

cis-Bromidobis(ethylene-1,2-diamine)(2-methylpropan-1-amine)cobalt(III) dibromide

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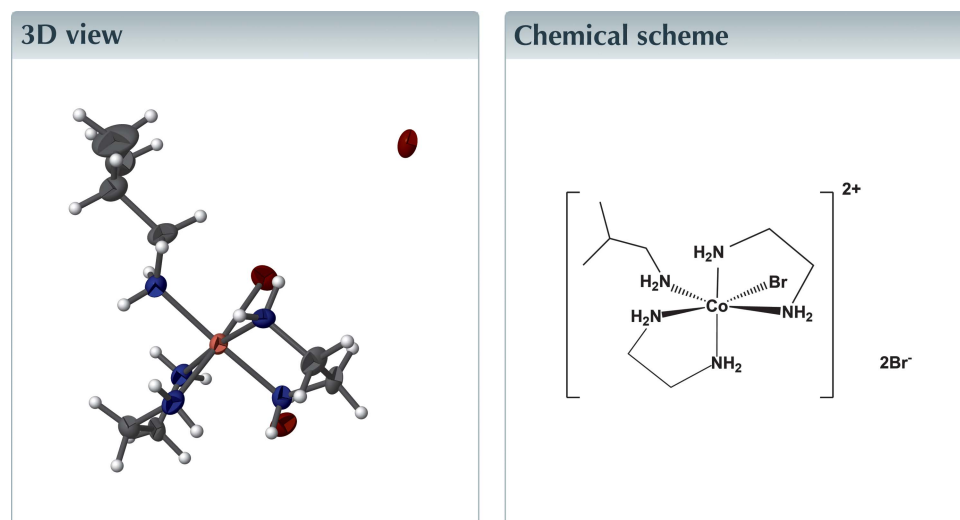
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Keywords: crystal structure; cobalt(III); dibromide; N—H...Br hydrogen bonding.

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

In the title compound, $[\text{CoBr}(\text{C}_2\text{H}_8\text{N}_2)_2(\text{C}_4\text{H}_{11}\text{N})]\text{Br}_2$, the cobalt(III) ion has a distorted octahedral coordination environment and is ligated by three N atoms and a bromine ion in the equatorial plane, and by two N atoms occupying the axial positions. In the crystal, the complex cation and the two Br^- counter-anions are linked by N—H...Br hydrogen bonds, forming a supramolecular framework.



Structure description

In recent years, considerable effort has been dedicated to the design and synthesis of supramolecular architectures of coordination complexes (Lehn, 1995; Khlobystov *et al.*, 2001). The primary reason for the interest in such complexes is their new and versatile topologies and potential applications in functional materials (Desiraju, 1995; Seo *et al.*, 2000). The interaction of transition metal polyamine complexes of cobalt(III) with DNA has received considerable attention in recent years. Using mixed-ligand complexes, it is possible to systematically vary parameters of interest by changing the properties of the interacting units either by the use of suitable substituents or by simply changing the nature of the ancillary ligand. In addition, cobalt(III) complexes have sustained a high level of attention because of their relevance in various redox processes in biological systems and their antitumor, anthelmintic, antiparasitic, antibiotic and antimicrobial activities, as well as their multiple applications in the fields of medicine and drug delivery (Chang *et al.*, 2010). Against this background and to ascertain the molecular structure and configuration of the title compound, the crystal structure determination has been carried out.

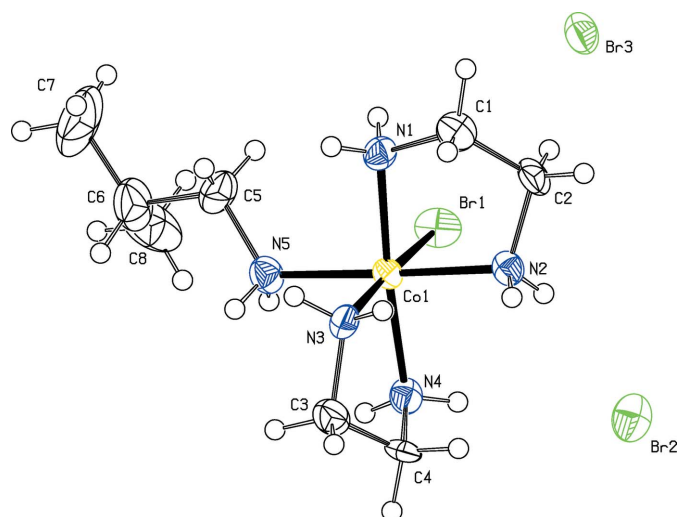


Figure 1
The molecular structure of the title complex, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

The molecular structure of the title compound is shown in Fig. 1. It is composed of a cobalt(III) complex with the metal atom being coordinated by two ethylene-1,2-diamine (*en*) and one 2-methylpropan-1-amine ligands, and a Br⁻ ion. The metal cation has a distorted hexagonal coordination sphere, being ligated to three N atoms, N2 and N3 of two *en* ligands and atom N5 of the 3-methylbutan-1-amine ligand, and a bromine atom (Br1) in the equatorial plane. The remaining *en* N atoms, N1 and N4, occupy the axial positions. This arrangement is very similar to that observed for *cis*-chlorido(ethylamine)bis(ethylene-1,2-diamine)cobalt(III) dichloride (Maheshwaran *et al.*, 2013). In the title complex cation, the Co–N_{en} bond lengths vary from 1.950 (4) to 1.963 (4) Å, while the Co–N5 bond length involving the

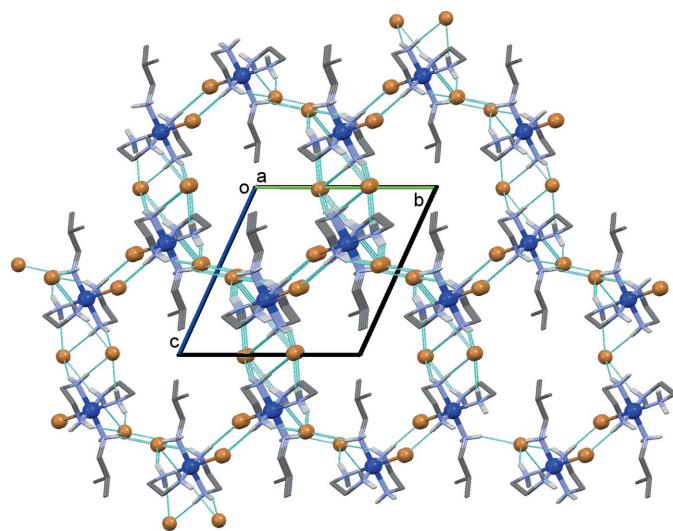


Figure 2
The crystal packing of the title compound, viewed along the *a* axis, showing the N–H···Br hydrogen bonds (see Table 1) as dashed lines. Only the N-bound H atoms have been included.

Table 1
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–H1NA···Br1 ⁱ	0.89	2.68	3.458 (5)	147
N1–H1NB···Br3 ^j	0.89	2.50	3.348 (5)	159
N2–H2NA···Br2 ⁱⁱ	0.89	2.57	3.430 (5)	164
N2–H2NB···Br2	0.89	2.60	3.436 (4)	158
N3–H3NA···Br2 ⁱⁱ	0.89	2.54	3.380 (5)	158
N3–H3NB···Br3 ^j	0.89	2.76	3.493 (4)	141
N4–H4NA···Br3 ⁱⁱⁱ	0.89	2.56	3.430 (4)	166
N4–H4NB···Br2	0.89	2.69	3.521 (5)	157
N5–H5NB···Br3 ⁱⁱⁱ	0.89	2.88	3.506 (4)	129
N5–H5NA···Br3 ^{iv}	0.89	2.67	3.509 (5)	159
C3–H3A···Br3 ^{iv}	0.97	2.88	3.647 (6)	137
C6–H6···Br3 ^{iv}	0.98	3.09	3.875 (8)	138

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

2-methylpropan-1-amine ligand is 1.998 (4) Å and the Co1–Br1 bond length is 2.4019 (11) Å. These bond lengths are comparable to the values reported in the literature for similar compounds (Lee *et al.*, 2007; Ramesh *et al.*, 2008; Anbalagan *et al.*, 2009; Ravichandran *et al.*, 2009). Both five-membered chelate rings, which are *cis* to each other, have twisted conformations on the C–C (C1–C2 and C3–C4) bonds and their mean planes are inclined to each other by 79.4 (3)°.

In the crystal, the cations and anions are linked by a number of N–H···Br hydrogen bonds forming a supramolecular framework (Table 1, Fig. 2), with small cavities as shown in Fig. 3. No residual electron density was observed in these regions in the final difference-Fourier map.

Synthesis and crystallization

A suspension of 2 g of *trans*-[Co^{III}(ethylene-1,2-diamine)₂-Br₂]Br was made into a paste using 3–4 drops of water. To this

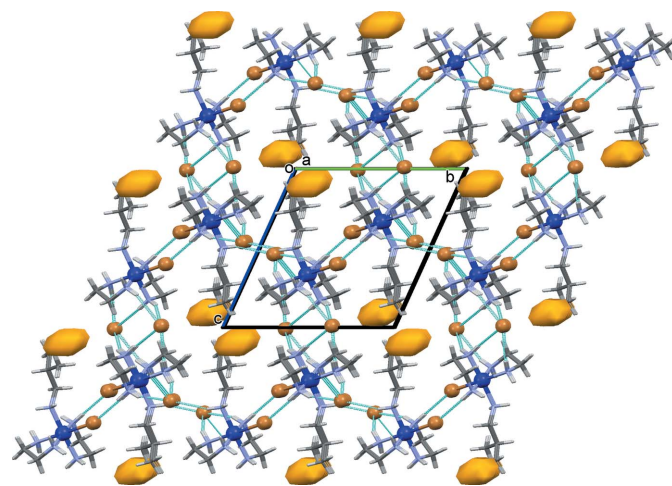


Figure 3
The crystal packing of the title compound, viewed along the *a* axis, showing the small voids (yellow regions) in the supramolecular framework (Mercury; Macrae *et al.*, 2008), and the N–H···Br hydrogen bonds (see Table 1) as dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	[CoBr(C ₂ H ₈ N ₂) ₂ (C ₄ H ₁₁ N)]Br ₂
<i>M</i> _r	492.00
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.3567 (7), 11.6172 (19), 11.7805 (15)
α , β , γ (°)	112.084 (13), 99.118 (9), 99.431 (10)
<i>V</i> (Å ³)	893.3 (2)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	7.66
Crystal size (mm)	0.23 × 0.17 × 0.11
Data collection	
Diffractionmeter	Bruker SMART APEXII area-detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2008)
<i>T</i> _{min} , <i>T</i> _{max}	0.165, 0.361
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	6158, 3318, 1911
<i>R</i> _{int}	0.052
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.606
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.043, 0.079, 0.83
No. of reflections	3318
No. of parameters	156
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.90, -0.63

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *pubCIF* (Westrip, 2010).

solid mass, ca 2 ml of 2-methylpropan-1-amine was added drop wise over 20 min and mixed well. Grinding was continued until the colour becomes dull-green to red. The reaction mixture was set aside until no further change was observed and the product was allowed to stand overnight. Finally, the solid was washed with ethanol then dissolved in 5–10 ml of water and pre-heated to 343 K. It was 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 giving finally pink plate-like crystals.

Refinement

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

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full crystallographic data

IUCrData (2018). 3, x181290 [https://doi.org/10.1107/S2414314618012907]

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Crystal data

[CoBr(C₂H₈N₂)₂(C₄H₁₁N)]Br₂

$M_r = 492.00$

Triclinic, *P* $\bar{1}$

$a = 7.3567$ (7) Å

$b = 11.6172$ (19) Å

$c = 11.7805$ (15) Å

$\alpha = 112.084$ (13)°

$\beta = 99.118$ (9)°

$\gamma = 99.431$ (10)°

$V = 893.3$ (2) Å³

$Z = 2$

$F(000) = 484$

$D_x = 1.829$ Mg m⁻³

Mo *K* α radiation, $\lambda = 0.71073$ Å

Cell parameters from 4095 reflections

$\theta = 2.9$ – 29.3 °

$\mu = 7.66$ mm⁻¹

$T = 293$ K

Plate, pink

$0.23 \times 0.17 \times 0.11$ mm

Data collection

Bruker SMART APEXII area-detector diffractometer

Graphite monochromator

ω and ϕ scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2008)

$T_{\min} = 0.165$, $T_{\max} = 0.361$

6158 measured reflections

3318 independent reflections

1911 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.052$

$\theta_{\max} = 25.5$ °, $\theta_{\min} = 2.9$ °

$h = -7 \rightarrow 8$

$k = -14 \rightarrow 11$

$l = -14 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.079$

$S = 0.83$

3318 reflections

156 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

$w = 1/[\sigma^2(F_o^2) + (0.0329P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.90$ e Å⁻³

$\Delta\rho_{\min} = -0.63$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.23622 (8)	0.50309 (7)	0.39902 (6)	0.0407 (2)
Co1	0.11284 (9)	0.65284 (7)	0.33292 (7)	0.0240 (2)
N1	-0.1140 (5)	0.6266 (4)	0.3951 (4)	0.0275 (12)
H1NA	-0.092806	0.592787	0.450851	0.033*
H1NB	-0.140672	0.701605	0.433825	0.033*
N2	-0.0369 (5)	0.5104 (4)	0.1749 (4)	0.0267 (12)
H2NA	-0.076525	0.540610	0.118748	0.032*
H2NB	0.035086	0.457655	0.143180	0.032*
N3	0.0362 (6)	0.7809 (4)	0.2775 (4)	0.0318 (13)
H3NA	-0.068590	0.744083	0.215246	0.038*
H3NB	0.010553	0.842021	0.341275	0.038*
N4	0.3228 (6)	0.6700 (5)	0.2517 (4)	0.0288 (12)
H4NA	0.429648	0.715828	0.310294	0.035*
H4NB	0.339174	0.592955	0.207580	0.035*
N5	0.2648 (6)	0.7926 (4)	0.4973 (4)	0.0310 (12)
H5NB	0.379876	0.778385	0.510958	0.037*
H5NA	0.279042	0.865595	0.487553	0.037*
C1	-0.2779 (7)	0.5397 (6)	0.2890 (6)	0.0389 (18)
H1A	-0.335725	0.587213	0.247390	0.047*
H1B	-0.372893	0.499418	0.319885	0.047*
C2	-0.2015 (7)	0.4402 (6)	0.1987 (5)	0.0331 (16)
H2A	-0.163159	0.383288	0.235438	0.040*
H2B	-0.297345	0.389624	0.120674	0.040*
C3	0.1892 (8)	0.8384 (6)	0.2331 (6)	0.0356 (16)
H3A	0.281827	0.907467	0.303933	0.043*
H3B	0.137264	0.872586	0.175150	0.043*
C4	0.2801 (8)	0.7335 (6)	0.1679 (6)	0.0325 (15)
H4A	0.194594	0.672553	0.088508	0.039*
H4B	0.395917	0.768860	0.150396	0.039*
C5	0.1973 (8)	0.8142 (7)	0.6138 (5)	0.0442 (18)
H5A	0.162352	0.733048	0.620283	0.053*
H5B	0.084679	0.846984	0.608494	0.053*
C6	0.3486 (11)	0.9092 (7)	0.7335 (6)	0.060 (2)
H6	0.396726	0.986063	0.720647	0.071*
C7	0.2505 (13)	0.9469 (9)	0.8421 (7)	0.100 (3)
H7A	0.218670	0.875620	0.863966	0.150*
H7B	0.136796	0.970529	0.816889	0.150*
H7C	0.334250	1.018126	0.913915	0.150*
C8	0.5128 (10)	0.8535 (8)	0.7599 (7)	0.081 (3)

H8A	0.601773	0.913826	0.836527	0.121*
H8B	0.574238	0.835317	0.691255	0.121*
H8C	0.467066	0.775759	0.768734	0.121*
Br2	0.26843 (8)	0.36505 (7)	0.01047 (6)	0.0434 (2)
Br3	0.27866 (8)	0.10929 (6)	0.53790 (6)	0.0379 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0363 (4)	0.0475 (5)	0.0489 (5)	0.0158 (3)	0.0119 (3)	0.0285 (4)
Co1	0.0204 (4)	0.0230 (5)	0.0245 (5)	0.0014 (4)	0.0038 (3)	0.0079 (4)
N1	0.031 (3)	0.030 (3)	0.021 (3)	0.007 (2)	0.005 (2)	0.011 (3)
N2	0.024 (3)	0.022 (3)	0.033 (3)	0.008 (2)	0.007 (2)	0.010 (2)
N3	0.032 (3)	0.030 (3)	0.023 (3)	0.002 (2)	0.009 (2)	0.002 (3)
N4	0.021 (2)	0.030 (3)	0.029 (3)	0.005 (2)	0.003 (2)	0.007 (3)
N5	0.030 (3)	0.030 (3)	0.029 (3)	0.002 (2)	0.001 (2)	0.011 (3)
C1	0.019 (3)	0.047 (5)	0.040 (4)	0.001 (3)	0.002 (3)	0.011 (4)
C2	0.023 (3)	0.025 (4)	0.039 (4)	−0.005 (3)	0.002 (3)	0.007 (3)
C3	0.040 (4)	0.032 (4)	0.033 (4)	0.001 (3)	0.006 (3)	0.016 (3)
C4	0.029 (3)	0.032 (4)	0.034 (4)	−0.007 (3)	0.014 (3)	0.015 (3)
C5	0.051 (4)	0.051 (5)	0.022 (4)	0.008 (4)	0.006 (3)	0.009 (4)
C6	0.082 (6)	0.045 (5)	0.033 (4)	−0.003 (4)	−0.003 (4)	0.011 (4)
C7	0.156 (9)	0.089 (8)	0.032 (5)	0.029 (7)	0.017 (5)	0.002 (5)
C8	0.066 (5)	0.095 (7)	0.063 (6)	−0.030 (5)	−0.019 (4)	0.046 (6)
Br2	0.0378 (4)	0.0469 (5)	0.0378 (4)	0.0144 (3)	0.0014 (3)	0.0107 (4)
Br3	0.0280 (3)	0.0276 (4)	0.0471 (4)	0.0035 (3)	0.0077 (3)	0.0055 (4)

Geometric parameters (Å, °)

Br1—Co1	2.4019 (11)	C1—H1A	0.9700
Co1—N1	1.950 (4)	C1—H1B	0.9700
Co1—N3	1.962 (5)	C2—H2A	0.9700
Co1—N4	1.962 (4)	C2—H2B	0.9700
Co1—N2	1.963 (4)	C3—C4	1.500 (8)
Co1—N5	1.998 (4)	C3—H3A	0.9700
N1—C1	1.486 (6)	C3—H3B	0.9700
N1—H1NA	0.8900	C4—H4A	0.9700
N1—H1NB	0.8900	C4—H4B	0.9700
N2—C2	1.472 (6)	C5—C6	1.541 (9)
N2—H2NA	0.8900	C5—H5A	0.9700
N2—H2NB	0.8900	C5—H5B	0.9700
N3—C3	1.479 (7)	C6—C8	1.505 (9)
N3—H3NA	0.8900	C6—C7	1.525 (10)
N3—H3NB	0.8900	C6—H6	0.9800
N4—C4	1.464 (7)	C7—H7A	0.9600
N4—H4NA	0.8900	C7—H7B	0.9600
N4—H4NB	0.8900	C7—H7C	0.9600
N5—C5	1.480 (7)	C8—H8A	0.9600

N5—H5NB	0.8900	C8—H8B	0.9600
N5—H5NA	0.8900	C8—H8C	0.9600
C1—C2	1.503 (7)		
N1—Co1—N3	93.07 (18)	C2—C1—H1A	110.4
N1—Co1—N4	173.73 (18)	N1—C1—H1B	110.4
N3—Co1—N4	84.75 (19)	C2—C1—H1B	110.4
N1—Co1—N2	84.76 (18)	H1A—C1—H1B	108.6
N3—Co1—N2	92.30 (19)	N2—C2—C1	106.4 (5)
N4—Co1—N2	89.44 (18)	N2—C2—H2A	110.5
N1—Co1—N5	94.20 (18)	C1—C2—H2A	110.5
N3—Co1—N5	89.98 (19)	N2—C2—H2B	110.5
N4—Co1—N5	91.69 (18)	C1—C2—H2B	110.5
N2—Co1—N5	177.5 (2)	H2A—C2—H2B	108.6
N1—Co1—Br1	92.15 (14)	N3—C3—C4	106.7 (5)
N3—Co1—Br1	174.59 (13)	N3—C3—H3A	110.4
N4—Co1—Br1	90.21 (14)	C4—C3—H3A	110.4
N2—Co1—Br1	89.62 (13)	N3—C3—H3B	110.4
N5—Co1—Br1	88.19 (14)	C4—C3—H3B	110.4
C1—N1—Co1	110.5 (3)	H3A—C3—H3B	108.6
C1—N1—H1NA	109.6	N4—C4—C3	107.6 (5)
Co1—N1—H1NA	109.6	N4—C4—H4A	110.2
C1—N1—H1NB	109.6	C3—C4—H4A	110.2
Co1—N1—H1NB	109.6	N4—C4—H4B	110.2
H1NA—N1—H1NB	108.1	C3—C4—H4B	110.2
C2—N2—Co1	109.8 (3)	H4A—C4—H4B	108.5
C2—N2—H2NA	109.7	N5—C5—C6	112.4 (5)
Co1—N2—H2NA	109.7	N5—C5—H5A	109.1
C2—N2—H2NB	109.7	C6—C5—H5A	109.1
Co1—N2—H2NB	109.7	N5—C5—H5B	109.1
H2NA—N2—H2NB	108.2	C6—C5—H5B	109.1
C3—N3—Co1	110.5 (3)	H5A—C5—H5B	107.9
C3—N3—H3NA	109.6	C8—C6—C7	112.3 (7)
Co1—N3—H3NA	109.6	C8—C6—C5	111.7 (6)
C3—N3—H3NB	109.6	C7—C6—C5	107.5 (6)
Co1—N3—H3NB	109.6	C8—C6—H6	108.4
H3NA—N3—H3NB	108.1	C7—C6—H6	108.4
C4—N4—Co1	109.6 (3)	C5—C6—H6	108.4
C4—N4—H4NA	109.7	C6—C7—H7A	109.5
Co1—N4—H4NA	109.7	C6—C7—H7B	109.5
C4—N4—H4NB	109.7	H7A—C7—H7B	109.5
Co1—N4—H4NB	109.7	C6—C7—H7C	109.5
H4NA—N4—H4NB	108.2	H7A—C7—H7C	109.5
C5—N5—Co1	120.2 (4)	H7B—C7—H7C	109.5
C5—N5—H5NB	107.3	C6—C8—H8A	109.5
Co1—N5—H5NB	107.3	C6—C8—H8B	109.5
C5—N5—H5NA	107.3	H8A—C8—H8B	109.5
Co1—N5—H5NA	107.3	C6—C8—H8C	109.5

H5NB—N5—H5NA	106.9	H8A—C8—H8C	109.5
N1—C1—C2	106.7 (4)	H8B—C8—H8C	109.5
N1—C1—H1A	110.4		
Co1—N1—C1—C2	37.1 (6)	N3—C3—C4—N4	-49.4 (6)
Co1—N2—C2—C1	41.1 (5)	Co1—N5—C5—C6	170.0 (5)
N1—C1—C2—N2	-50.2 (6)	N5—C5—C6—C8	-69.0 (8)
Co1—N3—C3—C4	36.3 (5)	N5—C5—C6—C7	167.4 (6)
Co1—N4—C4—C3	40.1 (5)		

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
N1—H1NA...Br1 ⁱ	0.89	2.68	3.458 (5)	147
N1—H1NB...Br3 ⁱ	0.89	2.50	3.348 (5)	159
N2—H2NA...Br2 ⁱⁱ	0.89	2.57	3.430 (5)	164
N2—H2NB...Br2	0.89	2.60	3.436 (4)	158
N3—H3NA...Br2 ⁱⁱ	0.89	2.54	3.380 (5)	158
N3—H3NB...Br3 ⁱ	0.89	2.76	3.493 (4)	141
N4—H4NA...Br3 ⁱⁱⁱ	0.89	2.56	3.430 (4)	166
N4—H4NB...Br2	0.89	2.69	3.521 (5)	157
N5—H5NB...Br3 ⁱⁱⁱ	0.89	2.88	3.506 (4)	129
N5—H5NA...Br3 ^{iv}	0.89	2.67	3.509 (5)	159
C3—H3A...Br3 ^{iv}	0.97	2.88	3.647 (6)	137
C6—H6...Br3 ^{iv}	0.98	3.09	3.875 (8)	138

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