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Dichlorido{*N*,*N*,*N*′-trimethyl-*N*′-(1*H*-pyrazol-1-yl-κN^2)methyl]ethane-1,2-diamine-$\kappa^2 N,N'$}copper(II) methanol monosolvate

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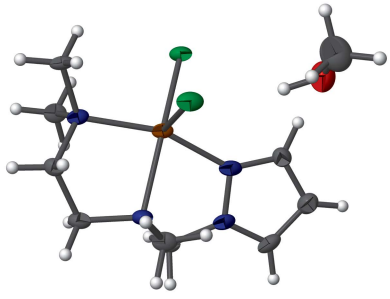
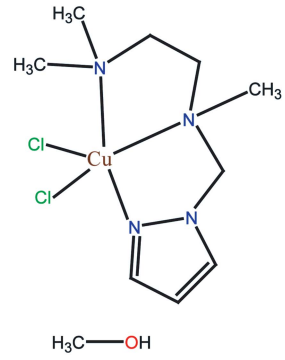
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[CuCl_2(C_9H_{18}N_4)]\cdot CH_3OH$, the central Cu^{II} ion is coordinated by three N atoms from the pyrazole derivative ligand and two chloride co-ligands. The coordination geometry around the Cu^{II} ion is distorted trigonal–bipyramidal. In the crystal, the molecules are linked by C—H···O, C—H···Cl and O—H···Cl hydrogen bonds, forming a three-dimensional framework with the lattice solvent molecule.

3D view



Chemical scheme



Structure description

Rigid ligands including pyrazole are some of the most desirable ligands to biologists and bioinorganic chemists for specific functions, such as catalysis and fluxional behaviour (Zhang *et al.*, 2009; Arroyo *et al.*, 2000), and also in electrochemistry (Morin *et al.*, 2011). Recently, there has been considerable interest in the use of multifunctional ligands containing substituted pyrazole groups because of their potential applications in catalysis, and their ability to form complexes that mimic structural and catalytic functions in metalloproteins (García-Antón *et al.*, 2003; Mukherjee, 2000; Pal *et al.*, 2005; Shaw *et al.*, 2004). In particular, the research field dealing with copper complexes embraces a wide range of topics, such as metastasis development (Turski *et al.*, 2009; Finney *et al.*, 2009), anticancer activity, and other aspects of bioinorganic chemistry.

As part of our continuing interest in coordination chemistry (Kumar *et al.*, 2018, 2019; Faizi *et al.*, 2014, 2018), we report herein the synthesis and structure of the title complex,

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···Cl1^{i}	0.93	2.98	3.841 (6)	156
C3—H3···O1^{ii}	0.93	2.62	3.305 (7)	131
C4—H4A···Cl2^{ii}	0.97	2.67	3.636 (5)	173
C4—H4B···Cl1^{iii}	0.97	2.94	3.902 (5)	170
C5—H5A···Cl2^{iv}	0.96	2.93	3.745 (5)	143
C7—H7A···O1^{v}	0.97	2.42	3.281 (6)	148
C7—H7B···Cl2^{iv}	0.97	2.83	3.632 (5)	140
C8—H8B···Cl1^{iii}	0.96	2.81	3.736 (5)	162
O1—H1O···Cl2	0.91 (2)	2.16 (3)	3.047 (4)	164 (7)

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

$[Cu(C_9H_{18}N_4)Cl_2]\cdot CH_4O$. In this mononuclear copper(II) compound (Fig. 1), the $CuCl_2$ group is bonded to a tridentate ligand, *N*,*N*,*N*′-trimethyl-*N*′-pyrazol-1-ylmethyl-ethane-1,2-diamine (TPED), and the asymmetric unit is completed by a methanol solvate molecule. The central Cu^{II} ion is coordinated by the tridentate N-chelating TPED ligand and two Cl^- ions in a distorted trigonal–bipyramidal geometry, with the chloride ligands and the central ethylenediamine N atom (N3) occupying the equatorial positions [Cu—Cl = 2.4630 (15) and 2.2914 (15) Å; Cu—N = 2.125 (4) Å], while the coordinating pyrazole N atom and the terminal ethylenediamine N atom (N4) are placed in axial positions [Cu—N = 1.991 (4) and 2.043 (4) Å]. In the crystal, the molecules are linked by weak O—H···Cl, C—H···O and C—H···Cl hydrogen bonds, forming a three dimensional network (Table 1; Figs. 2 and 3).

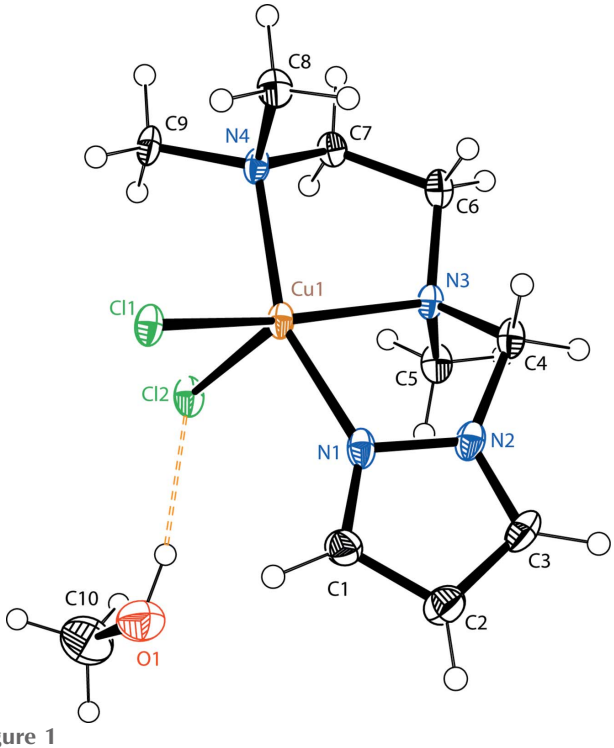


Figure 1
The asymmetric unit of the title compound, with displacement ellipsoids drawn at the 40% probability level. The intermolecular O—H···Cl hydrogen bond between the solvent molecule and the main complex is also shown.

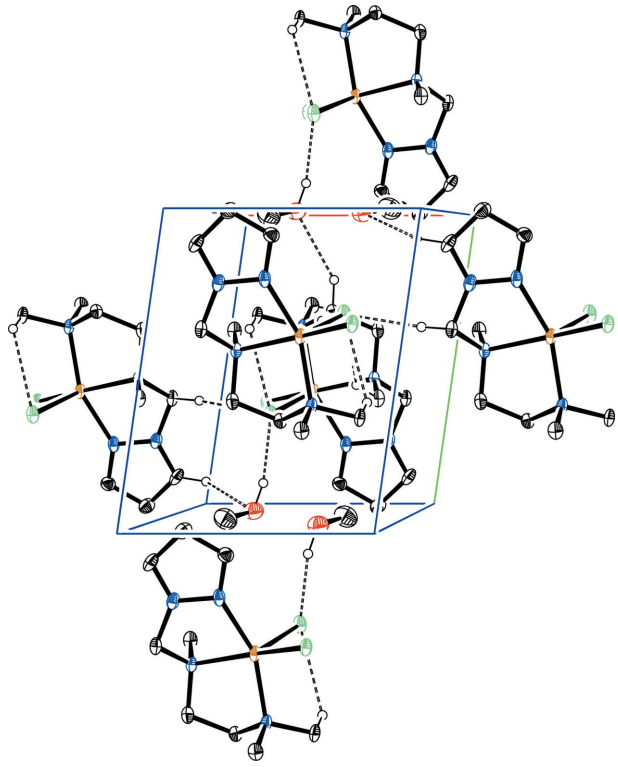


Figure 2
Part of the crystal structure showing the formation of a one-dimensional structure involving the lattice solvent and the main complex. Hydrogen bonds are shown as dashed lines.

Synthesis and crystallization

$[Cu^{II}(TPED)Cl_2]\cdot CH_3OH$: To a solution of TPED (0.050 g, 0.27 mmol) in 5 ml of methanol, solid $CuCl_2\cdot 2H_2O$ (0.046 g, 0.27 mmol) was added portionwise. The colour of the solution changed from light yellow to blue. The solution was stirred for 1 h at 298 K. The blue solid that formed was filtered and washed with a methanol/diethyl ether mixture (1:3 *v*/*v*). The resulting blue solid was recrystallized by diffusion of diethyl ether into a solution of the complex in methanol, and the crystals were dried *in vacuo*. Yield: 0.072 g, 70%. $C_{10}H_{22}Cl_2CuN_4O$: calculated C 34.44, H 6.36, N 16.06; found C

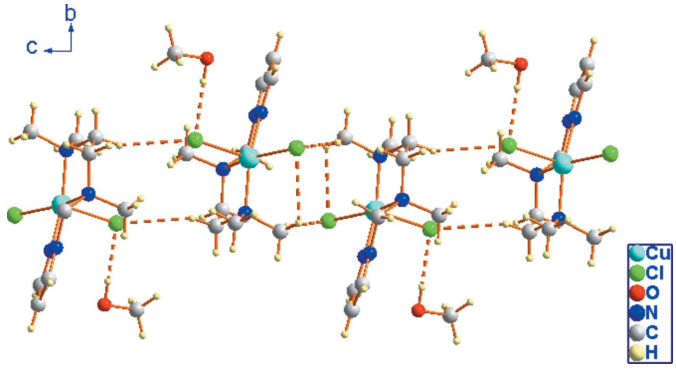


Figure 3
The crystal packing of the title compound, viewed along the *a* axis. Hydrogen bonds: molecules are linked by weak C—H···O, C—H···Cl and O—H···Cl interactions. See Table 1 for details.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[CuCl_2(C_9H_{18}N_4)]\cdot CH_4O$
M_r	348.75
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	7.240 (5), 9.260 (5), 11.649 (5)
α, β, γ (°)	87.438 (5), 78.987 (5), 81.887 (5)
V (Å^3)	758.8 (7)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.79
Crystal size (mm)	0.18 × 0.14 × 0.10
Data collection	
Diffractometer	Bruker *SMART APEX* CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.281, 0.397
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3864, 2599, 2169
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.596
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.158, 1.04
No. of reflections	2599
No. of parameters	168
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.53, −0.61

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006) and *publCIF* (Westrip, 2010).

34.94, H 6.86, N 16.78. UV–Vis [λ_{max}, nm (ε, $M^{-1}cm^{-1}$ in methanol)]: 680 (310), 290 (8900), 235 (16 800).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2019). **4**, x190692 [https://doi.org/10.1107/S2414314619006928]

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Crystal data

$[CuCl_2(C_9H_{18}N_4)]\cdot CH_4O$
$M_r = 348.75$
Triclinic, $P\overline{1}$
$a = 7.240$ (5) Å
$b = 9.260$ (5) Å
$c = 11.649$ (5) Å
$\alpha = 87.438$ (5)°
$\beta = 78.987$ (5)°
$\gamma = 81.887$ (5)°
$V = 758.8$ (7) Å^3
$Z = 2$
$F(000) = 362$
$D_x = 1.526$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2494 reflections
$\theta = 2.7$–24.6°
$\mu = 1.79$ mm^{-1}
$T = 296$ K
Prism, blue
0.18 × 0.14 × 0.10 mm

Data collection

Bruker SMART APEX CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2007)
$T_{min} = 0.281$, $T_{max} = 0.397$
3864 measured reflections
2599 independent reflections
2169 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 25.1°$, $\theta_{min} = 2.2°$
$h = -8\rightarrow7$
$k = -8\rightarrow11$
$l = -13\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.158$
$S = 1.04$
2599 reflections
168 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1044P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.53$ e Å^{-3}
$\Delta\rho_{min} = -0.61$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.45726 (7)	0.39934 (6)	0.79843 (4)	0.0189 (2)
Cl1	0.21622 (15)	0.35638 (12)	0.94918 (10)	0.0218 (3)
Cl2	0.34205 (16)	0.33139 (13)	0.62524 (10)	0.0254 (3)
O1	0.3144 (6)	0.0068 (4)	0.6629 (4)	0.0446 (10)
N1	0.6201 (5)	0.2174 (4)	0.8341 (3)	0.0221 (9)
N2	0.8060 (5)	0.2307 (4)	0.8190 (3)	0.0224 (9)
N3	0.7305 (5)	0.4460 (4)	0.7149 (3)	0.0198 (8)
N4	0.3760 (5)	0.6189 (4)	0.7857 (3)	0.0196 (8)
C1	0.6077 (7)	0.0801 (5)	0.8671 (4)	0.0269 (11)
H1	0.494998	0.039437	0.883402	0.032*
C2	0.7861 (7)	0.0041 (6)	0.8744 (5)	0.0309 (12)
H2	0.815459	−0.093094	0.896052	0.037*
C3	0.9082 (7)	0.1060 (5)	0.8423 (5)	0.0298 (12)
H3	1.039138	0.090345	0.837685	0.036*
C4	0.8589 (6)	0.3763 (5)	0.7913 (4)	0.0228 (10)
H4A	0.990186	0.370218	0.751313	0.027*
H4B	0.843582	0.431497	0.862068	0.027*
C5	0.7883 (7)	0.3862 (5)	0.5963 (4)	0.0248 (11)
H5A	0.703672	0.432445	0.547367	0.037*
H5B	0.915497	0.404192	0.564350	0.037*
H5C	0.783268	0.283036	0.600084	0.037*
C6	0.7179 (7)	0.6079 (5)	0.7113 (4)	0.0252 (11)
H6A	0.813789	0.638607	0.648547	0.030*
H6B	0.739459	0.642035	0.784564	0.030*
C7	0.5209 (6)	0.6717 (5)	0.6914 (4)	0.0203 (10)
H7A	0.507902	0.777404	0.691491	0.024*
H7B	0.502552	0.642083	0.615938	0.024*
C8	0.3699 (7)	0.6894 (5)	0.8977 (4)	0.0240 (11)
H8A	0.275110	0.653142	0.956793	0.036*
H8B	0.491658	0.667867	0.920385	0.036*
H8C	0.338952	0.793064	0.888771	0.036*
C9	0.1845 (6)	0.6579 (5)	0.7540 (4)	0.0238 (11)
H9A	0.183045	0.613796	0.681219	0.036*
H9B	0.090260	0.623030	0.814238	0.036*
H9C	0.157198	0.762008	0.746184	0.036*
C10	0.2343 (11)	−0.0099 (7)	0.5611 (6)	0.0552 (18)
H10A	0.099346	0.018269	0.579087	0.083*
H10B	0.261222	−0.109953	0.537796	0.083*
H10C	0.288970	0.050910	0.498446	0.083*
H1O	0.340 (12)	0.100 (4)	0.660 (8)	0.09 (3)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0138 (4)	0.0291 (4)	0.0137 (4)	−0.0029 (2)	−0.0019 (2)	−0.0033 (2)

Cl1	0.0148 (6)	0.0331 (7)	0.0169 (6)	−0.0028 (5)	−0.0014 (4)	−0.0012 (5)
Cl2	0.0205 (6)	0.0397 (7)	0.0172 (6)	−0.0054 (5)	−0.0045 (5)	−0.0061 (5)
O1	0.051 (3)	0.035 (2)	0.048 (3)	−0.004 (2)	−0.011 (2)	0.002 (2)
N1	0.015 (2)	0.034 (2)	0.017 (2)	−0.0042 (17)	−0.0016 (16)	−0.0066 (17)
N2	0.016 (2)	0.032 (2)	0.018 (2)	0.0005 (17)	−0.0003 (16)	−0.0051 (17)
N3	0.0137 (19)	0.027 (2)	0.018 (2)	−0.0030 (16)	−0.0018 (16)	0.0003 (16)
N4	0.014 (2)	0.029 (2)	0.016 (2)	−0.0010 (16)	−0.0043 (16)	−0.0031 (16)
C1	0.026 (3)	0.024 (3)	0.029 (3)	−0.005 (2)	0.000 (2)	−0.001 (2)
C2	0.029 (3)	0.029 (3)	0.032 (3)	0.001 (2)	−0.001 (2)	0.000 (2)
C3	0.021 (3)	0.034 (3)	0.031 (3)	0.009 (2)	−0.004 (2)	−0.005 (2)
C4	0.016 (2)	0.033 (3)	0.021 (3)	−0.003 (2)	−0.005 (2)	0.000 (2)
C5	0.022 (3)	0.037 (3)	0.015 (2)	−0.005 (2)	−0.002 (2)	−0.003 (2)
C6	0.017 (3)	0.032 (3)	0.026 (3)	−0.006 (2)	−0.004 (2)	0.002 (2)
C7	0.020 (2)	0.025 (3)	0.017 (2)	−0.0057 (19)	−0.0028 (19)	0.0032 (19)
C8	0.025 (3)	0.034 (3)	0.014 (2)	−0.005 (2)	−0.003 (2)	−0.007 (2)
C9	0.011 (2)	0.035 (3)	0.024 (3)	−0.001 (2)	−0.001 (2)	−0.002 (2)
C10	0.066 (5)	0.054 (4)	0.050 (4)	−0.015 (4)	−0.014 (4)	−0.002 (3)

Geometric parameters (Å, º)

Cu1—N1	1.991 (4)	C3—H3	0.9300
Cu1—N4	2.043 (4)	C4—H4A	0.9700
Cu1—N3	2.125 (4)	C4—H4B	0.9700
Cu1—Cl1	2.2914 (15)	C5—H5A	0.9600
Cu1—Cl2	2.4630 (15)	C5—H5B	0.9600
O1—C10	1.439 (7)	C5—H5C	0.9600
O1—H1O	0.91 (2)	C6—C7	1.522 (6)
N1—C1	1.322 (6)	C6—H6A	0.9700
N1—N2	1.346 (5)	C6—H6B	0.9700
N2—C3	1.327 (6)	C7—H7A	0.9700
N2—C4	1.459 (6)	C7—H7B	0.9700
N3—C4	1.473 (6)	C8—H8A	0.9600
N3—C5	1.473 (6)	C8—H8B	0.9600
N3—C6	1.488 (6)	C8—H8C	0.9600
N4—C8	1.475 (6)	C9—H9A	0.9600
N4—C7	1.484 (6)	C9—H9B	0.9600
N4—C9	1.493 (6)	C9—H9C	0.9600
C1—C2	1.396 (7)	C10—H10A	0.9600
C1—H1	0.9300	C10—H10B	0.9600
C2—C3	1.375 (7)	C10—H10C	0.9600
C2—H2	0.9300		
N1—Cu1—N4	156.67 (16)	N3—C4—H4A	110.6
N1—Cu1—N3	78.82 (16)	N2—C4—H4B	110.6
N4—Cu1—N3	85.33 (15)	N3—C4—H4B	110.6
N1—Cu1—Cl1	92.42 (12)	H4A—C4—H4B	108.7
N4—Cu1—Cl1	96.09 (11)	N3—C5—H5A	109.5
N3—Cu1—Cl1	157.90 (11)	N3—C5—H5B	109.5

N1—Cu1—Cl2	102.33 (12)	H5A—C5—H5B	109.5
N4—Cu1—Cl2	96.90 (11)	N3—C5—H5C	109.5
N3—Cu1—Cl2	98.84 (11)	H5A—C5—H5C	109.5
Cl1—Cu1—Cl2	102.86 (6)	H5B—C5—H5C	109.5
C10—O1—H1O	106 (5)	N3—C6—C7	108.4 (4)
C1—N1—N2	105.4 (4)	N3—C6—H6A	110.0
C1—N1—Cu1	140.6 (3)	C7—C6—H6A	110.0
N2—N1—Cu1	114.0 (3)	N3—C6—H6B	110.0
C3—N2—N1	111.5 (4)	C7—C6—H6B	110.0
C3—N2—C4	131.2 (4)	H6A—C6—H6B	108.4
N1—N2—C4	117.1 (4)	N4—C7—C6	109.2 (4)
C4—N3—C5	110.2 (4)	N4—C7—H7A	109.8
C4—N3—C6	112.7 (4)	C6—C7—H7A	109.8
C5—N3—C6	111.0 (4)	N4—C7—H7B	109.8
C4—N3—Cu1	104.4 (3)	C6—C7—H7B	109.8
C5—N3—Cu1	112.5 (3)	H7A—C7—H7B	108.3
C6—N3—Cu1	105.7 (3)	N4—C8—H8A	109.5
C8—N4—C7	111.4 (4)	N4—C8—H8B	109.5
C8—N4—C9	107.1 (4)	H8A—C8—H8B	109.5
C7—N4—C9	109.0 (3)	N4—C8—H8C	109.5
C8—N4—Cu1	110.6 (3)	H8A—C8—H8C	109.5
C7—N4—Cu1	105.1 (3)	H8B—C8—H8C	109.5
C9—N4—Cu1	113.6 (3)	N4—C9—H9A	109.5
N1—C1—C2	111.1 (5)	N4—C9—H9B	109.5
N1—C1—H1	124.4	H9A—C9—H9B	109.5
C2—C1—H1	124.4	N4—C9—H9C	109.5
C3—C2—C1	104.1 (5)	H9A—C9—H9C	109.5
C3—C2—H2	127.9	H9B—C9—H9C	109.5
C1—C2—H2	127.9	O1—C10—H10A	109.5
N2—C3—C2	107.8 (5)	O1—C10—H10B	109.5
N2—C3—H3	126.1	H10A—C10—H10B	109.5
C2—C3—H3	126.1	O1—C10—H10C	109.5
N2—C4—N3	105.9 (4)	H10A—C10—H10C	109.5
N2—C4—H4A	110.6	H10B—C10—H10C	109.5

C1—N1—N2—C3	−0.3 (5)	N1—N2—C4—N3	−36.6 (5)
Cu1—N1—N2—C3	−179.1 (3)	C5—N3—C4—N2	−75.1 (4)
C1—N1—N2—C4	−175.1 (4)	C6—N3—C4—N2	160.2 (4)
Cu1—N1—N2—C4	6.1 (5)	Cu1—N3—C4—N2	45.9 (4)
N2—N1—C1—C2	0.5 (5)	C4—N3—C6—C7	−149.4 (4)
Cu1—N1—C1—C2	178.8 (4)	C5—N3—C6—C7	86.4 (5)
N1—C1—C2—C3	−0.4 (6)	Cu1—N3—C6—C7	−35.9 (4)
N1—N2—C3—C2	0.0 (6)	C8—N4—C7—C6	72.7 (5)
C4—N2—C3—C2	173.9 (5)	C9—N4—C7—C6	−169.3 (4)
C1—C2—C3—N2	0.2 (6)	Cu1—N4—C7—C6	−47.2 (4)
C3—N2—C4—N3	149.9 (5)	N3—C6—C7—N4	57.5 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···Cl1^{i}	0.93	2.98	3.841 (6)	156
C3—H3···O1^{ii}	0.93	2.62	3.305 (7)	131
C4—H4*A*···Cl2^{ii}	0.97	2.67	3.636 (5)	173
C4—H4*B*···Cl1^{iii}	0.97	2.94	3.902 (5)	170
C5—H5*A*···Cl2^{iv}	0.96	2.93	3.745 (5)	143
C7—H7*A*···O1^{v}	0.97	2.42	3.281 (6)	148
C7—H7*B*···Cl2^{iv}	0.97	2.83	3.632 (5)	140
C8—H8*A*···Cl1	0.96	2.85	3.414 (5)	119
C8—H8*B*···Cl1^{iii}	0.96	2.81	3.736 (5)	162
C9—H9*A*···Cl2	0.96	2.76	3.387 (5)	124
O1—H1*O*···Cl2	0.91 (2)	2.16 (3)	3.047 (4)	164 (7)

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