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catena-Poly[[bis{2-[3-(carboxymethyl)adamantan-1-yl]acetato-κ^2O,O'}cadmium(II)]-μ-*N*,*N*′-bis-(pyridine-4-carboxamido)piperazine-κ^2N:*N*′]

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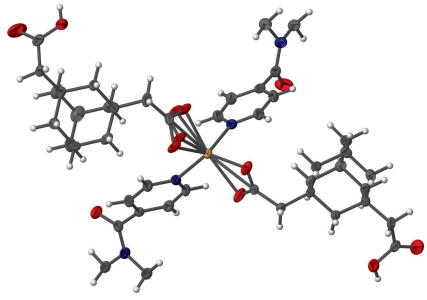
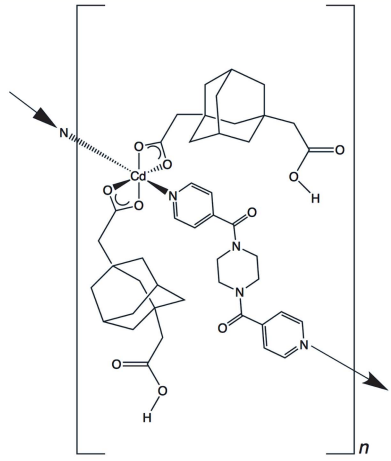
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[Cd(C_{14}H_{19}O_4)_2(C_{16}H_{16}N_4O_2)]_n$, the Cd^{II} cation is coordinated in a distorted octahedral fashion by *trans* pyridyl N-atom donors from two *N*,*N*′-bis(pyridine-4-carboxamido)piperazine (bpcp) ligands, and chelating carboxylate groups from two 2-[3-(carboxymethyl)adamantan-1-yl]acetate ligands. $[Cd(adaH)(bpcp)]_n$ coordination polymer chains are oriented along $[\bar{1}11]$ and aggregate into supramolecular layers parallel to (122) by O—H···O hydrogen-bonding interactions. The supramolecular three-dimensional crystal structure is then constructed by interlayer C—H···O non-classical interactions. The O atoms of one of the carboxylate groups were refined as disordered over two sets of sites, with occupancies 0.553 (7) and 0.447 (7).

3D view



Chemical scheme



Structure description

The title compound was isolated during an exploratory synthetic effort aiming to produce divalent metal coordination polymers containing both adamantanediacetate (ada) and *N*,*N*′-bis(4-pyridylcarboxamide)piperazine (bpcp) ligands. Coordination polymers containing both phthalate (pht) and bpcp ligands show significant topological differences depending on coordination-environment preferences at the divalent metal ion. $\{[Cd_2(pht)_2(bpcp)(H_2O)_2]_n$ displayed a 3-D structure built from the bpcp pillaring of $[Cd(pht)(H_2O)]_n$ layer motifs into a 4,5-connected binodal net with rare $(4^46^2)(4^46^6)$ **tcs** topology; this material fluoresced with a blue–violet hue upon UV excitation. $\{[Co(pht)(bpcp)(H_2O)_2]\cdot H_2O\}_n$ possesses an acentric (4,4) grid-layer topology. $\{[Cu_2(pht)_2(bpcp)(H_2O)_2]_n$ exhibits binding of bpcp C═O amide O atoms and a previously unreported 4,4-connected binodal layer structure with $(4.6^48)_2(4^26^4)$ topology (Wang *et al.*, 2011). It was hoped that the ada ligand would afford different coordination

Table 1
Selected geometric parameters (Å, °).

Cd1—O5	2.419 (2)	Cd1—O8	2.258 (9)
Cd1—O6	2.285 (2)	Cd1—N1	2.301 (3)
Cd1—O7	2.351 (6)	Cd1—N3	2.296 (3)
O6—Cd1—O5	54.87 (9)	O8—Cd1—N1	126.6 (2)
O6—Cd1—O7	115.9 (2)	O8—Cd1—N3	104.4 (3)
O6—Cd1—N1	100.50 (10)	N1—Cd1—O5	92.25 (11)
O6—Cd1—N3	131.49 (9)	N1—Cd1—O7	84.08 (19)
O7—Cd1—O5	169.4 (2)	N3—Cd1—O5	81.78 (9)
O8—Cd1—O5	136.7 (2)	N3—Cd1—O7	108.7 (2)
O8—Cd1—O6	95.4 (3)	N3—Cd1—N1	102.00 (10)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O5^{i}	0.84	1.75	2.588 (3)	175
O10—H10···O7^{ii}	0.84	1.89	2.725 (8)	171
O10—H10···O7*A*^{ii}	0.84	1.70	2.520 (6)	165
C39—H39*A*···O4	0.99	2.52	3.135 (4)	120
C47—H47*B*···O6	0.99	2.55	3.163 (4)	120
C55—H55*B*···O7*A*	0.99	2.46	3.009 (7)	115
C62—H62*B*···O10	0.99	2.53	3.115 (4)	117
C63—H63*B*···O8*A*	0.99	2.47	3.107 (8)	121

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

polymer topologies than previous pht analogs, due to its rigid non-aromatic adamantyl core along with its flexible pendant acetate arms.

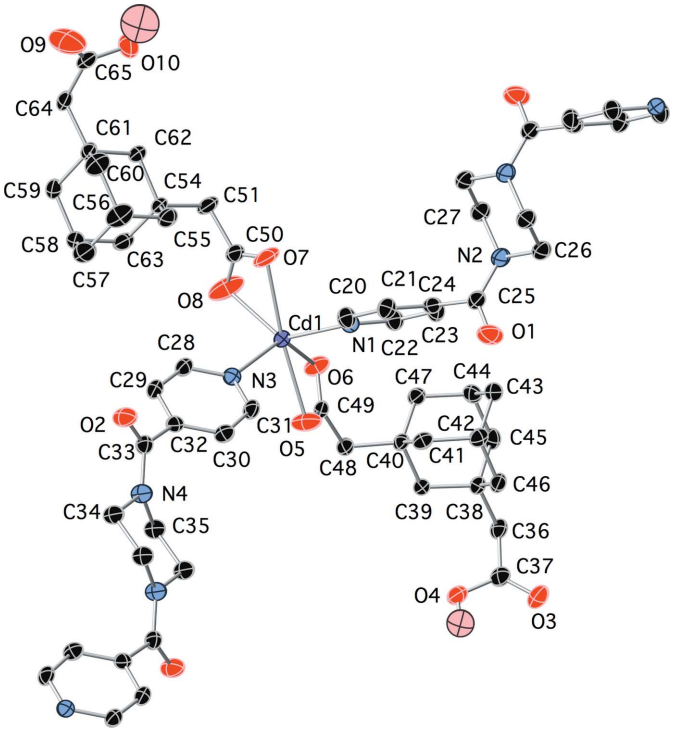


Figure 1
The coordination environment of the title compound, showing octahedral coordination at the Cd^{II} cation. Complete bpcp ligands are shown. Displacement ellipsoids are drawn at the 50% probability level. Most H atoms have been omitted for clarity. Color code: Cd, violet; N, blue; O, red; C, black; H, pink.

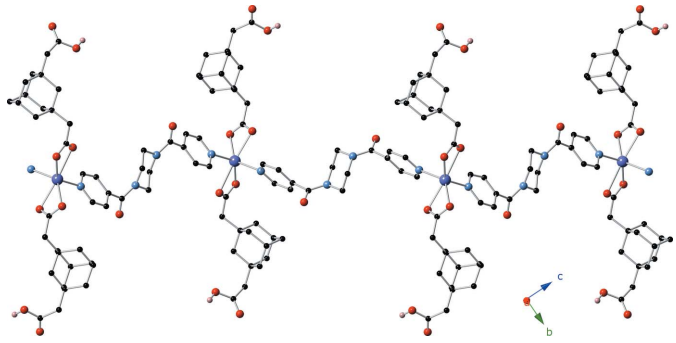


Figure 2
Coordination polymer chain in the title compound, oriented parallel to [$\bar{1}$11].

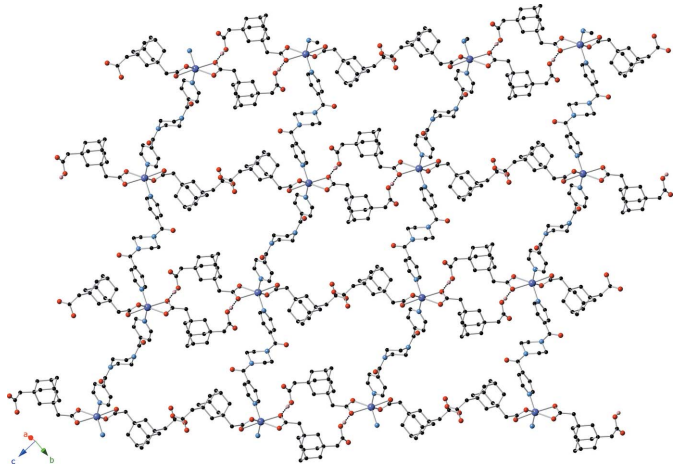


Figure 3
Supramolecular layer in the title compound, oriented parallel to the (122) plane. O—H···O hydrogen-bonding interactions are shown as dashed lines.

The asymmetric unit of the title compound contains a Cd^{II} cation, two anionic adaH ligands protonated at their unligated carboxylate termini, and halves of two crystallographically distinct bpcp ligands whose central piperazinyl rings are sited over crystallographic inversion centers (Fig. 1). The Cd^{II} ion is bound by *trans* pyridyl N atoms from two bpcp ligands, and chelating carboxylate groups from two adaH ligands. Each adaH ligand has a pendant, protonated carboxylate group that is unligated. Bond lengths and angles (Table 1) are consistent with an octahedral coordination environment for the Cd^{II} atom with two chelating groups. The dipodal bpcp ligands connect [Cd(adaH)$_2$] fragments into [Cd(adaH)$_2$(bpcp)]$_n$ coordination polymer chains that are oriented along the [$\bar{1}$11] direction (Fig. 2). The Cd···Cd distances through the crystallographically distinct *anti*-conformation bpcp ligands measure 16.53 (2) and 16.68 (2) Å.

Supramolecular O—H···O interactions (Table 2) anchor adjacent [Cd(adaH)$_2$(bpcp)]$_n$ coordination polymer chains into supramolecular layers parallel to the (122) plane (Fig. 3). These supramolecular layers stack and interdigitate in order to construct the three-dimensional crystal structure of the title compound, by means of C—H···O interactions between bpcp

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Cd(C_{14}H_{19}O_4)_2(C_{16}H_{16}N_4O_2)]$
M_r	911.31
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	173
a, b, c (Å)	6.3660 (11), 15.282 (3), 21.575 (4)
α, β, γ (°)	88.968 (2), 87.985 (2), 79.217 (2)
V (Å^3)	2060.4 (6)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.59
Crystal size (mm)	0.46 × 0.21 × 0.05
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*, Bruker, 2014)
T_{min}, T_{max}	0.663, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34440, 7598, 6439
R_{int}	0.054
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.115, 1.06
No. of reflections	7598
No. of parameters	535
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.66, −0.40

Computer programs: *COSMO* (Bruker, 2009), *APEX2* (Bruker, 2014), *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *CrystalMaker* (Palmer, 2013) and *OLEX2* (Dolomanov *et al.*, 2009).

piperazinyl carbon atoms and C═O moieties belonging to pendant adaH carboxylate groups (Fig. 4).

Synthesis and crystallization

$Cd(NO_3)_2{\cdot}4H_2O$ (114 mg, 0.37 mmol), 1,3-adamantanediacetic acid (93 mg, 0.37 mmol), bpcp (110 mg, 0.37 mmol) and 0.75 ml of a 1.0 *M* NaOH solution were placed into 10 ml distilled H_2O in a Teflon-lined acid digestion bomb. The bomb was sealed and heated in an oven at 393 K for 2 d, and then cooled slowly to 273 K. Colourless crystals of the title complex (107 mg, 32% yield based on 1,3-adamantanediacetic acid) were isolated after washing with distilled water and acetone, and drying in air.

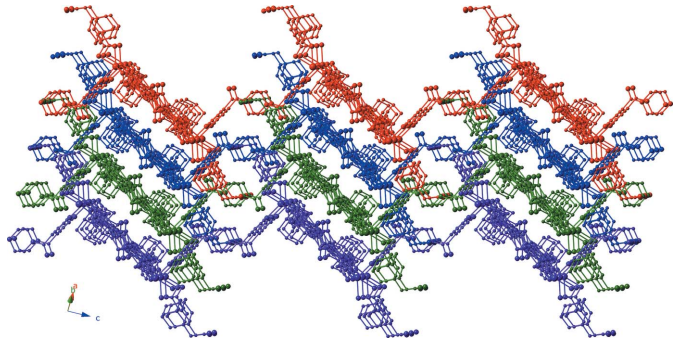


Figure 4
Stacking of supramolecular layer motifs in the title compound, mediated by interlayer C—H···O non-classical interactions.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The O atoms of one of the carboxylate groups were refined as disordered over two sets of sites, with occupancies 0.553 (7) and 0.447 (7).

Acknowledgements

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full crystallographic data

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Crystal data

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M_r = 911.31
Triclinic, $P\overline{1}$
a = 6.3660 (11) Å
b = 15.282 (3) Å
c = 21.575 (4) Å
α = 88.968 (2)°
β = 87.985 (2)°
γ = 79.217 (2)°
V = 2060.4 (6) Å^3
Z = 2
$F(000)$ = 948
D_x = 1.469 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9913 reflections
θ = 2.3–22.8°
μ = 0.59 mm^{-1}
T = 173 K
Rectangular, colourless
0.46 × 0.21 × 0.05 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 836.6 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS, Bruker, 2014)
T_{min} = 0.663, T_{max} = 0.745
34440 measured reflections
7598 independent reflections
6439 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 25.4°, θ_{min} = 1.4°
h = −7→7
k = −18→18
l = −25→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.115
S = 1.06
7598 reflections
535 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0658P)^2 + 0.9489P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Special details

Experimental. Data was collected using a BRUKER CCD (charge coupled device) based diffractometer equipped with an Oxford low-temperature apparatus operating at 173 K. A suitable crystal was chosen and mounted on a nylon loop using Paratone oil. Data were measured using omega and phi scans of 0.5° per frame for 30 s. The total number of images were based on results from the program COSMO where redundancy was expected to be 4 and completeness to 0.83Å to 100%. Cell parameters were retrieved using APEX II software and refined using SAINT on all observed reflections.Data reduction was performed using the SAINT software which corrects for Lp. Scaling and absorption corrections were applied using SADABS6 multi-scan technique, supplied by George Sheldrick. The structures are solved by the direct method using the SHELXS-97 program and refined by least squares method on F2, SHELXL-97, incorporated in OLEX2.

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cd1	1.01461 (4)	0.77868 (2)	0.76254 (2)	0.02423 (10)	
O1	0.3830 (5)	0.4755 (2)	0.64910 (13)	0.0519 (8)	
O2	0.0779 (4)	1.09521 (17)	0.85291 (12)	0.0419 (7)	
O3	1.2617 (5)	0.18816 (18)	1.02438 (13)	0.0523 (8)	
O4	1.2537 (4)	0.32992 (16)	1.04814 (12)	0.0389 (6)	
H4	1.1735	0.3178	1.0775	0.058*	
O5	0.9966 (5)	0.69784 (19)	0.85940 (12)	0.0485 (8)	
O6	1.2922 (4)	0.68106 (16)	0.80394 (11)	0.0351 (6)	
O7	1.0787 (14)	0.8339 (5)	0.6626 (3)	0.0366 (8)	0.447 (7)
O7A	0.9608 (11)	0.8550 (4)	0.6640 (2)	0.0366 (8)	0.553 (7)
O8	1.220 (2)	0.8710 (6)	0.7198 (4)	0.0366 (8)	0.447 (7)
O8A	1.2179 (16)	0.8909 (5)	0.7366 (3)	0.0366 (8)	0.553 (7)
O9	0.8949 (6)	1.3052 (3)	0.44493 (15)	0.0786 (12)	
O10	1.1218 (7)	1.17740 (19)	0.44569 (13)	0.0768 (12)	
H10	1.0737	1.1730	0.4104	0.115*	
N1	0.8480 (5)	0.68192 (18)	0.71065 (12)	0.0273 (6)	
N2	0.5755 (5)	0.47731 (19)	0.55966 (13)	0.0314 (7)	
N3	0.7295 (4)	0.87221 (17)	0.80842 (12)	0.0247 (6)	
N4	0.1051 (4)	1.02679 (19)	0.94668 (13)	0.0281 (6)	
C20	0.6470 (6)	0.7088 (2)	0.69111 (16)	0.0307 (8)	
H20	0.5761	0.7680	0.6995	0.037*	
C21	0.5399 (6)	0.6536 (2)	0.65924 (16)	0.0303 (8)	
H21	0.3986	0.6746	0.6459	0.036*	
C22	0.9459 (6)	0.5989 (2)	0.69811 (16)	0.0288 (7)	
H22	1.0877	0.5795	0.7116	0.035*	
C23	0.8506 (6)	0.5399 (2)	0.66644 (16)	0.0314 (8)	
H23	0.9265	0.4814	0.6580	0.038*	
C24	0.6436 (5)	0.5668 (2)	0.64722 (15)	0.0261 (7)	
C25	0.5219 (6)	0.5032 (2)	0.61819 (16)	0.0289 (8)	
C26	0.4487 (6)	0.4211 (2)	0.52913 (16)	0.0331 (8)	
H26A	0.3649	0.3932	0.5607	0.040*	

H26B	0.5452	0.3730	0.5064	0.040*
C27	0.7015 (5)	0.5238 (2)	0.51571 (16)	0.0310 (8)
H27A	0.8084	0.4799	0.4927	0.037*
H27B	0.7784	0.5630	0.5386	0.037*
C28	0.7140 (6)	0.9614 (2)	0.81094 (16)	0.0297 (8)
H28	0.8280	0.9871	0.7937	0.036*
C29	0.5407 (6)	1.0161 (2)	0.83741 (16)	0.0313 (8)
H29	0.5337	1.0788	0.8373	0.038*
C30	0.3922 (5)	0.8874 (2)	0.86200 (15)	0.0274 (7)
H30	0.2821	0.8596	0.8796	0.033*
C31	0.5701 (5)	0.8369 (2)	0.83379 (16)	0.0273 (7)
H31	0.5798	0.7742	0.8323	0.033*
C32	0.3744 (5)	0.9794 (2)	0.86457 (15)	0.0249 (7)
C33	0.1756 (5)	1.0396 (2)	0.88815 (16)	0.0282 (8)
C34	−0.0928 (5)	1.0825 (2)	0.96999 (16)	0.0297 (8)
H34A	−0.1723	1.1139	0.9350	0.036*
H34B	−0.0591	1.1277	0.9984	0.036*
C35	0.2294 (5)	0.9761 (2)	0.99571 (16)	0.0286 (7)
H35A	0.2745	1.0175	1.0251	0.034*
H35B	0.3595	0.9385	0.9774	0.034*
C36	1.4832 (5)	0.2699 (2)	0.96492 (16)	0.0292 (8)
H36A	1.5414	0.2106	0.9472	0.035*
H36B	1.6028	0.2909	0.9845	0.035*
C37	1.3202 (6)	0.2583 (2)	1.01475 (16)	0.0300 (8)
C38	1.4063 (5)	0.3342 (2)	0.91128 (15)	0.0234 (7)
C39	1.3826 (5)	0.4327 (2)	0.93002 (14)	0.0214 (7)
H39A	1.2745	0.4456	0.9644	0.026*
H39B	1.5207	0.4434	0.9451	0.026*
C40	1.3142 (5)	0.4960 (2)	0.87499 (14)	0.0219 (7)
C41	1.1010 (5)	0.4776 (2)	0.85260 (15)	0.0246 (7)
H41A	1.0526	0.5180	0.8175	0.030*
H41B	0.9911	0.4891	0.8866	0.030*
C42	1.1275 (5)	0.3800 (2)	0.83188 (15)	0.0262 (7)
H42	0.9882	0.3692	0.8166	0.031*
C43	1.2974 (6)	0.3612 (2)	0.77995 (16)	0.0308 (8)
H43A	1.2535	0.4002	0.7437	0.037*
H43B	1.3138	0.2985	0.7668	0.037*
C44	1.5108 (5)	0.3787 (2)	0.80314 (16)	0.0291 (8)
H44	1.6230	0.3663	0.7692	0.035*
C45	1.5764 (5)	0.3171 (2)	0.85828 (16)	0.0289 (8)
H45A	1.7151	0.3272	0.8732	0.035*
H45B	1.5950	0.2544	0.8451	0.035*
C46	1.1921 (5)	0.3186 (2)	0.88754 (16)	0.0271 (7)
H46A	1.2056	0.2557	0.8752	0.032*
H46B	1.0805	0.3308	0.9210	0.032*
C47	1.4843 (5)	0.4763 (2)	0.82269 (15)	0.0250 (7)
H47A	1.6224	0.4881	0.8370	0.030*
H47B	1.4414	0.5159	0.7867	0.030*

C48	1.2923 (6)	0.5928 (2)	0.89746 (15)	0.0267 (7)
H48A	1.2059	0.5996	0.9367	0.032*
H48B	1.4362	0.6044	0.9063	0.032*
C49	1.1894 (6)	0.6612 (2)	0.85122 (15)	0.0265 (7)
C50	1.1503 (7)	0.8897 (2)	0.67748 (19)	0.0422 (10)
C51	1.2182 (8)	0.9543 (2)	0.62969 (19)	0.0495 (12)
H51A	1.2008	0.9327	0.5876	0.059*
H51B	1.3716	0.9561	0.6343	0.059*
C54	1.0852 (6)	1.0500 (2)	0.63679 (15)	0.0284 (8)
C55	0.8450 (6)	1.0508 (2)	0.63406 (17)	0.0353 (9)
H55A	0.8136	1.0249	0.5945	0.042*
H55B	0.7998	1.0141	0.6685	0.042*
C56	0.7213 (6)	1.1458 (3)	0.6391 (2)	0.0425 (10)
H56	0.5647	1.1454	0.6376	0.051*
C57	0.7669 (7)	1.1850 (3)	0.69993 (19)	0.0457 (10)
H57A	0.7217	1.1491	0.7349	0.055*
H57B	0.6847	1.2465	0.7035	0.055*
C58	1.0049 (7)	1.1856 (2)	0.70306 (16)	0.0374 (9)
H58	1.0351	1.2116	0.7433	0.045*
C59	1.0709 (7)	1.2423 (2)	0.64891 (16)	0.0360 (9)
H59A	1.2254	1.2438	0.6508	0.043*
H59B	0.9904	1.3041	0.6525	0.043*
C60	0.7866 (6)	1.2033 (3)	0.58516 (19)	0.0403 (9)
H60A	0.7527	1.1790	0.5453	0.048*
H60B	0.7050	1.2649	0.5888	0.048*
C61	1.0261 (5)	1.2038 (2)	0.58651 (15)	0.0254 (7)
C62	1.1482 (6)	1.1075 (2)	0.58227 (15)	0.0277 (7)
H62A	1.3039	1.1071	0.5826	0.033*
H62B	1.1170	1.0816	0.5427	0.033*
C63	1.1315 (6)	1.0908 (2)	0.69754 (16)	0.0316 (8)
H63A	1.2864	1.0914	0.6992	0.038*
H63B	1.0918	1.0541	0.7328	0.038*
C64	1.0972 (6)	1.2643 (2)	0.53469 (16)	0.0320 (8)
H64A	1.0449	1.3271	0.5464	0.038*
H64B	1.2555	1.2543	0.5330	0.038*
C65	1.0233 (7)	1.2516 (2)	0.47122 (17)	0.0377 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03120 (16)	0.01866 (14)	0.02213 (15)	−0.00346 (10)	0.00096 (10)	0.00224 (9)
O1	0.065 (2)	0.066 (2)	0.0358 (16)	−0.0418 (17)	0.0161 (14)	−0.0080 (14)
O2	0.0466 (16)	0.0373 (15)	0.0335 (15)	0.0112 (12)	0.0066 (12)	0.0099 (12)
O3	0.080 (2)	0.0363 (16)	0.0477 (17)	−0.0291 (15)	0.0000 (15)	0.0065 (13)
O4	0.0488 (17)	0.0282 (14)	0.0371 (15)	−0.0036 (12)	0.0140 (12)	0.0059 (11)
O5	0.0503 (18)	0.0446 (16)	0.0373 (15)	0.0199 (14)	0.0143 (13)	0.0214 (13)
O6	0.0327 (14)	0.0330 (14)	0.0382 (15)	−0.0044 (11)	0.0001 (11)	0.0164 (11)
O7	0.0536 (16)	0.038 (2)	0.0242 (15)	−0.024 (2)	−0.015 (2)	0.0141 (15)

O7A	0.0536 (16)	0.038 (2)	0.0242 (15)	−0.024 (2)	−0.015 (2)	0.0141 (15)
O8	0.0536 (16)	0.038 (2)	0.0242 (15)	−0.024 (2)	−0.015 (2)	0.0141 (15)
O8A	0.0536 (16)	0.038 (2)	0.0242 (15)	−0.024 (2)	−0.015 (2)	0.0141 (15)
O9	0.082 (3)	0.099 (3)	0.0389 (19)	0.027 (2)	−0.0125 (17)	0.0103 (18)
O10	0.170 (4)	0.0308 (17)	0.0270 (16)	−0.008 (2)	−0.020 (2)	0.0007 (13)
N1	0.0369 (17)	0.0242 (15)	0.0224 (14)	−0.0103 (13)	−0.0001 (12)	0.0005 (11)
N2	0.0412 (18)	0.0311 (16)	0.0267 (16)	−0.0193 (14)	−0.0009 (13)	0.0005 (12)
N3	0.0270 (15)	0.0230 (14)	0.0232 (14)	−0.0031 (12)	0.0020 (11)	−0.0001 (11)
N4	0.0227 (15)	0.0291 (15)	0.0282 (16)	0.0050 (12)	0.0026 (12)	0.0042 (12)
C20	0.0310 (19)	0.0261 (18)	0.034 (2)	−0.0018 (15)	−0.0024 (15)	−0.0030 (15)
C21	0.0297 (19)	0.0267 (18)	0.034 (2)	−0.0037 (15)	−0.0035 (15)	0.0018 (15)
C22	0.0283 (18)	0.0264 (18)	0.0308 (19)	−0.0024 (14)	−0.0014 (14)	−0.0007 (14)
C23	0.036 (2)	0.0235 (18)	0.034 (2)	−0.0024 (15)	−0.0035 (16)	−0.0019 (14)
C24	0.0308 (19)	0.0282 (18)	0.0206 (17)	−0.0094 (15)	0.0005 (14)	0.0025 (13)
C25	0.035 (2)	0.0247 (18)	0.0281 (19)	−0.0086 (15)	−0.0025 (15)	0.0040 (14)
C26	0.042 (2)	0.0326 (19)	0.0291 (19)	−0.0186 (17)	−0.0002 (16)	0.0013 (15)
C27	0.0293 (18)	0.034 (2)	0.033 (2)	−0.0160 (16)	0.0038 (15)	−0.0008 (15)
C28	0.035 (2)	0.0223 (17)	0.0317 (19)	−0.0061 (15)	0.0072 (15)	0.0027 (14)
C29	0.041 (2)	0.0198 (17)	0.033 (2)	−0.0071 (15)	0.0060 (16)	0.0012 (14)
C30	0.0265 (18)	0.0274 (18)	0.0287 (18)	−0.0064 (14)	0.0007 (14)	0.0050 (14)
C31	0.0316 (19)	0.0174 (16)	0.0321 (19)	−0.0029 (14)	0.0001 (15)	0.0040 (14)
C32	0.0295 (18)	0.0236 (17)	0.0201 (17)	−0.0021 (14)	0.0010 (13)	0.0011 (13)
C33	0.0315 (19)	0.0213 (17)	0.0307 (19)	−0.0030 (14)	0.0045 (15)	−0.0002 (14)
C34	0.0263 (18)	0.0291 (18)	0.0297 (19)	0.0033 (14)	0.0036 (14)	0.0049 (14)
C35	0.0232 (17)	0.0308 (19)	0.0293 (18)	0.0009 (14)	−0.0019 (14)	0.0035 (14)
C36	0.0313 (19)	0.0191 (17)	0.0337 (19)	0.0039 (14)	−0.0008 (15)	0.0042 (14)
C37	0.036 (2)	0.0261 (18)	0.0281 (18)	−0.0047 (15)	−0.0086 (15)	0.0079 (14)
C38	0.0261 (17)	0.0184 (16)	0.0248 (17)	−0.0024 (13)	−0.0011 (13)	0.0018 (13)
C39	0.0231 (16)	0.0204 (16)	0.0206 (16)	−0.0040 (13)	−0.0005 (13)	0.0009 (13)
C40	0.0242 (17)	0.0188 (16)	0.0229 (17)	−0.0049 (13)	−0.0024 (13)	0.0041 (13)
C41	0.0236 (17)	0.0244 (17)	0.0252 (17)	−0.0030 (13)	−0.0029 (13)	0.0075 (13)
C42	0.0235 (17)	0.0294 (18)	0.0283 (18)	−0.0116 (14)	−0.0032 (14)	0.0025 (14)
C43	0.040 (2)	0.0284 (19)	0.0264 (18)	−0.0118 (16)	0.0002 (15)	−0.0013 (14)
C44	0.0302 (19)	0.0289 (18)	0.0286 (18)	−0.0072 (15)	0.0075 (14)	−0.0046 (14)
C45	0.0258 (18)	0.0226 (17)	0.036 (2)	0.0006 (14)	0.0006 (15)	−0.0022 (14)
C46	0.0308 (19)	0.0193 (16)	0.0317 (19)	−0.0067 (14)	0.0002 (15)	0.0019 (14)
C47	0.0272 (18)	0.0243 (17)	0.0243 (17)	−0.0070 (14)	−0.0018 (13)	0.0026 (13)
C48	0.0366 (19)	0.0208 (17)	0.0225 (17)	−0.0039 (14)	−0.0050 (14)	0.0020 (13)
C49	0.041 (2)	0.0167 (16)	0.0233 (17)	−0.0082 (15)	−0.0025 (15)	0.0007 (13)
C50	0.066 (3)	0.0191 (18)	0.035 (2)	0.0014 (18)	0.025 (2)	0.0020 (16)
C51	0.074 (3)	0.024 (2)	0.043 (2)	0.0037 (19)	0.030 (2)	0.0120 (17)
C54	0.041 (2)	0.0177 (16)	0.0254 (18)	−0.0040 (14)	0.0086 (15)	0.0039 (13)
C55	0.046 (2)	0.035 (2)	0.031 (2)	−0.0236 (18)	−0.0005 (16)	0.0025 (16)
C56	0.0224 (19)	0.050 (2)	0.055 (3)	−0.0083 (17)	0.0019 (17)	0.015 (2)
C57	0.053 (3)	0.031 (2)	0.047 (2)	0.0049 (18)	0.022 (2)	0.0045 (18)
C58	0.065 (3)	0.0276 (19)	0.0221 (18)	−0.0155 (18)	0.0006 (17)	−0.0005 (14)
C59	0.060 (3)	0.0227 (18)	0.0292 (19)	−0.0158 (17)	−0.0044 (17)	−0.0005 (15)
C60	0.037 (2)	0.040 (2)	0.044 (2)	−0.0055 (17)	−0.0073 (17)	0.0111 (18)

C61	0.0344 (19)	0.0189 (16)	0.0242 (17)	−0.0077 (14)	−0.0045 (14)	0.0040 (13)
C62	0.0349 (19)	0.0219 (17)	0.0258 (18)	−0.0056 (14)	0.0052 (14)	0.0040 (13)
C63	0.0318 (19)	0.037 (2)	0.0271 (19)	−0.0091 (16)	−0.0022 (15)	0.0107 (15)
C64	0.049 (2)	0.0180 (17)	0.0308 (19)	−0.0099 (15)	−0.0045 (16)	0.0040 (14)
C65	0.058 (3)	0.030 (2)	0.029 (2)	−0.0184 (18)	0.0004 (18)	0.0094 (16)

Geometric parameters (Å, º)

Cd1—O5	2.419 (2)	C36—C38	1.538 (4)
Cd1—O6	2.285 (2)	C38—C39	1.545 (4)
Cd1—O7	2.351 (6)	C38—C45	1.538 (5)
Cd1—O7A	2.411 (5)	C38—C46	1.534 (5)
Cd1—O8	2.258 (9)	C39—H39A	0.9900
Cd1—O8A	2.382 (7)	C39—H39B	0.9900
Cd1—N1	2.301 (3)	C39—C40	1.540 (4)
Cd1—N3	2.296 (3)	C40—C41	1.532 (4)
O1—C25	1.222 (4)	C40—C47	1.530 (4)
O2—C33	1.224 (4)	C40—C48	1.545 (4)
O3—C37	1.211 (4)	C41—H41A	0.9900
O4—H4	0.8400	C41—H41B	0.9900
O4—C37	1.315 (4)	C41—C42	1.542 (5)
O5—C49	1.258 (4)	C42—H42	1.0000
O6—C49	1.256 (4)	C42—C43	1.522 (5)
O7—C50	1.097 (8)	C42—C46	1.530 (5)
O7A—C50	1.445 (8)	C43—H43A	0.9900
O8—C50	1.040 (9)	C43—H43B	0.9900
O8A—C50	1.361 (8)	C43—C44	1.535 (5)
O9—C65	1.194 (5)	C44—H44	1.0000
O10—H10	0.8400	C44—C45	1.524 (5)
O10—C65	1.309 (5)	C44—C47	1.535 (5)
N1—C20	1.348 (4)	C45—H45A	0.9900
N1—C22	1.333 (4)	C45—H45B	0.9900
N2—C25	1.343 (4)	C46—H46A	0.9900
N2—C26	1.463 (4)	C46—H46B	0.9900
N2—C27	1.478 (4)	C47—H47A	0.9900
N3—C28	1.350 (4)	C47—H47B	0.9900
N3—C31	1.333 (4)	C48—H48A	0.9900
N4—C33	1.348 (4)	C48—H48B	0.9900
N4—C34	1.461 (4)	C48—C49	1.507 (4)
N4—C35	1.465 (4)	C50—C51	1.523 (5)
C20—H20	0.9500	C51—H51A	0.9900
C20—C21	1.386 (5)	C51—H51B	0.9900
C21—H21	0.9500	C51—C54	1.553 (5)
C21—C24	1.392 (5)	C54—C55	1.530 (5)
C22—H22	0.9500	C54—C62	1.542 (4)
C22—C23	1.380 (5)	C54—C63	1.523 (5)
C23—H23	0.9500	C55—H55A	0.9900
C23—C24	1.381 (5)	C55—H55B	0.9900

C24—C25	1.508 (5)	C55—C56	1.520 (5)
C26—H26A	0.9900	C56—H56	1.0000
C26—H26B	0.9900	C56—C57	1.511 (6)
C26—C27^{i}	1.514 (5)	C56—C60	1.538 (5)
C27—C26^{i}	1.514 (5)	C57—H57A	0.9900
C27—H27A	0.9900	C57—H57B	0.9900
C27—H27B	0.9900	C57—C58	1.521 (6)
C28—H28	0.9500	C58—H58	1.0000
C28—C29	1.368 (5)	C58—C59	1.535 (5)
C29—H29	0.9500	C58—C63	1.526 (5)
C29—C32	1.395 (5)	C59—H59A	0.9900
C30—H30	0.9500	C59—H59B	0.9900
C30—C31	1.375 (5)	C59—C61	1.536 (5)
C30—C32	1.391 (5)	C60—H60A	0.9900
C31—H31	0.9500	C60—H60B	0.9900
C32—C33	1.497 (5)	C60—C61	1.527 (5)
C34—H34A	0.9900	C61—C62	1.533 (4)
C34—H34B	0.9900	C61—C64	1.547 (4)
C34—C35^{ii}	1.526 (5)	C62—H62A	0.9900
C35—C34^{ii}	1.526 (5)	C62—H62B	0.9900
C35—H35A	0.9900	C63—H63A	0.9900
C35—H35B	0.9900	C63—H63B	0.9900
C36—H36A	0.9900	C64—H64A	0.9900
C36—H36B	0.9900	C64—H64B	0.9900
C36—C37	1.499 (5)	C64—C65	1.491 (5)

O6—Cd1—O5	54.87 (9)	C42—C41—H41B	109.7
O6—Cd1—O7	115.9 (2)	C41—C42—H42	109.2
O6—Cd1—O7A	134.05 (19)	C43—C42—C41	110.2 (3)
O6—Cd1—O8A	95.5 (2)	C43—C42—H42	109.2
O6—Cd1—N1	100.50 (10)	C43—C42—C46	110.1 (3)
O6—Cd1—N3	131.49 (9)	C46—C42—C41	108.9 (3)
O7—Cd1—O5	169.4 (2)	C46—C42—H42	109.2
O7—Cd1—O8A	53.4 (2)	C42—C43—H43A	109.8
O7A—Cd1—O5	168.65 (17)	C42—C43—H43B	109.8
O8—Cd1—O5	136.7 (2)	C42—C43—C44	109.3 (3)
O8—Cd1—O6	95.4 (3)	H43A—C43—H43B	108.3
O8—Cd1—O7A	54.1 (3)	C44—C43—H43A	109.8
O8—Cd1—N1	126.6 (2)	C44—C43—H43B	109.8
O8—Cd1—N3	104.4 (3)	C43—C44—H44	109.5
O8A—Cd1—O5	128.67 (17)	C43—C44—C47	109.4 (3)
N1—Cd1—O5	92.25 (11)	C45—C44—C43	108.9 (3)
N1—Cd1—O7	84.08 (19)	C45—C44—H44	109.5
N1—Cd1—O7A	79.53 (15)	C45—C44—C47	110.0 (3)
N1—Cd1—O8A	137.31 (16)	C47—C44—H44	109.5
N3—Cd1—O5	81.78 (9)	C38—C45—H45A	109.5
N3—Cd1—O7	108.7 (2)	C38—C45—H45B	109.5
N3—Cd1—O7A	92.20 (19)	C44—C45—C38	110.8 (3)

N3—Cd1—O8A	96.2 (2)	C44—C45—H45A	109.5
N3—Cd1—N1	102.00 (10)	C44—C45—H45B	109.5
C37—O4—H4	109.5	H45A—C45—H45B	108.1
C49—O5—Cd1	89.69 (19)	C38—C46—H46A	109.7
C49—O6—Cd1	96.0 (2)	C38—C46—H46B	109.7
C50—O7—Cd1	96.5 (5)	C42—C46—C38	109.7 (3)
C50—O7A—Cd1	85.2 (3)	C42—C46—H46A	109.7
C50—O8—Cd1	103.9 (7)	C42—C46—H46B	109.7
C50—O8A—Cd1	88.1 (4)	H46A—C46—H46B	108.2
C65—O10—H10	109.5	C40—C47—C44	110.0 (3)
C20—N1—Cd1	120.2 (2)	C40—C47—H47A	109.7
C22—N1—Cd1	121.8 (2)	C40—C47—H47B	109.7
C22—N1—C20	118.0 (3)	C44—C47—H47A	109.7
C25—N2—C26	119.0 (3)	C44—C47—H47B	109.7
C25—N2—C27	124.3 (3)	H47A—C47—H47B	108.2
C26—N2—C27	113.3 (3)	C40—C48—H48A	108.9
C28—N3—Cd1	123.5 (2)	C40—C48—H48B	108.9
C31—N3—Cd1	118.5 (2)	H48A—C48—H48B	107.7
C31—N3—C28	118.0 (3)	C49—C48—C40	113.3 (3)
C33—N4—C34	119.2 (3)	C49—C48—H48A	108.9
C33—N4—C35	126.2 (3)	C49—C48—H48B	108.9
C34—N4—C35	113.1 (3)	O5—C49—Cd1	62.76 (17)
N1—C20—H20	118.7	O5—C49—C48	119.6 (3)
N1—C20—C21	122.6 (3)	O6—C49—Cd1	56.67 (17)
C21—C20—H20	118.7	O6—C49—O5	119.4 (3)
C20—C21—H21	120.7	O6—C49—C48	121.0 (3)
C20—C21—C24	118.6 (3)	C48—C49—Cd1	176.8 (2)
C24—C21—H21	120.7	O7—C50—Cd1	59.7 (4)
N1—C22—H22	118.5	O7—C50—O8A	119.6 (5)
N1—C22—C23	123.0 (3)	O7—C50—C51	120.2 (5)
C23—C22—H22	118.5	O7A—C50—Cd1	62.6 (2)
C22—C23—H23	120.4	O7A—C50—C51	116.1 (4)
C22—C23—C24	119.2 (3)	O8—C50—Cd1	54.1 (5)
C24—C23—H23	120.4	O8—C50—O7A	116.8 (6)
C21—C24—C25	119.2 (3)	O8—C50—C51	127.1 (7)
C23—C24—C21	118.6 (3)	O8A—C50—Cd1	61.7 (3)
C23—C24—C25	122.0 (3)	O8A—C50—C51	118.9 (5)
O1—C25—N2	122.7 (3)	C51—C50—Cd1	177.8 (3)
O1—C25—C24	119.0 (3)	C50—C51—H51A	109.2
N2—C25—C24	118.3 (3)	C50—C51—H51B	109.2
N2—C26—H26A	109.6	C50—C51—C54	112.1 (3)
N2—C26—H26B	109.6	H51A—C51—H51B	107.9
N2—C26—C27^{i}	110.3 (3)	C54—C51—H51A	109.2
H26A—C26—H26B	108.1	C54—C51—H51B	109.2
C27^{i}—C26—H26A	109.6	C55—C54—C51	111.7 (3)
C27^{i}—C26—H26B	109.6	C55—C54—C62	107.8 (3)
N2—C27—C26^{i}	108.9 (3)	C62—C54—C51	108.1 (3)
N2—C27—H27A	109.9	C63—C54—C51	110.9 (3)

N2—C27—H27B	109.9	C63—C54—C55	109.3 (3)
C26^{i}—C27—H27A	109.9	C63—C54—C62	109.0 (3)
C26^{i}—C27—H27B	109.9	C54—C55—H55A	109.7
H27A—C27—H27B	108.3	C54—C55—H55B	109.7
N3—C28—H28	118.7	H55A—C55—H55B	108.2
N3—C28—C29	122.6 (3)	C56—C55—C54	110.0 (3)
C29—C28—H28	118.7	C56—C55—H55A	109.7
C28—C29—H29	120.2	C56—C55—H55B	109.7
C28—C29—C32	119.6 (3)	C55—C56—H56	109.2
C32—C29—H29	120.2	C55—C56—C60	110.2 (3)
C31—C30—H30	120.2	C57—C56—C55	109.7 (3)
C31—C30—C32	119.6 (3)	C57—C56—H56	109.2
C32—C30—H30	120.2	C57—C56—C60	109.4 (3)
N3—C31—C30	122.8 (3)	C60—C56—H56	109.2
N3—C31—H31	118.6	C56—C57—H57A	109.7
C30—C31—H31	118.6	C56—C57—H57B	109.7
C29—C32—C33	119.6 (3)	C56—C57—C58	109.8 (3)
C30—C32—C29	117.4 (3)	H57A—C57—H57B	108.2
C30—C32—C33	122.6 (3)	C58—C57—H57A	109.7
O2—C33—N4	122.6 (3)	C58—C57—H57B	109.7
O2—C33—C32	119.1 (3)	C57—C58—H58	109.7
N4—C33—C32	118.2 (3)	C57—C58—C59	108.8 (3)
N4—C34—H34A	109.8	C57—C58—C63	109.7 (3)
N4—C34—H34B	109.8	C59—C58—H58	109.7
N4—C34—C35^{ii}	109.2 (3)	C63—C58—H58	109.7
H34A—C34—H34B	108.3	C63—C58—C59	109.1 (3)
C35^{ii}—C34—H34A	109.8	C58—C59—H59A	109.5
C35^{ii}—C34—H34B	109.8	C58—C59—H59B	109.5
N4—C35—C34^{ii}	109.4 (3)	C58—C59—C61	110.7 (3)
N4—C35—H35A	109.8	H59A—C59—H59B	108.1
N4—C35—H35B	109.8	C61—C59—H59A	109.5
C34^{ii}—C35—H35A	109.8	C61—C59—H59B	109.5
C34^{ii}—C35—H35B	109.8	C56—C60—H60A	109.7
H35A—C35—H35B	108.2	C56—C60—H60B	109.7
H36A—C36—H36B	107.3	H60A—C60—H60B	108.2
C37—C36—H36A	108.1	C61—C60—C56	109.8 (3)
C37—C36—H36B	108.1	C61—C60—H60A	109.7
C37—C36—C38	116.8 (3)	C61—C60—H60B	109.7
C38—C36—H36A	108.1	C59—C61—C64	107.4 (3)
C38—C36—H36B	108.1	C60—C61—C59	107.9 (3)
O3—C37—O4	123.5 (3)	C60—C61—C62	108.6 (3)
O3—C37—C36	122.5 (3)	C60—C61—C64	111.6 (3)
O4—C37—C36	113.9 (3)	C62—C61—C59	108.8 (3)
C36—C38—C39	112.2 (3)	C62—C61—C64	112.3 (3)
C36—C38—C45	107.7 (3)	C54—C62—H62A	109.4
C45—C38—C39	107.6 (3)	C54—C62—H62B	109.4
C46—C38—C36	111.3 (3)	C61—C62—C54	111.3 (3)
C46—C38—C39	109.0 (3)	C61—C62—H62A	109.4

C46—C38—C45	109.0 (3)	C61—C62—H62B	109.4
C38—C39—H39A	109.4	H62A—C62—H62B	108.0
C38—C39—H39B	109.4	C54—C63—C58	110.4 (3)
H39A—C39—H39B	108.0	C54—C63—H63A	109.6
C40—C39—C38	111.4 (2)	C54—C63—H63B	109.6
C40—C39—H39A	109.4	C58—C63—H63A	109.6
C40—C39—H39B	109.4	C58—C63—H63B	109.6
C39—C40—C48	108.2 (2)	H63A—C63—H63B	108.1
C41—C40—C39	108.1 (2)	C61—C64—H64A	108.2
C41—C40—C48	111.4 (3)	C61—C64—H64B	108.2
C47—C40—C39	108.7 (3)	H64A—C64—H64B	107.4
C47—C40—C41	109.4 (3)	C65—C64—C61	116.2 (3)
C47—C40—C48	110.9 (3)	C65—C64—H64A	108.2
C40—C41—H41A	109.7	C65—C64—H64B	108.2
C40—C41—H41B	109.7	O9—C65—O10	123.1 (4)
C40—C41—C42	110.0 (3)	O9—C65—C64	123.8 (4)
H41A—C41—H41B	108.2	O10—C65—C64	113.1 (3)
C42—C41—H41A	109.7		

Cd1—O5—C49—O6	1.1 (3)	C38—C39—C40—C47	−59.9 (3)
Cd1—O5—C49—C48	−177.5 (3)	C38—C39—C40—C48	179.6 (3)
Cd1—O6—C49—O5	−1.2 (3)	C39—C38—C45—C44	−59.0 (3)
Cd1—O6—C49—C48	177.4 (3)	C39—C38—C46—C42	59.1 (3)
Cd1—O7—C50—O8A	15.7 (8)	C39—C40—C41—C42	−60.0 (3)
Cd1—O7—C50—C51	−177.5 (3)	C39—C40—C47—C44	58.5 (3)
Cd1—O7A—C50—O8	−1.8 (8)	C39—C40—C48—C49	−170.0 (3)
Cd1—O7A—C50—C51	−178.1 (3)	C40—C41—C42—C43	−58.9 (3)
Cd1—O8—C50—O7A	1.9 (9)	C40—C41—C42—C46	62.0 (3)
Cd1—O8—C50—C51	177.8 (3)	C40—C48—C49—O5	102.6 (4)
Cd1—O8A—C50—O7	−15.4 (8)	C40—C48—C49—O6	−76.1 (4)
Cd1—O8A—C50—C51	177.6 (3)	C41—C40—C47—C44	−59.3 (3)
Cd1—N1—C20—C21	179.5 (3)	C41—C40—C48—C49	−51.3 (4)
Cd1—N1—C22—C23	−179.2 (3)	C41—C42—C43—C44	59.5 (4)
Cd1—N3—C28—C29	178.7 (3)	C41—C42—C46—C38	−61.0 (3)
Cd1—N3—C31—C30	−179.6 (3)	C42—C43—C44—C45	60.2 (4)
O7—C50—C51—C54	115.1 (7)	C42—C43—C44—C47	−60.1 (4)
O7A—C50—C51—C54	80.1 (5)	C43—C42—C46—C38	59.8 (3)
O8—C50—C51—C54	−95.7 (10)	C43—C44—C45—C38	−60.0 (4)
O8A—C50—C51—C54	−78.0 (7)	C43—C44—C47—C40	60.4 (3)
N1—C20—C21—C24	0.3 (5)	C45—C38—C39—C40	59.4 (3)
N1—C22—C23—C24	−0.8 (5)	C45—C38—C46—C42	−58.0 (3)
N3—C28—C29—C32	1.8 (5)	C45—C44—C47—C40	−59.2 (3)
C20—N1—C22—C23	−0.2 (5)	C46—C38—C39—C40	−58.6 (3)
C20—C21—C24—C23	−1.3 (5)	C46—C38—C45—C44	59.0 (3)
C20—C21—C24—C25	174.1 (3)	C46—C42—C43—C44	−60.6 (3)
C21—C24—C25—O1	−71.0 (4)	C47—C40—C41—C42	58.2 (3)
C21—C24—C25—N2	110.8 (4)	C47—C40—C48—C49	70.8 (4)
C22—N1—C20—C21	0.5 (5)	C47—C44—C45—C38	59.9 (4)

C22—C23—C24—C21	1.5 (5)	C48—C40—C41—C42	−178.8 (3)
C22—C23—C24—C25	−173.7 (3)	C48—C40—C47—C44	177.4 (3)
C23—C24—C25—O1	104.2 (4)	C50—C51—C54—C55	−55.4 (5)
C23—C24—C25—N2	−73.9 (4)	C50—C51—C54—C62	−173.8 (4)
C25—N2—C26—C27^{i}	102.6 (4)	C50—C51—C54—C63	66.7 (5)
C25—N2—C27—C26^{i}	−102.1 (4)	C51—C54—C55—C56	−178.2 (3)
C26—N2—C25—O1	6.5 (5)	C51—C54—C62—C61	−179.1 (3)
C26—N2—C25—C24	−175.4 (3)	C51—C54—C63—C58	178.3 (3)
C26—N2—C27—C26^{i}	56.8 (4)	C54—C55—C56—C57	−60.0 (4)
C27—N2—C25—O1	164.4 (4)	C54—C55—C56—C60	60.5 (4)
C27—N2—C25—C24	−17.5 (5)	C55—C54—C62—C61	60.1 (4)
C27—N2—C26—C27^{i}	−57.6 (4)	C55—C54—C63—C58	−58.2 (4)
C28—N3—C31—C30	0.2 (5)	C55—C56—C57—C58	60.2 (4)
C28—C29—C32—C30	−1.4 (5)	C55—C56—C60—C61	−59.5 (4)
C28—C29—C32—C33	−174.2 (3)	C56—C57—C58—C59	59.9 (4)
C29—C32—C33—O2	55.0 (5)	C56—C57—C58—C63	−59.4 (4)
C29—C32—C33—N4	−128.7 (4)	C56—C60—C61—C59	−59.7 (4)
C30—C32—C33—O2	−117.5 (4)	C56—C60—C61—C62	58.2 (4)
C30—C32—C33—N4	58.9 (5)	C56—C60—C61—C64	−177.5 (3)
C31—N3—C28—C29	−1.1 (5)	C57—C56—C60—C61	61.2 (4)
C31—C30—C32—C29	0.5 (5)	C57—C58—C59—C61	−59.9 (4)
C31—C30—C32—C33	173.1 (3)	C57—C58—C63—C54	58.7 (4)
C32—C30—C31—N3	0.1 (5)	C58—C59—C61—C60	59.7 (4)
C33—N4—C34—C35^{ii}	135.2 (3)	C58—C59—C61—C62	−58.1 (4)
C33—N4—C35—C34^{ii}	−136.2 (3)	C58—C59—C61—C64	−179.9 (3)
C34—N4—C33—O2	−1.5 (5)	C59—C58—C63—C54	−60.4 (4)
C34—N4—C33—C32	−177.8 (3)	C59—C61—C62—C54	57.5 (4)
C34—N4—C35—C34^{ii}	58.0 (4)	C59—C61—C64—C65	−166.6 (3)
C35—N4—C33—O2	−166.5 (3)	C60—C56—C57—C58	−60.8 (4)
C35—N4—C33—C32	17.2 (5)	C60—C61—C62—C54	−59.7 (4)
C35—N4—C34—C35^{ii}	−57.9 (4)	C60—C61—C64—C65	−48.5 (4)
C36—C38—C39—C40	177.7 (3)	C61—C64—C65—O9	110.9 (4)
C36—C38—C45—C44	179.9 (3)	C61—C64—C65—O10	−72.3 (5)
C36—C38—C46—C42	−176.7 (3)	C62—C54—C55—C56	−59.6 (4)
C37—C36—C38—C39	76.8 (4)	C62—C54—C63—C58	59.4 (4)
C37—C36—C38—C45	−165.0 (3)	C62—C61—C64—C65	73.8 (4)
C37—C36—C38—C46	−45.6 (4)	C63—C54—C55—C56	58.8 (4)
C38—C36—C37—O3	115.1 (4)	C63—C54—C62—C61	−58.4 (4)
C38—C36—C37—O4	−67.4 (4)	C63—C58—C59—C61	59.7 (4)
C38—C39—C40—C41	58.8 (3)	C64—C61—C62—C54	176.3 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O5^{iii}	0.84	1.75	2.588 (3)	175
O10—H10···O7^{iv}	0.84	1.89	2.725 (8)	171

O10—H10···O7*A*^{iv}	0.84	1.70	2.520 (6)	165
C39—H39*A*···O4	0.99	2.52	3.135 (4)	120
C47—H47*B*···O6	0.99	2.55	3.163 (4)	120
C55—H55*B*···O7*A*	0.99	2.46	3.009 (7)	115
C62—H62*B*···O10	0.99	2.53	3.115 (4)	117
C63—H63*B*···O8*A*	0.99	2.47	3.107 (8)	121

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