

Chloridobis(ethane-1,2-diamine)(4*H*-1,2,4-triazole- κ N¹)cobalt(III) dichloride

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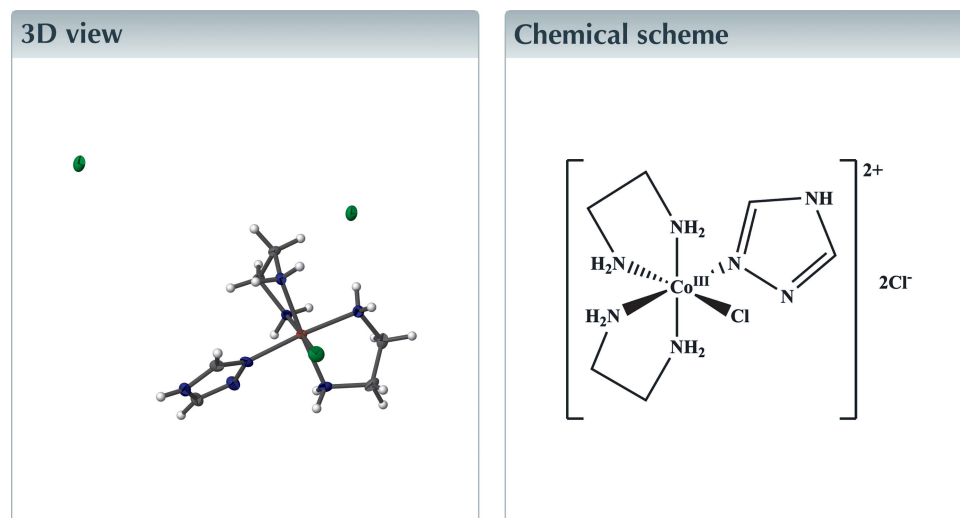
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Keywords: crystal structure; ethane-1,2-diamine; triazole ligand; cobalt(III) complex; hydrogen bonding; N—H···N; N—H···Cl and C—H···Cl interactions.

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

In the title complex, [Co^{III}Cl(C₂H₈N₂)₂(C₂H₃N₃)]Cl₂, the Co^{III} ion has a distorted octahedral environment. It is surrounded by four N atoms in the equatorial plane, with another N atom and a Cl atom occupying the axial positions. Both five-membered Co—N—C—C—N rings adopt a twist conformation. The Co—N bond lengths range from 1.941 (2) to 1.954 (1) Å, while the Co—Cl bond length is 2.257 (1) Å. In the crystal, molecules are linked by N—H···N, N—H···Cl and C—H···Cl hydrogen bonds. Dimers are formed by N—H···Cl hydrogen-bonding interactions between amine H-atom donors and chloride ions resulting in an R₄²(8) ring motif. These dimers are further connected in a head-to-tail fashion *via* N—H···Cl and C—H···Cl hydrogen bonds. All the interactions together combine to link the molecules into a three-dimensional framework.



Structure description

Appropriate tailoring of the coordination environment and specific incorporation of ligands around transition metal ions are of key importance in the modification of the properties of metal complexes with respect to spectroscopic, redox activity in interfacial electron-transfer reactions, catalytic and photocatalytic properties (Xu *et al.*, 2008; Anbalagan, 2011). As a result of the excellent coordination ability of nitrogen-containing ligands, research on transition metal complexes involving ligands that coordinate through an N atom, such as simple amines (Mitzi, 1996; Deeth *et al.*, 1984), cyanides (Wu *et al.*, 2003; Shores *et al.*, 2002), or N-heterocyclic rings (Hagrman *et al.*, 1999; Willett *et al.*, 2001), has always been an active area in coordination chemistry. Polydentate amine ligands generally coordinate to transition metal ions using all of the available nitrogen atoms as donors. Metal–chelate complexes (Tweedy, 1964; Králová *et al.*, 2004) find

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1A\cdots Cl3^i$	0.89	2.39	3.2202 (17)	155
$N3-H3B\cdots Cl2^i$	0.89	2.57	3.2833 (17)	138
$C3-H3C\cdots Cl2^i$	0.97	2.79	3.382 (2)	120
$N2-H2A\cdots Cl3^{ii}$	0.89	2.40	3.2311 (17)	156
$N7-H7\cdots Cl2^{iii}$	0.86	2.17	3.0326 (17)	177
$N4-H4B\cdots Cl2^{iv}$	0.89	2.36	3.1891 (16)	156
$N4-H4A\cdots Cl2^v$	0.89	2.50	3.3364 (17)	157
$N2-H2B\cdots N6$	0.89	2.37	2.898 (2)	118
$N1-H1B\cdots Cl3$	0.89	2.45	3.3103 (17)	162

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

potential applications in the research fields of antitumor activity, enzyme catalysis, functioning of micro organisms and in the respiration processes of biological systems (Parekh *et al.*, 2005; Rajavel *et al.*, 2008). Chelating ligands such as ethylenediamine have been widely used to prepare a number of cobalt(III) complexes (Bailar & Clapp, 1945; Bailar & Rollinson, 1946). It acts as a bidentate ligand in the majority of its complexes, chelating to one metal ion through both nitrogen atoms, and there are few complexes in which it coordinates as a monodentate ligand. This paper reports the synthesis and X-ray structural characterization of $[Co^{III}(en)_2(tzl)Cl]Cl_2$ in order to determine the bonding mode and geometric features of two ethylenediamine (en) ligands, a triazole (tzl) and a chloride ligand.

An ORTEP representation of the title compound is given in Fig. 1. The coordination environment around the Co^{III} ion can be described as a slightly distorted octahedron. The coordination sphere of cobalt is formed by one triazole, one chloride ion and two ethylenediamine ligands. The Co^{III} ion and four N atoms almost lie in same plane whereas another N and the Cl atom are approximately perpendicular to this plane. The coordination octahedron shows a slight but significant distortion: the $N(en)-Co-N(en)$ angles within the five-membered

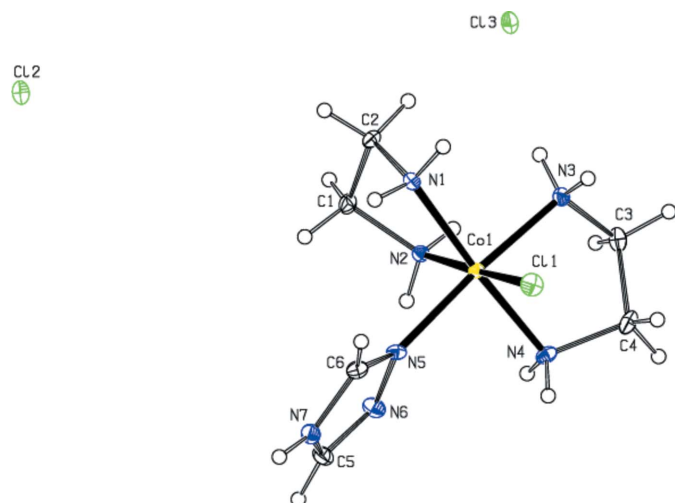


Figure 1
A view of the molecular structure of the title salt, showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

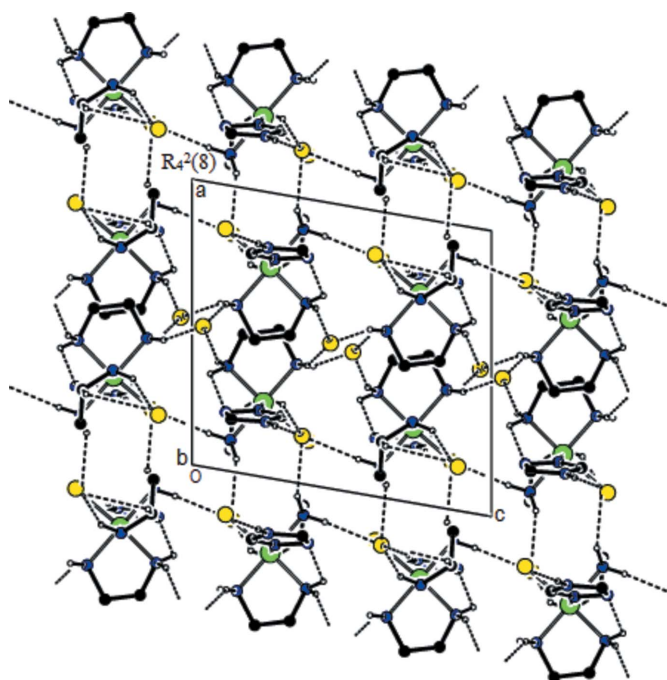


Figure 2
A view along the b axis of the crystal packing of the title complex. The $N-H\cdots N$, $N-H\cdots Cl$ and $C-H\cdots Cl$ hydrogen bonds are shown as dashed lines (see Table 1 for details; H atoms not involved in hydrogen bonding have been omitted for clarity). $N-H\cdots Cl$ hydrogen bonds form dimers resulting in an $R_4^2(8)$ ring motif.

rings are smaller [$85.5(7)$ and $85.6(7)^\circ$] than those between two nitrogen atoms of different ethylenediamine ligands. The bond lengths and angles also confirm the distortion from a regular octahedron. Both five-membered rings in the molecule adopt a twist conformation.

All of the amine H atoms of the triazole and en ligands except H3A, and additionally the carbon H3C atom are involved in hydrogen bonds with chlorine and a triazole N-atom acceptor [$D\cdots A$ distances in the range 2.898 (2)–3.382 (2) Å; Table 1]. The $N-H\cdots Cl$ hydrogen-bonding

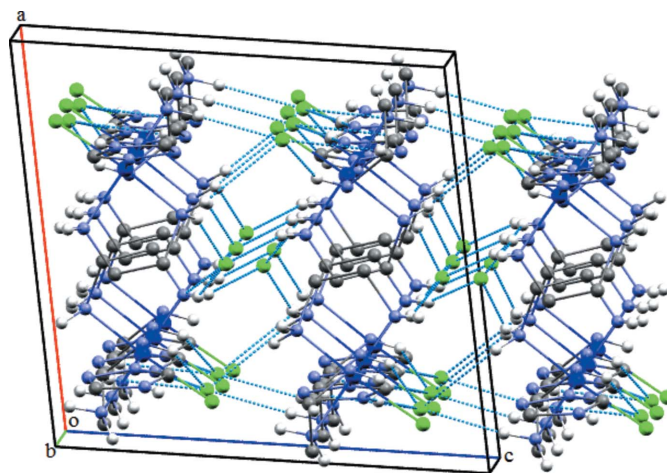


Figure 3
Partial packing diagram of the title structure viewed parallel to (100). $N-H\cdots Cl$ and $C-H\cdots Cl$ hydrogen bonds are drawn as dashed light-blue lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	[CoCl(C ₂ H ₈ N ₂) ₂ (C ₂ H ₃ N ₃)]Cl ₂
<i>M_r</i>	354.56
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.9170 (3), 11.0714 (3), 11.6172 (3)
β (°)	99.822 (2)
<i>V</i> (Å ³)	1383.55 (6)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	1.81
Crystal size (mm)	0.22 × 0.12 × 0.10
Data collection	
Diffractometer	Oxford Diffraction Xcalibur diffractometer with Eos detector
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Oxford Diffraction, 2009)
<i>T</i> _{min} , <i>T</i> _{max}	0.771, 0.834
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	6386, 2422, 2202
<i>R</i> _{int}	0.025
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.594
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.023, 0.058, 1.05
No. of reflections	2422
No. of parameters	154
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.29, -0.26

Computer programs: *CrysAlis CCD* and *CrysAlis RED* (Oxford Diffraction, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

interactions between amine H-atom donors and chlorine-atom acceptors result in an *R*₄²(8) ring motif, as shown in Fig. 2. Further N—H...Cl and C—H...Cl hydrogen bonds connect the molecules in a head-to-tail fashion *via* these dimers (Fig. 2, Table 1). All these interactions combine to link the molecules into a three-dimensional framework (Fig. 3). It is remarkable that the chlorine ligand bonded to Co is not involved in hydrogen bonding. No π – π stacking interactions are observed.

Synthesis and crystallization

The title complex was synthesized by the reported method (Ravichandran *et al.*, 2009) by taking 2 g of the *trans*-[Co^{III}(en)₂Cl₂]Cl complex and 0.5 g of 1,2,4-triazole. The cobalt(III) complex was recrystallized by addition of few drops of concentrated HCl in 10 ml of water containing 1 g of the complex. The solution was heated at 343 K with stirring for

30 min and cooled. The pure crystals were obtained by filtration, washed with ethanol after 2–3 weeks and dried under vacuum.

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2017). 2, x171728 [https://doi.org/10.1107/S241431461701728X]

Chloridobis(ethane-1,2-diamine)(4*H*-1,2,4-triazole- κ N¹)cobalt(III) dichloride

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Chloridobis(ethane-1,2-diamine)(4*H*-1,2,4-triazole- κ N¹)cobalt(III) dichloride*Crystal data*

[CoCl(C₂H₈N₂)₂(C₂H₃N₃)]Cl₂

M_r = 354.56

Monoclinic, *P*2₁/*c*

a = 10.9170 (3) Å

b = 11.0714 (3) Å

c = 11.6172 (3) Å

β = 99.822 (2)°

V = 1383.55 (6) Å³

Z = 4

F(000) = 728

D_x = 1.702 Mg m⁻³

Mo *K* α radiation, λ = 0.71073 Å

Cell parameters from 2202 reflections

θ = 2.6–25.0°

μ = 1.81 mm⁻¹

T = 293 K

Block, pink

0.22 × 0.12 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur

diffractometer with Eos detector

Radiation source: fine-focus sealed tube

ω and ϕ scans

Absorption correction: multi-scan

(CrysAlis Pro; Oxford Diffraction, 2009)

T_{min} = 0.771, *T_{max}* = 0.834

6386 measured reflections

2422 independent reflections

2202 reflections with *I* > 2 σ (*I*)

R_{int} = 0.025

θ_{\max} = 25.0°, θ_{\min} = 2.6°

h = -12→10

k = -13→12

l = -13→13

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2 σ (*F*²)] = 0.023

wR(*F*²) = 0.058

S = 1.05

2422 reflections

154 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-atom parameters constrained

w = 1/[$\sigma^2(F_o^2) + (0.0275P)^2 + 0.4893P$]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} = 0.001

$\Delta\rho_{\max}$ = 0.29 e Å⁻³

$\Delta\rho_{\min}$ = -0.26 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.

Refinement. All H atoms were refined using a ring model with methylene C—H = 0.97 Å, aromatic C—H = 0.93 Å, aromatic N—H = 0.86 Å and remaining N—H = 0.89 Å. *U_{iso}*(H) was set to 1.2 *U_{eq}*(C,N).

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.48819 (19)	0.53430 (18)	0.17319 (17)	0.0179 (5)
H1C	0.4817	0.6209	0.1834	0.022*
H1D	0.5501	0.5188	0.1242	0.022*
C2	0.52424 (19)	0.47293 (18)	0.29027 (18)	0.0179 (4)
H2C	0.5439	0.3886	0.2799	0.022*
H2D	0.5963	0.5120	0.3355	0.022*
C3	0.1958 (2)	0.24086 (18)	0.13512 (17)	0.0195 (5)
H3C	0.1825	0.1554	0.1467	0.023*
H3D	0.2297	0.2511	0.0638	0.023*
C4	0.07586 (19)	0.30938 (19)	0.12812 (18)	0.0212 (5)
H4C	0.0192	0.2887	0.0572	0.025*
H4D	0.0363	0.2906	0.1947	0.025*
C5	0.1827 (2)	0.80491 (19)	0.13127 (17)	0.0200 (5)
H5	0.1615	0.8620	0.0725	0.024*
C6	0.22500 (18)	0.72412 (18)	0.30049 (17)	0.0168 (4)
H6	0.2395	0.7130	0.3810	0.020*
N1	0.41523 (15)	0.48390 (15)	0.35022 (14)	0.0141 (3)
H1A	0.4166	0.5556	0.3851	0.017*
H1B	0.4189	0.4270	0.4048	0.017*
N2	0.36590 (15)	0.48335 (14)	0.11867 (13)	0.0127 (3)
H2A	0.3767	0.4115	0.0875	0.015*
H2B	0.3294	0.5320	0.0621	0.015*
N3	0.28179 (15)	0.29178 (15)	0.23624 (13)	0.0154 (4)
H3A	0.3599	0.2736	0.2305	0.019*
H3B	0.2653	0.2601	0.3023	0.019*
N4	0.10919 (15)	0.43907 (15)	0.12816 (14)	0.0158 (4)
H4A	0.0479	0.4833	0.1480	0.019*
H4B	0.1198	0.4612	0.0569	0.019*
N5	0.23054 (15)	0.63932 (15)	0.22306 (13)	0.0142 (4)
N6	0.20391 (16)	0.69145 (15)	0.11309 (14)	0.0203 (4)
N7	0.19539 (15)	0.82883 (15)	0.24633 (14)	0.0188 (4)
H7	0.1863	0.8976	0.2783	0.023*
Co1	0.26132 (2)	0.46688 (2)	0.23849 (2)	0.01067 (9)
Cl1	0.15406 (5)	0.45606 (5)	0.38793 (4)	0.02057 (13)
Cl2	0.83310 (5)	0.93314 (4)	0.63180 (4)	0.01813 (13)
Cl3	0.49114 (5)	0.25953 (4)	0.53712 (4)	0.02029 (13)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0133 (10)	0.0191 (11)	0.0226 (11)	-0.0023 (9)	0.0065 (8)	0.0005 (9)
C2	0.0106 (10)	0.0184 (11)	0.0238 (11)	-0.0006 (8)	0.0004 (8)	-0.0006 (9)
C3	0.0246 (12)	0.0173 (11)	0.0178 (10)	-0.0055 (9)	0.0071 (9)	-0.0017 (9)
C4	0.0148 (11)	0.0280 (12)	0.0205 (10)	-0.0081 (10)	0.0020 (8)	-0.0005 (9)
C5	0.0223 (11)	0.0161 (11)	0.0217 (10)	0.0025 (9)	0.0042 (9)	0.0052 (9)

C6	0.0144 (10)	0.0209 (11)	0.0158 (10)	0.0032 (9)	0.0044 (8)	-0.0009 (9)
N1	0.0156 (9)	0.0121 (8)	0.0147 (8)	0.0001 (7)	0.0027 (7)	0.0010 (7)
N2	0.0123 (8)	0.0129 (8)	0.0135 (8)	0.0013 (7)	0.0036 (7)	0.0004 (7)
N3	0.0146 (9)	0.0144 (9)	0.0179 (8)	-0.0007 (7)	0.0042 (7)	0.0014 (7)
N4	0.0106 (8)	0.0232 (9)	0.0140 (8)	0.0018 (7)	0.0033 (7)	0.0005 (7)
N5	0.0128 (8)	0.0164 (9)	0.0137 (7)	0.0046 (7)	0.0031 (6)	0.0018 (7)
N6	0.0252 (10)	0.0186 (10)	0.0171 (8)	0.0034 (8)	0.0038 (7)	0.0020 (8)
N7	0.0176 (9)	0.0138 (9)	0.0260 (9)	0.0018 (7)	0.0065 (7)	-0.0044 (7)
Co1	0.00960 (15)	0.01248 (16)	0.01046 (14)	0.00105 (10)	0.00321 (10)	0.00064 (10)
Cl1	0.0225 (3)	0.0254 (3)	0.0164 (2)	0.0008 (2)	0.0106 (2)	0.0021 (2)
Cl2	0.0226 (3)	0.0163 (3)	0.0168 (2)	-0.0051 (2)	0.0069 (2)	-0.0023 (2)
Cl3	0.0215 (3)	0.0150 (3)	0.0240 (3)	-0.0043 (2)	0.0030 (2)	0.0004 (2)

Geometric parameters (Å, °)

C1—N2	1.488 (2)	C6—N7	1.332 (3)
C1—C2	1.511 (3)	C6—H6	0.9300
C1—H1C	0.9700	N1—Co1	1.9492 (16)
C1—H1D	0.9700	N1—H1A	0.8900
C2—N1	1.483 (3)	N1—H1B	0.8900
C2—H2C	0.9700	N2—Co1	1.9536 (15)
C2—H2D	0.9700	N2—H2A	0.8900
C3—N3	1.484 (2)	N2—H2B	0.8900
C3—C4	1.504 (3)	N3—Co1	1.9522 (16)
C3—H3C	0.9700	N3—H3A	0.8900
C3—H3D	0.9700	N3—H3B	0.8900
C4—N4	1.481 (3)	N4—Co1	1.9416 (16)
C4—H4C	0.9700	N4—H4A	0.8900
C4—H4D	0.9700	N4—H4B	0.8900
C5—N6	1.301 (3)	N5—N6	1.387 (2)
C5—N7	1.346 (3)	N5—Co1	1.9414 (17)
C5—H5	0.9300	N7—H7	0.8600
C6—N5	1.309 (3)	Co1—Cl1	2.2568 (5)
N2—C1—C2	106.84 (16)	Co1—N2—H2A	109.9
N2—C1—H1C	110.4	C1—N2—H2B	109.9
C2—C1—H1C	110.4	Co1—N2—H2B	109.9
N2—C1—H1D	110.4	H2A—N2—H2B	108.3
C2—C1—H1D	110.4	C3—N3—Co1	109.24 (12)
H1C—C1—H1D	108.6	C3—N3—H3A	109.8
N1—C2—C1	106.22 (16)	Co1—N3—H3A	109.8
N1—C2—H2C	110.5	C3—N3—H3B	109.8
C1—C2—H2C	110.5	Co1—N3—H3B	109.8
N1—C2—H2D	110.5	H3A—N3—H3B	108.3
C1—C2—H2D	110.5	C4—N4—Co1	109.66 (12)
H2C—C2—H2D	108.7	C4—N4—H4A	109.7
N3—C3—C4	106.17 (16)	Co1—N4—H4A	109.7
N3—C3—H3C	110.5	C4—N4—H4B	109.7

C4—C3—H3C	110.5	Co1—N4—H4B	109.7
N3—C3—H3D	110.5	H4A—N4—H4B	108.2
C4—C3—H3D	110.5	C6—N5—N6	107.92 (16)
H3C—C3—H3D	108.7	C6—N5—Co1	132.03 (14)
N4—C4—C3	106.10 (16)	N6—N5—Co1	120.01 (12)
N4—C4—H4C	110.5	C5—N6—N5	105.51 (16)
C3—C4—H4C	110.5	C6—N7—C5	105.86 (17)
N4—C4—H4D	110.5	C6—N7—H7	127.1
C3—C4—H4D	110.5	C5—N7—H7	127.1
H4C—C4—H4D	108.7	N5—Co1—N4	88.85 (7)
N6—C5—N7	111.10 (18)	N5—Co1—N1	94.73 (7)
N6—C5—H5	124.4	N4—Co1—N1	176.42 (7)
N7—C5—H5	124.4	N5—Co1—N3	173.57 (7)
N5—C6—N7	109.61 (17)	N4—Co1—N3	85.45 (7)
N5—C6—H6	125.2	N1—Co1—N3	90.99 (7)
N7—C6—H6	125.2	N5—Co1—N2	87.45 (7)
C2—N1—Co1	110.43 (12)	N4—Co1—N2	94.73 (7)
C2—N1—H1A	109.6	N1—Co1—N2	85.60 (7)
Co1—N1—H1A	109.6	N3—Co1—N2	90.06 (7)
C2—N1—H1B	109.6	N5—Co1—Cl1	91.08 (5)
Co1—N1—H1B	109.6	N4—Co1—Cl1	90.10 (5)
H1A—N1—H1B	108.1	N1—Co1—Cl1	89.67 (5)
C1—N2—Co1	108.86 (11)	N3—Co1—Cl1	91.90 (5)
C1—N2—H2A	109.9	N2—Co1—Cl1	174.91 (5)
N2—C1—C2—N1	-50.6 (2)	C6—N5—Co1—Cl1	36.86 (18)
N3—C3—C4—N4	52.03 (19)	N6—N5—Co1—Cl1	-140.35 (13)
C1—C2—N1—Co1	37.29 (18)	C4—N4—Co1—N5	-168.10 (13)
C2—C1—N2—Co1	41.09 (18)	C4—N4—Co1—N3	14.88 (13)
C4—C3—N3—Co1	-40.20 (17)	C4—N4—Co1—N2	104.56 (13)
C3—C4—N4—Co1	-40.50 (18)	C4—N4—Co1—Cl1	-77.02 (12)
N7—C6—N5—N6	0.3 (2)	C2—N1—Co1—N5	-99.16 (13)
N7—C6—N5—Co1	-177.12 (13)	C2—N1—Co1—N3	77.89 (13)
N7—C5—N6—N5	0.6 (2)	C2—N1—Co1—N2	-12.09 (13)
C6—N5—N6—C5	-0.6 (2)	C2—N1—Co1—Cl1	169.78 (12)
Co1—N5—N6—C5	177.23 (13)	C3—N3—Co1—N4	14.58 (13)
N5—C6—N7—C5	0.0 (2)	C3—N3—Co1—N1	-165.76 (13)
N6—C5—N7—C6	-0.4 (2)	C3—N3—Co1—N2	-80.15 (13)
C6—N5—Co1—N4	126.94 (19)	C3—N3—Co1—Cl1	104.54 (12)
N6—N5—Co1—N4	-50.27 (14)	C1—N2—Co1—N5	78.37 (13)
C6—N5—Co1—N1	-52.90 (19)	C1—N2—Co1—N4	166.99 (13)
N6—N5—Co1—N1	129.89 (14)	C1—N2—Co1—N1	-16.57 (12)
C6—N5—Co1—N2	-138.28 (19)	C1—N2—Co1—N3	-107.56 (13)
N6—N5—Co1—N2	44.51 (14)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H1 <i>A</i> ···C13 ⁱ	0.89	2.39	3.2202 (17)	155
N3—H3 <i>B</i> ···C12 ⁱ	0.89	2.57	3.2833 (17)	138
C3—H3 <i>C</i> ···C12 ⁱ	0.97	2.79	3.382 (2)	120
N2—H2 <i>A</i> ···C13 ⁱⁱ	0.89	2.40	3.2311 (17)	156
N7—H7···C12 ⁱⁱⁱ	0.86	2.17	3.0326 (17)	177
N4—H4 <i>B</i> ···C12 ^{iv}	0.89	2.36	3.1891 (16)	156
N4—H4 <i>A</i> ···C12 ^v	0.89	2.50	3.3364 (17)	157
N2—H2 <i>B</i> ···N6	0.89	2.37	2.898 (2)	118
N1—H1 <i>B</i> ···C13	0.89	2.45	3.3103 (17)	162

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, -y+1/2, z-1/2$; (iii) $-x+1, -y+2, -z+1$; (iv) $-x+1, y-1/2, -z+1/2$; (v) $x-1, -y+3/2, z-1/2$.