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cis-Bromido(*n*-butylamine-κN)bis(ethene-1,2-diamine-$\kappa^2 N,N'$)cobalt(III) dibromide

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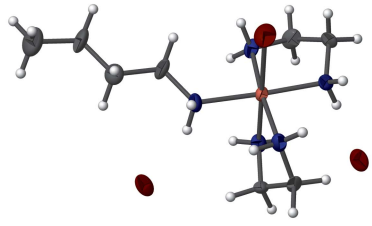
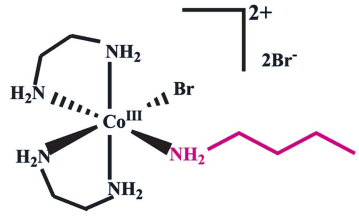
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[CoBr(C_2H_8N_2)_2(C_4H_{11}N)]Br_2$, the cobalt(III) ion has a distorted octahedral coordination environment and is surrounded by four N atoms in the equatorial plane made up of three N atoms from the two ethylenediamine ligands and the remaining N from the *n*-butyl substituent, with the other N atom from the ethylenediamine ligand and the Br atom occupying the axial positions. In the crystal, the complex cation and the two counter-anions are linked *via* N—H···Br and C—H···Br hydrogen bonds, forming a three-dimensional network. The crystal studied was refined as a two-component inversion twin.

3D view



Chemical scheme



Structure description

Mixed-ligand cobalt(III) complexes exhibit antitumor, antibacterial, antimicrobial, radiosenzitation and cytotoxicity activities (Sayed *et al.*, 1992; Teicher *et al.*, 1990; Arslan *et al.*, 2009; Delehanty *et al.*, 2008). Cobalt is an essential and integral component of vitamin B12 and is therefore found physiologically in most tissues. Complexes of cobalt are useful for nutritional supplementation to provide cobalt in a form, which effectively increases its bioavailability, for instance, vitamin B12 by microorganisms present in the gut. In addition, cobalt(III) complexes are known for electron-transfer and ligand-substitution reactions, which find applications in chemical and biological systems. Our present research concerns the design and synthesis of cobalt(III) complexes with the objective of understanding the structure–reactivity correlation. Substituting a different amino ligand for the $MeNH_2$ moiety can yield complexes of similar structure, but with

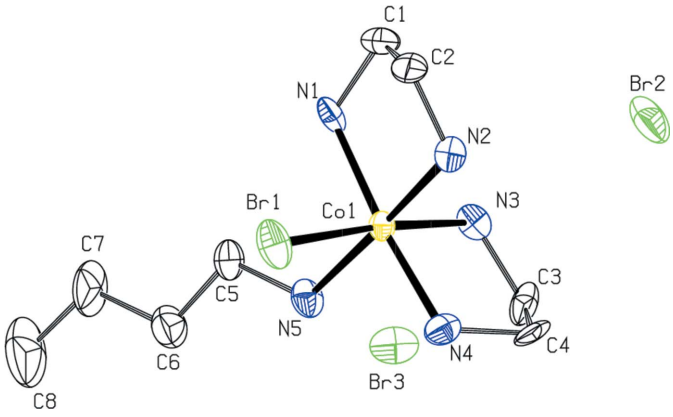


Figure 1
Molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

differing electron-transfer rates (Anbalagan, 2011; Anbalagan *et al.*, 2011). Against this background and to ascertain the molecular conformation, the structure determination of the title compound has been carried out.

X-ray analysis confirms the molecular structure and atom connectivity as illustrated in Fig. 1. The Co—N bond lengths are comparable with literature values [1.9722 (2)–1.988 (2) Å: Manimaran *et al.*, 2018; 1.948 (7)–1.963 (7) Å: Lee *et al.*, 2007; Ramesh *et al.*, 2008; Anbalagan *et al.*, 2009; Ravichandran *et al.*, 2009]. The whole molecule is not planar, the dihedral angle between the two chelate rings being 79.4 (4)°. One of the five-membered rings in the molecule adopts a half-chair conformation.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Br3^{i}	0.90	2.51	3.348 (9)	156
N1—H1*B*···Br1^{ii}	0.90	2.71	3.467 (8)	143
N2—H2*A*···Br2^{iii}	0.90	2.50	3.335 (8)	154
N2—H2*B*···Br2	0.90	2.50	3.392 (8)	173
N3—H3*A*···Br3	0.90	3.03	3.680 (9)	131
N3—H3*A*···Br3^{i}	0.90	3.01	3.695 (9)	134
N3—H3*B*···Br2	0.90	2.57	3.372 (9)	148
N4—H4*C*···Br2^{iii}	0.90	2.65	3.468 (9)	151
N4—H4*D*···Br3^{iv}	0.90	2.49	3.359 (9)	163
N5—H5*A*···Br3	0.90	2.61	3.458 (9)	158
N5—H5*B*···Br3^{iv}	0.90	2.88	3.487 (9)	126
C3—H3*D*···Br3	0.99	2.84	3.594 (11)	134
C4—H4*B*···Br2	0.99	3.00	3.739 (11)	132
C5—H5*D*···Br1	0.99	3.10	3.607 (12)	114
C5—H5*D*···Br1^{ii}	0.99	3.10	3.884 (13)	137

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

In the crystal, C—H···Br and N—H···Br hydrogen bonds (Table 1) link the molecules into a three-dimensional framework, as shown in Figs 2 and 3.

Synthesis and crystallization

trans-[Co(en)$_2$Br$_2$]Br solid (2 g) was made into a paste using 3–4 drops of water. To the solid mass, about 2 ml of *N*-butyl-

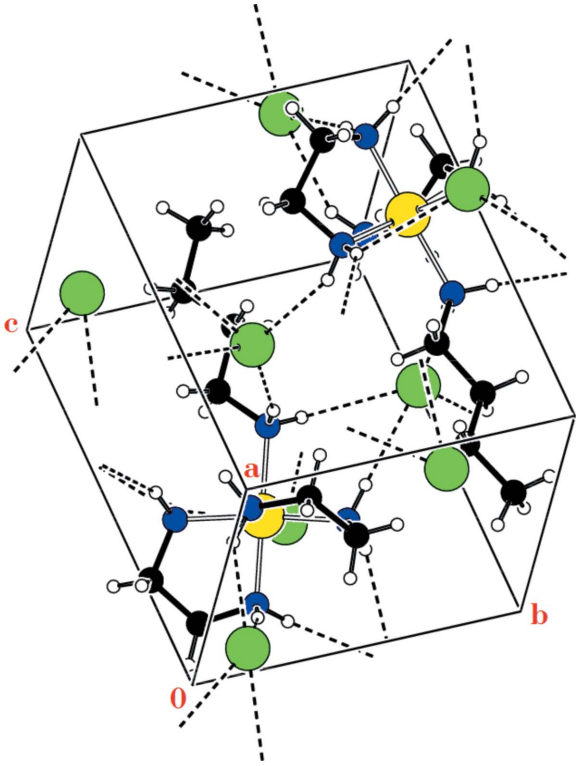


Figure 2
The packing of the title compound viewed along the *a* axis. Dashed lines indicate hydrogen bonds.

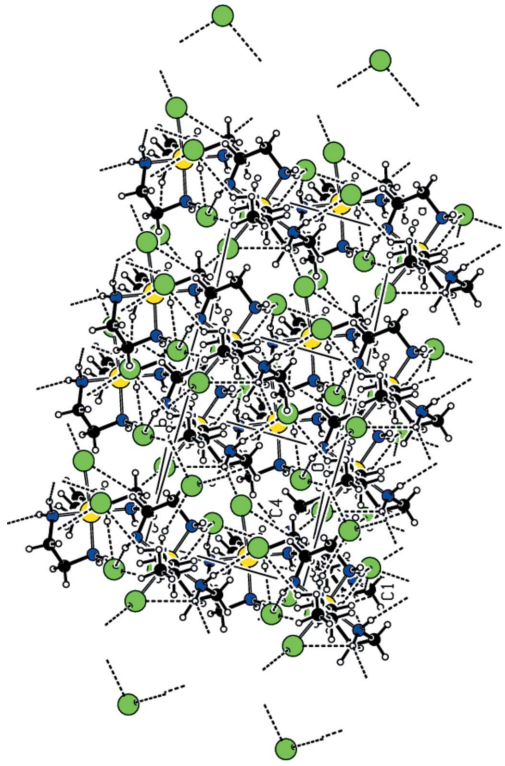


Figure 3
The packing of the title compound viewed along the *a* axis. Dashed lines indicate hydrogen bonds.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[CoBr(C_2H_8N_2)_2(C_4H_{11}N)]Br_2$
M_r	492.00
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	123
a, b, c (Å)	10.6336 (7), 7.5810 (3), 12.0809 (7)
β (°)	114.028 (7)
V (Å^3)	889.49 (10)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	7.69
Crystal size (mm)	0.23 × 0.17 × 0.11
Data collection	
Diffractometer	Bruker SMART APEXII area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.165, 0.361
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2398, 2398, 1769
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.085, 0.92
No. of reflections	2398
No. of parameters	156
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.78, −0.72
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.08 (3)

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXTL* (Sheldrick, 2008) and *SHELXL2018* (Sheldrick, 2015).

amine was dropped for 20 min and mixed well. The mixing was continued until the colour changed from dull green to red. The reaction mixture was set aside until no further change was observed and the mixture was allowed to stand overnight. Finally, the obtained solid was washed with ethanol and dissolved in 5–10 ml of water pre-heated to 70°C and allowed to crystallize using hot acidified water (yield 0.85 g). The crystals were filtered, washed with ethanol and dried under vacuum. X-ray quality crystals were obtained by repeated recrystallization from hot acidified distilled water. Microcrystalline pink crystals were obtained for analysis.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal studied was refined as a two-component inversion twin.

Acknowledgements

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full crystallographic data

IUCrData (2018). **3**, x181022 [https://doi.org/10.1107/S2414314618010222]

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cis-Bromido(*n*-butylamine-κN)bis(ethene-1,2-diamine-κ^2N,N')cobalt(III) dibromide

Crystal data

$[CoBr(C_2H_8N_2)_2(C_4H_{11}N)]Br_2$
M_r = 492.00
Monoclinic, $P2_1$
a = 10.6336 (7) Å
b = 7.5810 (3) Å
c = 12.0809 (7) Å
β = 114.028 (7)°
V = 889.49 (10) Å^3
Z = 2
$F(000)$ = 484
D_x = 1.837 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2458 reflections
θ = 2.9–25.0°
μ = 7.69 mm^{-1}
T = 123 K
Block, pink
0.23 × 0.17 × 0.11 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.165, T_{max} = 0.361
2398 measured reflections
2398 independent reflections
1769 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 25.0°, θ_{min} = 3.3°
h = −7→12
k = −8→8
l = −14→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.085
S = 0.92
2398 reflections
156 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.72 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.08 (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. Refined as a 2-component inversion twin.
The H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = ranging from 0.95 to 0.99 Å and N—H 0.90 Å. U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H atoms and 1.2 for all other C and N bound H atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	1.03734 (13)	0.48014 (17)	0.62170 (11)	0.0420 (4)
Co1	0.86142 (14)	0.3543 (2)	0.67319 (11)	0.0192 (3)
N1	0.8910 (9)	0.1217 (11)	0.6194 (7)	0.026 (2)
H1A	0.808973	0.070057	0.577554	0.032*
H1B	0.934073	0.133357	0.569254	0.032*
N2	1.0045 (8)	0.2816 (11)	0.8297 (7)	0.024 (2)
H2A	1.063969	0.370871	0.862055	0.029*
H2B	0.965869	0.253471	0.881155	0.029*
N3	0.7102 (9)	0.2722 (11)	0.7171 (8)	0.026 (2)
H3A	0.645306	0.217550	0.653245	0.031*
H3B	0.743506	0.194250	0.778545	0.031*
N4	0.8408 (10)	0.5759 (11)	0.7439 (8)	0.028 (2)
H4C	0.924563	0.621362	0.788221	0.034*
H4D	0.794962	0.652962	0.684421	0.034*
N5	0.7236 (9)	0.4307 (12)	0.5110 (7)	0.029 (2)
H5A	0.640727	0.432547	0.514638	0.035*
H5B	0.743627	0.542937	0.499738	0.035*
C1	0.9733 (13)	0.0091 (15)	0.7212 (10)	0.040 (3)
H1C	1.019060	−0.085105	0.694447	0.048*
H1D	0.914632	−0.046286	0.757530	0.048*
C2	1.0779 (12)	0.1281 (16)	0.8109 (9)	0.034 (3)
H2C	1.127138	0.065188	0.888472	0.041*
H2D	1.146204	0.166546	0.779520	0.041*
C3	0.6490 (11)	0.4226 (15)	0.7535 (10)	0.035 (3)
H3C	0.603590	0.382502	0.806183	0.042*
H3D	0.579195	0.480660	0.681181	0.042*
C4	0.7650 (12)	0.5509 (14)	0.8220 (10)	0.032 (3)
H4A	0.727491	0.664551	0.835414	0.039*
H4B	0.826389	0.501359	0.901613	0.039*
C5	0.7084 (12)	0.3309 (18)	0.4017 (8)	0.036 (3)
H5C	0.663946	0.216313	0.402205	0.044*
H5D	0.800965	0.306121	0.404319	0.044*
C6	0.6245 (12)	0.4262 (16)	0.2852 (9)	0.041 (3)
H6A	0.532247	0.451988	0.283059	0.049*
H6B	0.669402	0.540265	0.284472	0.049*
C7	0.6072 (14)	0.325 (2)	0.1734 (9)	0.059 (4)
H7A	0.699580	0.290312	0.179469	0.071*
H7B	0.555810	0.215341	0.171365	0.071*
C8	0.5347 (16)	0.420 (2)	0.0568 (11)	0.086 (7)
H8A	0.519280	0.339169	−0.010801	0.129*

H8B	0.591162	0.519581	0.052262	0.129*
H8C	0.446030	0.463682	0.052249	0.129*
Br2	0.84875 (14)	0.1393 (2)	1.00875 (12)	0.0503 (4)
Br3	0.38253 (12)	0.35525 (18)	0.45593 (11)	0.0385 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0407 (9)	0.0524 (8)	0.0383 (7)	−0.0145 (7)	0.0215 (7)	0.0064 (7)
Co1	0.0198 (8)	0.0217 (7)	0.0150 (7)	−0.0008 (8)	0.0060 (6)	−0.0012 (8)
N1	0.034 (6)	0.027 (5)	0.019 (5)	−0.006 (5)	0.011 (4)	0.006 (5)
N2	0.017 (6)	0.030 (5)	0.023 (5)	−0.004 (4)	0.007 (4)	−0.002 (4)
N3	0.022 (6)	0.027 (5)	0.026 (6)	−0.007 (4)	0.007 (5)	0.001 (5)
N4	0.028 (6)	0.028 (6)	0.023 (5)	0.006 (4)	0.004 (5)	−0.003 (5)
N5	0.023 (6)	0.039 (5)	0.019 (5)	0.001 (4)	0.003 (4)	0.003 (5)
C1	0.060 (10)	0.024 (7)	0.034 (7)	0.017 (6)	0.018 (7)	0.007 (6)
C2	0.033 (8)	0.040 (7)	0.028 (6)	0.025 (7)	0.010 (6)	0.011 (7)
C3	0.024 (7)	0.061 (9)	0.022 (6)	0.015 (6)	0.011 (5)	−0.002 (6)
C4	0.042 (8)	0.028 (6)	0.019 (6)	0.021 (6)	0.006 (6)	−0.009 (5)
C5	0.049 (8)	0.042 (8)	0.015 (5)	0.004 (7)	0.011 (6)	−0.001 (6)
C6	0.041 (9)	0.049 (8)	0.032 (7)	0.005 (6)	0.015 (6)	0.007 (6)
C7	0.065 (11)	0.090 (12)	0.015 (6)	0.014 (10)	0.010 (6)	−0.002 (8)
C8	0.077 (13)	0.14 (2)	0.033 (8)	0.017 (12)	0.020 (8)	0.015 (10)
Br2	0.0412 (9)	0.0702 (9)	0.0393 (8)	0.0142 (8)	0.0161 (7)	0.0307 (8)
Br3	0.0263 (7)	0.0326 (6)	0.0448 (7)	−0.0020 (7)	0.0023 (6)	−0.0047 (7)

Geometric parameters (Å, º)

Br1—Co1	2.3967 (18)	C1—H1C	0.9900
Co1—N4	1.937 (8)	C1—H1D	0.9900
Co1—N1	1.949 (9)	C2—H2C	0.9900
Co1—N2	1.962 (8)	C2—H2D	0.9900
Co1—N3	1.988 (9)	C3—C4	1.524 (15)
Co1—N5	1.996 (8)	C3—H3C	0.9900
N1—C1	1.460 (13)	C3—H3D	0.9900
N1—H1A	0.8999	C4—H4A	0.9900
N1—H1B	0.9001	C4—H4B	0.9900
N2—C2	1.469 (13)	C5—C6	1.509 (14)
N2—H2A	0.9001	C5—H5C	0.9900
N2—H2B	0.8993	C5—H5D	0.9900
N3—C3	1.467 (13)	C6—C7	1.498 (15)
N3—H3A	0.8998	C6—H6A	0.9900
N3—H3B	0.9003	C6—H6B	0.9900
N4—C4	1.481 (13)	C7—C8	1.487 (16)
N4—H4C	0.9006	C7—H7A	0.9900
N4—H4D	0.9002	C7—H7B	0.9900
N5—C5	1.473 (13)	C8—H8A	0.9800
N5—H5A	0.9002	C8—H8B	0.9800

N5—H5B	0.9005	C8—H8C	0.9800
C1—C2	1.498 (16)		

N4—Co1—N1	174.0 (4)	C2—C1—H1C	110.6
N4—Co1—N2	90.1 (4)	N1—C1—H1D	110.6
N1—Co1—N2	84.3 (3)	C2—C1—H1D	110.6
N4—Co1—N3	84.5 (4)	H1C—C1—H1D	108.7
N1—Co1—N3	93.6 (4)	N2—C2—C1	107.7 (9)
N2—Co1—N3	92.8 (4)	N2—C2—H2C	110.2
N4—Co1—N5	90.6 (4)	C1—C2—H2C	110.2
N1—Co1—N5	95.1 (4)	N2—C2—H2D	110.2
N2—Co1—N5	177.0 (4)	C1—C2—H2D	110.2
N3—Co1—N5	90.2 (4)	H2C—C2—H2D	108.5
N4—Co1—Br1	90.6 (3)	N3—C3—C4	107.4 (9)
N1—Co1—Br1	91.4 (3)	N3—C3—H3C	110.2
N2—Co1—Br1	88.9 (2)	C4—C3—H3C	110.2
N3—Co1—Br1	174.8 (3)	N3—C3—H3D	110.2
N5—Co1—Br1	88.2 (3)	C4—C3—H3D	110.2
C1—N1—Co1	111.7 (7)	H3C—C3—H3D	108.5
C1—N1—H1A	109.3	N4—C4—C3	105.4 (9)
Co1—N1—H1A	109.2	N4—C4—H4A	110.7
C1—N1—H1B	109.3	C3—C4—H4A	110.7
Co1—N1—H1B	109.3	N4—C4—H4B	110.7
H1A—N1—H1B	107.9	C3—C4—H4B	110.7
C2—N2—Co1	109.0 (6)	H4A—C4—H4B	108.8
C2—N2—H2A	109.8	N5—C5—C6	113.5 (10)
Co1—N2—H2A	109.8	N5—C5—H5C	108.9
C2—N2—H2B	109.9	C6—C5—H5C	108.9
Co1—N2—H2B	109.9	N5—C5—H5D	108.9
H2A—N2—H2B	108.4	C6—C5—H5D	108.9
C3—N3—Co1	110.0 (6)	H5C—C5—H5D	107.7
C3—N3—H3A	109.6	C7—C6—C5	113.9 (10)
Co1—N3—H3A	109.6	C7—C6—H6A	108.8
C3—N3—H3B	109.7	C5—C6—H6A	108.8
Co1—N3—H3B	109.6	C7—C6—H6B	108.8
H3A—N3—H3B	108.2	C5—C6—H6B	108.8
C4—N4—Co1	111.0 (7)	H6A—C6—H6B	107.7
C4—N4—H4C	109.5	C8—C7—C6	115.6 (13)
Co1—N4—H4C	109.4	C8—C7—H7A	108.4
C4—N4—H4D	109.5	C6—C7—H7A	108.4
Co1—N4—H4D	109.4	C8—C7—H7B	108.4
H4C—N4—H4D	108.0	C6—C7—H7B	108.4
C5—N5—Co1	120.0 (7)	H7A—C7—H7B	107.4
C5—N5—H5A	107.4	C7—C8—H8A	109.5
Co1—N5—H5A	107.4	C7—C8—H8B	109.5
C5—N5—H5B	107.2	H8A—C8—H8B	109.5
Co1—N5—H5B	107.4	C7—C8—H8C	109.5
H5A—N5—H5B	106.8	H8A—C8—H8C	109.5

N1—C1—C2	105.7 (9)	H8B—C8—H8C	109.5
N1—C1—H1C	110.6		
Co1—N1—C1—C2	−37.0 (11)	N3—C3—C4—N4	49.8 (11)
Co1—N2—C2—C1	−40.7 (10)	Co1—N5—C5—C6	−167.2 (8)
N1—C1—C2—N2	50.1 (12)	N5—C5—C6—C7	−179.5 (11)
Co1—N3—C3—C4	−36.4 (10)	C5—C6—C7—C8	−175.3 (12)
Co1—N4—C4—C3	−41.3 (10)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Br3^{i}	0.90	2.51	3.348 (9)	156
N1—H1*B*···Br1^{ii}	0.90	2.71	3.467 (8)	143
N2—H2*A*···Br2^{iii}	0.90	2.50	3.335 (8)	154
N2—H2*B*···Br2	0.90	2.50	3.392 (8)	173
N3—H3*A*···Br3	0.90	3.03	3.680 (9)	131
N3—H3*A*···Br3^{i}	0.90	3.01	3.695 (9)	134
N3—H3*B*···Br2	0.90	2.57	3.372 (9)	148
N4—H4*C*···Br2^{iii}	0.90	2.65	3.468 (9)	151
N4—H4*D*···Br3^{iv}	0.90	2.49	3.359 (9)	163
N5—H5*A*···Br3	0.90	2.61	3.458 (9)	158
N5—H5*B*···Br3^{iv}	0.90	2.88	3.487 (9)	126
C3—H3*D*···Br3	0.99	2.84	3.594 (11)	134
C4—H4*B*···Br2	0.99	3.00	3.739 (11)	132
C5—H5*D*···Br1	0.99	3.10	3.607 (12)	114
C5—H5*D*···Br1^{ii}	0.99	3.10	3.884 (13)	137

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