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catena-Poly[[[diaqua(dimethylformamide-κO)-cobalt(II)]-μ-4,4′-(hexafluoroisopropylidene)-dibenzoato-$\kappa^2 O$:O'] dihydrate]

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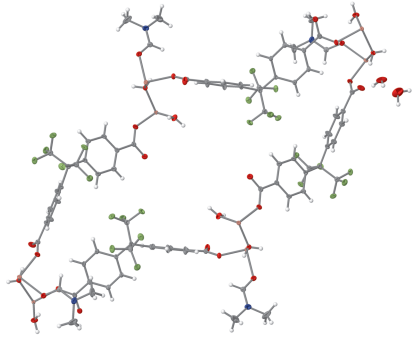
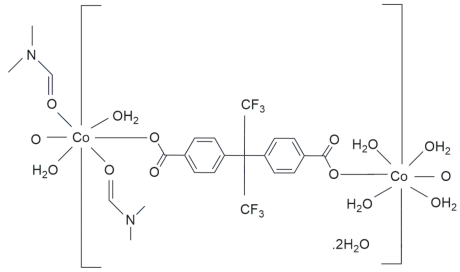
Structural data: full structural data are available from iucrdata.iucr.org

The title cobalt(II) coordination polymer, $\{[Co(C_{17}H_8F_6O_4)(C_3H_7NO)(H_2O)_2]\cdot 2H_2O\}_n$, assembled from 4,4′-(hexafluoroisopropylidene)bis(benzoic acid) (H_2L), crystallizes in the monoclinic space group $P2_1/n$. The two crystallographically independent Co^{II} sites are both situated on inversion centres and exhibit six-coordinate, slightly distorted octahedral O-donor environments. One Co is coordinated by O atoms from a carboxylate group, dimethylformamide and aqua ligands, whereas the other is coordinated by O atoms from a carboxylate group and by aqua ligands. The H_2L-derived dicarboxylate anion links in abis-monodentate manner two Co^{II} atoms, while the μ_2-bridging ligands link adjacent Co^{II} ions perpendicular to this direction. Hydrogen-bonding interactions between the solvent water molecules and aqua ligands as donors and other O atoms consolidate the packing.

3D view



Chemical scheme



Structure description

The title compound crystallizes in the monoclinic space group $P2_1/n$. Both Co atoms lie on inversion centres. Co1 is surrounded by two carboxylate donors (O1), two DMF donors (O5) and two symmetry-related water donors (O6) (Fig. 1). The Co1—O1, Co1—O5 and Co1—O6 bond lengths are 1.9928 (7), 2.1317 (7) and 2.1727 (7) Å, respectively. Co2 is coordinated by two carboxylate donors (O3) and four water donors (O6, O7), with Co2—O3, Co2—O7 and Co2—O6 bond lengths of 2.0261 (7), 2.0737 (8) and 2.1573 (7) Å, respectively. The inversion-related donor pairs generate *trans* angles of 180°, while the remaining *cis* angles deviate modestly from 90°, consistent with slightly distorted octahedral coordination (Wang *et al.*, 2007).

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6A···O2^{i}	0.844 (16)	1.857 (16)	2.6826 (11)	165.6 (14)
O6—H6B···O4^{ii}	0.803 (16)	1.926 (16)	2.6991 (11)	161.3 (15)
O7—H7A···O5^{i}	0.816 (18)	1.899 (18)	2.6868 (11)	161.8 (17)
O7—H7B···O8^{iii}	0.844 (17)	1.899 (17)	2.7314 (12)	168.8 (16)
O8—H8···O2	0.84 (2)	1.95 (2)	2.7107 (12)	150 (2)
O8—H8A···O9	0.82 (2)	1.97 (2)	2.7283 (14)	155 (2)
O9—H1···O4^{iv}	0.87 (3)	1.96 (3)	2.7983 (14)	161 (2)
O9—H1A···O8^{v}	0.86 (2)	1.96 (2)	2.812 (2)	177 (2)

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

The H_2L-derived ligand retains its V-shaped (Jiang *et al.*, 2009) aromatic backbone. The carboxylate C—O distances are C8—O1 = 1.2696 (12) Å, C8—O2 = 1.2511 (12) Å and C15—O3 = 1.2600 (12) Å, C15—O4 = 1.2636 (12) Å, with O—C—O angles of 124.84 (9) and 125.35 (9)° at C8 and C15, respectively. The coordinating DMF fragment is characterized by O5—C18 = 1.2487 (13) Å and C18—N1 = 1.3150 (13) Å.

The primary covalent connectivity is generated by Co—O coordination involving the monodentately binding carboxylate groups and the μ_2-bridging aqua ligands with alternating Co1 and Co2 atoms. The resulting framework (Fig. 2) is consolidated by hydrogen bonds between aqua ligands and solvent water molecules as donors and carboxylate O atoms, DMF O atoms and solvent water O atoms as acceptors (Table 1).

Synthesis and crystallization

Cobalt(II) acetate was dissolved in distilled water and 4,4′-(hexafluoroisopropylidene)bis(benzoic acid) was dissolved separately in DMF. The solutions were combined and the reaction mixture was left undisturbed at room temperature to allow slow crystal growth. Crystals suitable for single-crystal X-ray diffraction were isolated from the mother liquor and used for the diffraction experiment.

Refinement

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

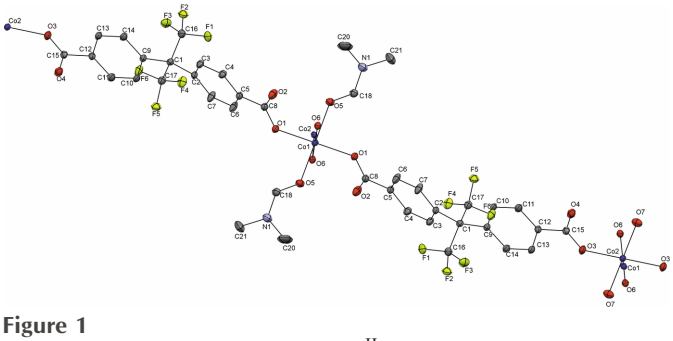

Figure 1
The molecular structure of the title Co^{II} coordination polymer, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity. Symmetry codes: (i) x, y, z; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x, -y, -z$; (iv) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Co(C_{17}H_8F_6O_4)(C_3H_7NO)(H_2O)_2]\cdot 2H_2O$
M_r	594.32
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	120
a, b, c (Å)	7.68581 (14), 29.2312 (5), 10.9718 (2)
β (°)	94.1830 (17)
V (Å^3)	2458.42 (8)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.79
Crystal size (mm)	0.18 × 0.15 × 0.08
Data collection	
Diffractometer	ROD, SynergyCustom DW system, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2026)
T_{min}, T_{max}	0.622, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34772, 8871, 7285
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.787
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.083, 1.05
No. of reflections	8871
No. of parameters	363
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.50, −0.63

Computer programs: *CrysAlis PRO* (Rigaku OD, 2026), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

Acknowledgements

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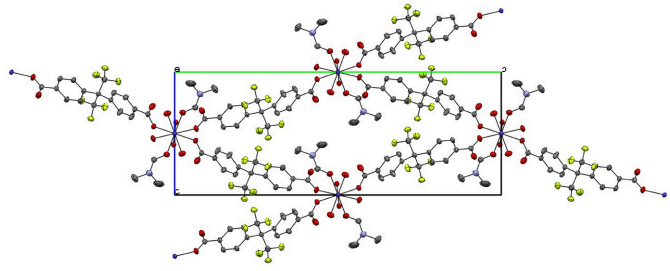

Figure 2
Crystal packing in a projection along [100].

Rigaku OD (2026). *CrysAlis PRO*. Rigaku Corporation, Wroclaw, Poland.
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full crystallographic data

IUCrData (2026). **11**, x261222 [https://doi.org/10.1107/S2414314626012228]

catena-Poly[[[diaqua(dimethylformamide-κO)cobalt(II)]-μ-4,4′-(hexafluoroisopropylidene)dibenzoato-κ^2O:O'] dihydrate]

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Crystal data

$[Co(C_{17}H_8F_6O_4)(C_3H_7NO)(H_2O)_2]\cdot 2H_2O$
M_r = 594.32
Monoclinic, $P2_1/n$
a = 7.68581 (14) Å
b = 29.2312 (5) Å
c = 10.9718 (2) Å
β = 94.1830 (17)°
V = 2458.42 (8) Å^3
Z = 4
$F(000)$ = 1212
D_x = 1.606 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 20549 reflections
θ = 2.3–34.2°
μ = 0.79 mm^{-1}
T = 120 K
Prism, pink
0.18 × 0.15 × 0.08 mm

Data collection

ROD, SynergyCustom DW system, HyPix diffractometer
Radiation source: Rotating-anode X-ray tube
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2026)
T_{min} = 0.622, T_{max} = 1.000
34772 measured reflections
8871 independent reflections
7285 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 34.0°, θ_{min} = 2.3°
h = −12→11
k = −45→43
l = −16→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.083
S = 1.05
8871 reflections
363 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.5153P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.50 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.

Refinement. Coordinates of the H atoms bonded to O were freely refined with U_{iso}(H) = 1.5 U_{eq}(O). Hydrogen atoms bonded to C atoms were placed at calculated positions and were refined in the riding-model approximation with $C_{aromatic}$–H = 0.95 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) or with C_{methyl}–H = 0.98 Å, and with U_{iso}(H) = 1.5 U_{eq}(C). The methyl groups were allowed to rotate but not to tip.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.500000	0.000000	0.500000	0.01066 (5)
Co2	0.500000	0.500000	1.000000	0.01063 (5)
F1	−0.02374 (10)	0.17287 (2)	0.92429 (6)	0.02412 (14)
F2	0.16110 (9)	0.21350 (2)	1.03350 (6)	0.02183 (14)
F3	−0.09333 (9)	0.24057 (2)	0.97785 (6)	0.02321 (14)
F4	−0.16273 (8)	0.21425 (2)	0.71818 (6)	0.02150 (13)
F5	0.01282 (9)	0.25677 (2)	0.62219 (6)	0.02056 (13)
F6	−0.12482 (9)	0.28457 (2)	0.76898 (6)	0.02115 (13)
O1	0.47379 (10)	0.06411 (3)	0.55767 (6)	0.01533 (14)
O2	0.66525 (10)	0.06889 (3)	0.72046 (7)	0.02110 (16)
O3	0.43640 (10)	0.43422 (3)	0.95918 (7)	0.01739 (14)
O4	0.61567 (10)	0.41680 (3)	0.81369 (7)	0.01863 (15)
O5	0.57599 (9)	0.02461 (3)	0.32887 (6)	0.01621 (14)
O6	0.26057 (10)	0.50352 (3)	1.09068 (7)	0.01286 (13)
H6A	0.2460 (19)	0.4818 (5)	1.1396 (14)	0.019*
H6B	0.2819 (19)	0.5261 (5)	1.1309 (13)	0.019*
O7	0.37648 (10)	0.52263 (3)	0.83672 (7)	0.01882 (15)
H7A	0.288 (2)	0.5079 (6)	0.8181 (16)	0.028*
H7B	0.420 (2)	0.5310 (5)	0.7721 (15)	0.028*
O8	0.94688 (13)	0.04117 (4)	0.86474 (8)	0.0352 (2)
H8	0.868 (3)	0.0586 (7)	0.835 (2)	0.053*
H8A	1.001 (3)	0.0519 (7)	0.9249 (19)	0.053*
O9	1.14930 (17)	0.04874 (5)	1.07862 (10)	0.0471 (3)
H1	1.129 (3)	0.0649 (9)	1.142 (2)	0.071*
N1	0.55779 (13)	0.07751 (4)	0.17747 (8)	0.02191 (19)
C1	0.11460 (13)	0.23420 (3)	0.82318 (8)	0.01250 (16)
C2	0.22574 (13)	0.19538 (3)	0.77397 (9)	0.01312 (17)
C3	0.38996 (13)	0.18641 (4)	0.83285 (9)	0.01536 (18)
H3	0.432774	0.205251	0.898932	0.018*
C4	0.49105 (13)	0.15028 (4)	0.79581 (9)	0.01567 (18)
H4	0.601877	0.144461	0.836992	0.019*
C5	0.43045 (13)	0.12255 (3)	0.69843 (9)	0.01380 (17)
C6	0.26835 (14)	0.13172 (4)	0.63923 (10)	0.0205 (2)
H6	0.226735	0.113196	0.572175	0.025*
C7	0.16628 (14)	0.16748 (4)	0.67644 (10)	0.0205 (2)
H7	0.055208	0.173028	0.635318	0.025*
C8	0.53269 (13)	0.08223 (3)	0.65746 (9)	0.01406 (17)
C9	0.22066 (12)	0.27854 (3)	0.84630 (8)	0.01259 (17)
C10	0.35024 (14)	0.28934 (4)	0.76782 (9)	0.01591 (18)
H10	0.377302	0.268130	0.706384	0.019*

C11	0.44005 (14)	0.33062 (4)	0.77827 (9)	0.01693 (19)
H11	0.527611	0.337355	0.724164	0.020*
C12	0.40205 (13)	0.36210 (3)	0.86780 (9)	0.01307 (17)
C13	0.27424 (13)	0.35122 (3)	0.94712 (9)	0.01477 (18)
H13	0.248578	0.372284	1.009254	0.018*
C14	0.18406 (13)	0.31011 (4)	0.93667 (9)	0.01514 (18)
H14	0.097017	0.303382	0.991199	0.018*
C15	0.49235 (13)	0.40786 (3)	0.88001 (9)	0.01349 (17)
C16	0.03894 (14)	0.21536 (4)	0.94035 (9)	0.01687 (19)
C17	−0.04182 (14)	0.24721 (4)	0.73245 (9)	0.01583 (18)
C18	0.53038 (13)	0.06296 (4)	0.28786 (9)	0.01613 (18)
H18	0.472113	0.082923	0.339759	0.019*
C20	0.6445 (3)	0.04908 (6)	0.09166 (13)	0.0454 (4)
H20A	0.587438	0.052985	0.009507	0.068*
H20B	0.637389	0.016930	0.116126	0.068*
H20C	0.767265	0.058157	0.091503	0.068*
C21	0.4974 (2)	0.12247 (5)	0.13586 (13)	0.0384 (3)
H21A	0.597572	0.141133	0.116345	0.058*
H21B	0.436632	0.137417	0.200503	0.058*
H21C	0.417308	0.119115	0.062713	0.058*
H1A	1.118 (3)	0.0217 (8)	1.098 (2)	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01078 (8)	0.01049 (9)	0.01067 (8)	0.00139 (6)	0.00060 (6)	−0.00120 (6)
Co2	0.01123 (8)	0.00912 (9)	0.01162 (8)	−0.00133 (6)	0.00154 (6)	−0.00133 (6)
F1	0.0315 (4)	0.0163 (3)	0.0249 (3)	−0.0103 (3)	0.0043 (3)	0.0002 (2)
F2	0.0269 (3)	0.0247 (4)	0.0135 (3)	−0.0039 (3)	−0.0015 (2)	0.0024 (2)
F3	0.0225 (3)	0.0256 (4)	0.0228 (3)	−0.0007 (3)	0.0103 (3)	−0.0017 (3)
F4	0.0157 (3)	0.0207 (3)	0.0273 (3)	−0.0031 (2)	−0.0038 (2)	−0.0038 (3)
F5	0.0232 (3)	0.0239 (3)	0.0141 (3)	0.0037 (3)	−0.0018 (2)	0.0015 (2)
F6	0.0199 (3)	0.0174 (3)	0.0257 (3)	0.0068 (2)	−0.0016 (2)	−0.0047 (2)
O1	0.0191 (3)	0.0126 (3)	0.0141 (3)	0.0022 (3)	−0.0003 (3)	−0.0025 (2)
O2	0.0190 (4)	0.0214 (4)	0.0219 (4)	0.0068 (3)	−0.0051 (3)	−0.0068 (3)
O3	0.0207 (3)	0.0114 (3)	0.0205 (3)	−0.0027 (3)	0.0043 (3)	−0.0042 (3)
O4	0.0186 (3)	0.0170 (4)	0.0209 (3)	−0.0047 (3)	0.0050 (3)	−0.0038 (3)
O5	0.0155 (3)	0.0182 (4)	0.0152 (3)	0.0026 (3)	0.0026 (3)	0.0020 (3)
O6	0.0129 (3)	0.0120 (3)	0.0137 (3)	−0.0019 (2)	0.0013 (2)	0.0001 (2)
O7	0.0143 (3)	0.0259 (4)	0.0161 (3)	−0.0043 (3)	0.0001 (3)	0.0037 (3)
O8	0.0266 (5)	0.0608 (7)	0.0173 (4)	0.0176 (5)	−0.0043 (3)	−0.0082 (4)
O9	0.0505 (7)	0.0690 (9)	0.0208 (5)	−0.0068 (6)	−0.0041 (4)	−0.0075 (5)
N1	0.0269 (5)	0.0221 (5)	0.0169 (4)	−0.0020 (4)	0.0022 (3)	0.0037 (3)
C1	0.0142 (4)	0.0114 (4)	0.0117 (4)	−0.0004 (3)	0.0000 (3)	−0.0010 (3)
C2	0.0159 (4)	0.0093 (4)	0.0139 (4)	0.0000 (3)	−0.0002 (3)	−0.0021 (3)
C3	0.0168 (4)	0.0143 (5)	0.0145 (4)	0.0005 (4)	−0.0026 (3)	−0.0041 (3)
C4	0.0156 (4)	0.0155 (5)	0.0153 (4)	0.0015 (3)	−0.0026 (3)	−0.0027 (3)
C5	0.0153 (4)	0.0108 (4)	0.0152 (4)	0.0005 (3)	0.0006 (3)	−0.0018 (3)

C6	0.0203 (5)	0.0174 (5)	0.0226 (5)	0.0040 (4)	−0.0063 (4)	−0.0098 (4)
C7	0.0180 (5)	0.0174 (5)	0.0247 (5)	0.0041 (4)	−0.0079 (4)	−0.0093 (4)
C8	0.0154 (4)	0.0120 (4)	0.0150 (4)	0.0000 (3)	0.0020 (3)	−0.0008 (3)
C9	0.0149 (4)	0.0101 (4)	0.0127 (4)	−0.0005 (3)	0.0003 (3)	−0.0016 (3)
C10	0.0213 (5)	0.0123 (4)	0.0148 (4)	−0.0021 (4)	0.0055 (4)	−0.0044 (3)
C11	0.0202 (5)	0.0143 (5)	0.0170 (4)	−0.0022 (4)	0.0060 (4)	−0.0030 (3)
C12	0.0141 (4)	0.0106 (4)	0.0143 (4)	−0.0003 (3)	−0.0002 (3)	−0.0010 (3)
C13	0.0174 (4)	0.0118 (4)	0.0154 (4)	0.0002 (3)	0.0030 (3)	−0.0042 (3)
C14	0.0171 (4)	0.0137 (4)	0.0151 (4)	−0.0005 (3)	0.0045 (3)	−0.0032 (3)
C15	0.0142 (4)	0.0120 (4)	0.0139 (4)	−0.0004 (3)	−0.0019 (3)	−0.0003 (3)
C16	0.0192 (5)	0.0153 (5)	0.0162 (4)	−0.0033 (4)	0.0018 (4)	−0.0008 (3)
C17	0.0160 (4)	0.0144 (5)	0.0170 (4)	0.0010 (3)	0.0000 (3)	−0.0022 (3)
C18	0.0158 (4)	0.0173 (5)	0.0152 (4)	−0.0019 (4)	0.0005 (3)	−0.0002 (3)
C20	0.0622 (10)	0.0557 (10)	0.0204 (6)	0.0197 (8)	0.0179 (6)	0.0058 (6)
C21	0.0612 (10)	0.0226 (7)	0.0306 (6)	−0.0024 (6)	−0.0013 (6)	0.0115 (5)

Geometric parameters (Å, º)

Co1—O1^{i}	1.9928 (7)	O5—C18	1.2487 (13)
Co1—O1	1.9929 (7)	N1—C18	1.3150 (13)
Co1—O5	2.1317 (7)	N1—C20	1.4537 (18)
Co1—O5^{i}	2.1317 (7)	N1—C21	1.4560 (17)
Co1—O6^{ii}	2.1727 (7)	C1—C2	1.5415 (14)
Co1—O6^{iii}	2.1727 (7)	C1—C9	1.5423 (14)
Co2—O3^{iv}	2.0261 (7)	C1—C16	1.5502 (14)
Co2—O3	2.0261 (7)	C1—C17	1.5512 (14)
Co2—O7	2.0737 (8)	C2—C7	1.3955 (14)
Co2—O7^{iv}	2.0737 (8)	C2—C3	1.4001 (14)
Co2—O6	2.1573 (7)	C3—C4	1.3892 (14)
Co2—O6^{iv}	2.1573 (7)	C4—C5	1.3940 (13)
F1—C16	1.3394 (12)	C5—C6	1.3885 (14)
F2—C16	1.3375 (12)	C5—C8	1.5033 (14)
F3—C16	1.3440 (13)	C6—C7	1.3862 (15)
F4—C17	1.3398 (12)	C9—C14	1.3979 (13)
F5—C17	1.3386 (12)	C9—C10	1.3994 (14)
F6—C17	1.3406 (12)	C10—C11	1.3906 (14)
O1—C8	1.2696 (12)	C11—C12	1.3925 (14)
O2—C8	1.2511 (12)	C12—C13	1.3958 (14)
O3—C15	1.2600 (12)	C12—C15	1.5084 (14)
O4—C15	1.2636 (12)	C13—C14	1.3879 (14)
O1^{i}—Co1—O1	180.0	C9—C1—C17	105.96 (8)
O1^{i}—Co1—O5	89.84 (3)	C16—C1—C17	107.41 (8)
O1—Co1—O5	90.16 (3)	C7—C2—C3	118.57 (9)
O1^{i}—Co1—O5^{i}	90.16 (3)	C7—C2—C1	122.68 (9)
O1—Co1—O5^{i}	89.84 (3)	C3—C2—C1	118.70 (8)
O5—Co1—O5^{i}	180.0	C4—C3—C2	120.79 (9)
O1^{i}—Co1—O6^{ii}	89.41 (3)	C3—C4—C5	120.24 (9)

O1—Co1—O6^{ii}	90.59 (3)	C6—C5—C4	118.98 (9)
O5—Co1—O6^{ii}	96.70 (3)	C6—C5—C8	118.83 (9)
O5^{i}—Co1—O6^{ii}	83.30 (3)	C4—C5—C8	122.17 (9)
O1^{i}—Co1—O6^{iii}	90.59 (3)	C7—C6—C5	121.04 (9)
O1—Co1—O6^{iii}	89.41 (3)	C6—C7—C2	120.38 (10)
O5—Co1—O6^{iii}	83.30 (3)	O2—C8—O1	124.84 (9)
O5^{i}—Co1—O6^{iii}	96.70 (3)	O2—C8—C5	120.10 (9)
O6^{ii}—Co1—O6^{iii}	180.0	O1—C8—C5	115.07 (9)
O3^{iv}—Co2—O3	180.0	C14—C9—C10	118.46 (9)
O3^{iv}—Co2—O7	88.63 (3)	C14—C9—C1	122.69 (9)
O3—Co2—O7	91.37 (3)	C10—C9—C1	118.67 (8)
O3^{iv}—Co2—O7^{iv}	91.37 (3)	C11—C10—C9	121.08 (9)
O3—Co2—O7^{iv}	88.63 (3)	C10—C11—C12	120.22 (9)
O7—Co2—O7^{iv}	180.00 (5)	C11—C12—C13	118.84 (9)
O3^{iv}—Co2—O6	93.04 (3)	C11—C12—C15	122.00 (9)
O3—Co2—O6	86.96 (3)	C13—C12—C15	119.14 (9)
O7—Co2—O6	91.78 (3)	C14—C13—C12	121.05 (9)
O7^{iv}—Co2—O6	88.22 (3)	C13—C14—C9	120.33 (9)
O3^{iv}—Co2—O6^{iv}	86.96 (3)	O3—C15—O4	125.35 (9)
O3—Co2—O6^{iv}	93.04 (3)	O3—C15—C12	115.18 (9)
O7—Co2—O6^{iv}	88.22 (3)	O4—C15—C12	119.47 (9)
O7^{iv}—Co2—O6^{iv}	91.78 (3)	F2—C16—F1	106.76 (9)
O6—Co2—O6^{iv}	180.00 (4)	F2—C16—F3	107.04 (8)
C8—O1—Co1	128.92 (7)	F1—C16—F3	106.01 (8)
C15—O3—Co2	130.07 (7)	F2—C16—C1	111.30 (8)
C18—O5—Co1	122.18 (7)	F1—C16—C1	111.92 (8)
Co2—O6—Co1^{v}	125.12 (3)	F3—C16—C1	113.40 (9)
C18—N1—C20	121.56 (11)	F5—C17—F4	107.76 (8)
C18—N1—C21	120.79 (11)	F5—C17—F6	106.72 (8)
C20—N1—C21	117.63 (11)	F4—C17—F6	106.23 (8)
C2—C1—C9	112.12 (8)	F5—C17—C1	110.58 (8)
C2—C1—C16	106.26 (8)	F4—C17—C1	113.40 (8)
C9—C1—C16	112.81 (8)	F6—C17—C1	111.80 (8)
C2—C1—C17	112.28 (8)	O5—C18—N1	124.24 (10)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6*A*···O2^{vi}	0.844 (16)	1.857 (16)	2.6826 (11)	165.6 (14)
O6—H6*B*···O4^{iv}	0.803 (16)	1.926 (16)	2.6991 (11)	161.3 (15)
O7—H7*A*···O5^{vi}	0.816 (18)	1.899 (18)	2.6868 (11)	161.8 (17)
O7—H7*B*···O8^{vii}	0.844 (17)	1.899 (17)	2.7314 (12)	168.8 (16)
O8—H8···O2	0.84 (2)	1.95 (2)	2.7107 (12)	150 (2)
O8—H8*A*···O9	0.82 (2)	1.97 (2)	2.7283 (14)	155 (2)

O9—H1···O4^{viii}	0.87 (3)	1.96 (3)	2.7983 (14)	161 (2)
O9—H1*A*···O8^{ix}	0.86 (2)	1.96 (2)	2.812 (2)	177 (2)

Symmetry codes: (iv) −*x*+1, −*y*+1, −*z*+2; (vi) *x*−1/2, −*y*+1/2, *z*+1/2; (vii) −*x*+3/2, *y*+1/2, −*z*+3/2; (viii) *x*+1/2, −*y*+1/2, *z*+1/2; (ix) −*x*+2, −*y*, −*z*+2.