.218 (2)	110

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

Short interatomic contacts (Å)

Contact	Distance	Symmetry operation
Cl1···H6C	3.15	1+x,y,z
Cl2···H7C	3.07	x,1+y,z
H3A···N1	2.08	-x,1-y,1-z
H6A···Cl2	3.08	-x,1-y,2-z
H5A···N2	2.54	1-x,1-y,2-z