Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS
ISSN 2056-9890

Crystal structure of bis[(*S*)-2-(2-hydroxybenzylamino)-4-methylpentanoato-κ^2N,O^1](1,10-phenanthroline-κ^2N,N')cadmium dihydrate

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Received 3 September 2018
Accepted 1 October 2018

Edited by M. Weil, Vienna University of Technology, Austria

Keywords: crystal structure; Cd^{II} complex; distorted octahedral coordination; O— H···O hydrogen bonding; π—π stacking interactions.; crystal structure.

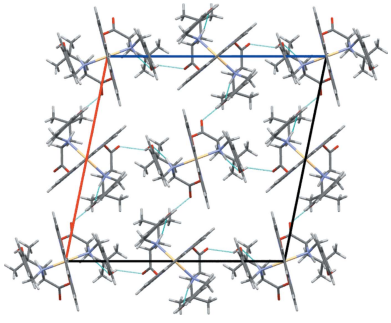
CCDC reference: 1534691

Supporting information: this article has supporting information at journals.iucr.org/e

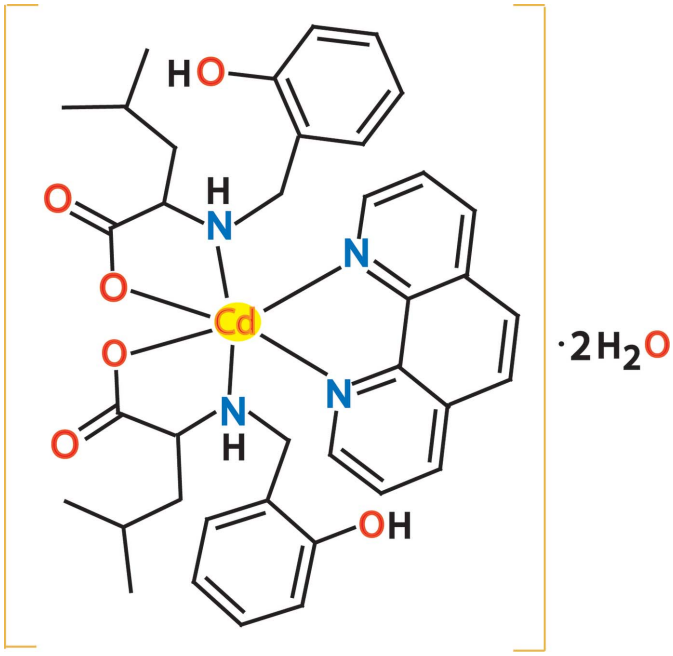
The asymmetric unit of the mononuclear mixed-ligand title complex, $[Cd(C_{13}H_{18}NO_3)_2(C_{12}H_8N_2)]\cdot 2H_2O$, contains two crystallographically independent molecules that differ insignificantly in their geometrical parameters. In both, the Cd^{II} cation lies on a twofold rotation axis and is coordinated in a distorted octahedral fashion to two monodeprotonated residues of the L-leucine-derived ligand (*S*)-2-(2-hydroxybenzylamino)-4-methylpentanoic acid (**L**), as well as to a 1,10-phenanthroline ligand in a κ^2N,N' mode. The former coordinate in an *N*,*O*-chelating mode, exhibiting a *trans*-*N*,*N*′ mutual disposition. The phenolic oxygen donor groups remain protonated and do not coordinate to the cation but take part in intra- and intermolecular hydrogen bonds. In the crystal, O—H···O hydrogen bonding results in the formation of a three-dimensional network structure. The contribution to the electron density of two disordered water molecules was removed with the SQUEEZE procedure in *PLATON* [Spek (2015). *Acta Cryst.* C**71**, 9–18]. The studied crystal was refined as a two-component inversion twin. The title complex was also characterized by IR and ^{1}H NMR spectroscopic methods.

1. Chemical context

Schiff base metal complexes are an important research area with respect to inorganic and supramolecular chemistry (Burkhardt *et al.*, 2008; Przybylski *et al.*, 2009; Moroz *et al.*, 2012). Such compounds have been found to exhibit a number of properties among which are antibacterial, antifungal, antitumor, herbicidal activities (Asadi *et al.*, 2011), as well as having applications in pharmaceutical, agricultural and industrial chemistry (Anis *et al.*, 2013). Unlike oximes, another azomethine ligand family (Sliva *et al.*, 1997; Penkova *et al.*, 2010; Pavlishchuk *et al.*, 2010), Schiff base ligands containing additional polar or acidic groups are known for their enhanced reactivity and, as a consequence, instability upon coordination to metals (Casella & Gullotti, 1983). Thus, attempts to isolate Schiff bases derived from aminohydroxamic acids resulted in cyclization under the formation of 2-substituted 3-hydroxyimidazolidine-4-ones (Iskenderov *et al.*, 2009). In attempts to achieve stable polydentate ligand systems retaining the initial donor sets, it was found that reduction of Schiff bases to amines allows the formation of stable complexes (Koh *et al.*, 1996). Phenanthroline and phenanthroline-derived ligands also have important roles in many fields (Faizi & Sharkina, 2015; Faizi *et al.*, 2017). Herein we report the synthesis and



structure of a new hydrated cadmium complex, $[Cd(C_{13}H_{18}NO_3)_2(C_{12}H_8N_2)]\cdot 2H_2O$, with a phenanthroline ligand and two ligands derived from L-leucine.



2. Structural commentary

The asymmetric unit of the title complex contains two mononuclear molecules (Fig. 1). In each, the metal cation is located on a twofold rotation axis and is coordinated by three chelating ligands, leading to a distorted octahedral N_4O_2 coordination sphere. The mixed-ligand complex is made up from one neutral phenanthroline ligand and two residues of the monodeprotonated L-leucine-derived ligand **L**. The **L** ligands of each complex are *trans-N,N′* disposed with respect to each other and comprise the chiral atoms C8 for the first and C27 for the second molecule. The Cd—O and Cd—N bond lengths in the first molecule are virtually the same in the $Cd1O_4N_2$ octahedron with Cd1—O1, Cd1—N1 and Cd1—N2 = 2.346 (3), 2.341 (4) and 2.315 (4) Å, respectively. The second molecule also exhibits similar geometrical parameters [Cd2—O4, Cd2—N3 and Cd2—N4 = 2.322 (4), 2.351 (5) and 2.339 (4) Å, respectively]. All three sets of ligands form five-membered chelate rings. Unlike the essentially planar chelate rings formed by the phenanthroline ligands, the ones involving the L-leucine-derived ligands exhibit a λ-conformation in both complex molecules. The deviations of the carbon atoms from the planes defined by the central atom and donor atoms are 0.258 (6) Å for C7, 0.599 (7) Å for C8, −0.417 (7) Å for C26 and 0.632 (5) Å for C27. In the second molecule, the highest deviations are found to be 0.160 and 0.232 Å for O4 and N4, respectively. The N—Cd—O and N—Cd—N bite angles are 73.01 (13) and 71.2 (2)°, respectively, for the first molecule and 72.40 (14) and 70.8 (2)° for the second. The phenolic O—H group remains protonated and is non-coordinating, albeit participating in an extensive intermolecular hydrogen-bonding network. Intramolecular hydrogen bonds are also found to exist and take place between atoms H2*A* and O3 as well as between H4 and O6 of the L-leucine-derived ligands. To a minor extent, intramolecular C—H···O interactions are also present between a methylene group and O4 (Table 1).

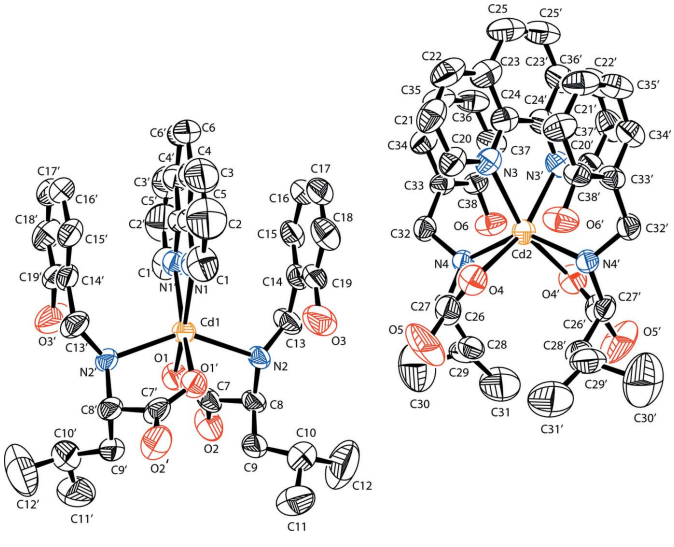


Figure 1
Structures of the two complex molecules in the title compound. Displacement ellipsoids are drawn at the 40% probability level. Atoms with primed labels are generated by the symmetry operations $-x+1, y, -z+1$ for complex Cd1 and $-x+1, y, -z+2$ for complex Cd2.

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6*A*···O2^{i}	0.82	1.83	2.645 (5)	174
N4—H4···O6	0.98	2.07	2.763 (5)	126
N2—H2*A*···O3	0.98	2.09	2.795 (6)	127
O3—H3*A*···O5	0.82	2.33	2.951 (9)	133
C28—H28*A*···O4^{ii}	0.97	2.67	3.470 (7)	141

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

3. Supramolecular features

In the crystal structure, the complex molecules are linked *via* hydrogen-bonding interactions between phenolic O—H and C—O groups of L-leucine-derived ligands (Table 1, Fig. 2). π–π interactions take place between the central phenanthroline ring and the C14–C19 rings of two leucine-derived **L** ligands with distances between the centroids of the aromatic fragments being 3.813 (4) Å for the first molecule. The stacking interactions of the second molecule are between C33–C38 rings of two L-leucine-derived ligands **L** and the C23–C25/C23′–C25′($-x+1, y, -z+2$) phenanthroline fragment with a centroid-to-centroid distance of 3.773 (4) Å.

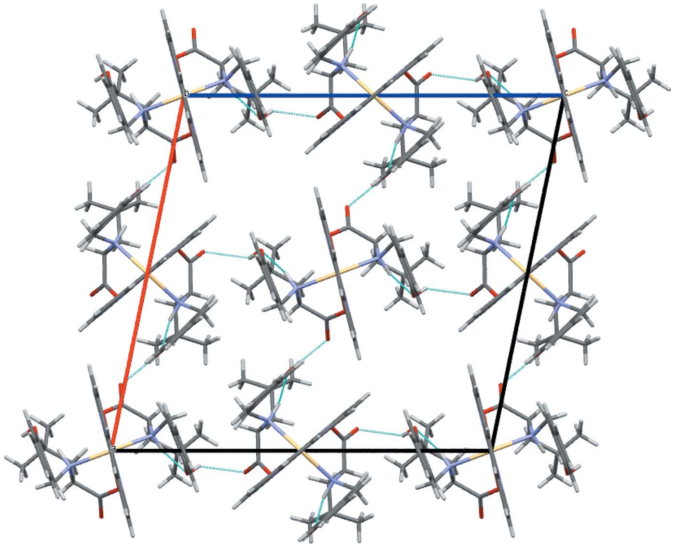


Figure 2
The crystal packing of the title compound viewed along [010]. Hydrogen bonds are shown as dashed lines (see Table 1 for numerical details).

4. Database survey

A search in the Cambridge Structural Database (Version 5.39, last update February 2018; Groom *et al.*, 2016) revealed only one precedent of a Cd^{II} complex with a 2-hydroxybenzyl derivative of an amino acid (refcode WARLIL). In this mononuclear complex, the phenolic and β-carboxylic groups are deprotonated. The *N*-(2-hydroxybenzyl)-D,L-aspartic acid residue coordinates in an (*O*,*N*,*O*′)-tridentate mode including the phenolic O atom (Lou *et al.*, 2005). This differs from the title compound in which the phenolic group is protonated and is non-coordinating. The second O atom of the β-carboxylic group bridges the neighbouring Cd^{II} units into a polymeric chain. In addition, there are four structures of complexes of homologous zinc and with 2-hydroxybenzyl derivatives of alanine (refcodes AZIROQ, AZIRUW, NOLYIW, NOLYOC). These compounds have a Zn_2O_2 binuclear core, and the ligands also coordinate in an (*O*,*N*,*O*′)-tridentate manner, with an additional μ_2-mode for the phenolic O atom (Lou *et al.*, 2004; Ranford *et al.*, 1998).

5. Synthesis and crystallization

Synthesis of (*S*)-2-(2-hydroxybenzylamino)-4-methylpentanoic acid (L)

A mixture of L-leucine (1.00 g, 7.62 mmol) and $LiOH{\cdot}H_2O$ (0.323 g, 7.62 mmol) in methanol (25 ml) was stirred for 10 min to dissolve. A methanolic solution of *o*-salicylaldehyde (0.930 g, 7.62 mmol) was added dropwise to the above solution whereby the colour of the solution turned to yellow. Stirring was continued for 30 min before the solution was treated with $NaBH_4$ (0.580 g, 15.3 mmol), leading to a colourless solution. The solvent was evaporated under reduced pressure, and the resulting solid was dissolved in water. The clear solution was then acidified with diluted HCl (pH ∼5–7). The ligand precipitated as a white solid. The suspension was filtered, and the residue was washed thoroughly with water. The solid was dried in a vacuum desiccator (yield 1.65 g, 88%). Because of its poor solubility, the ^{1}H NMR spectrum for the ligand was recorded as the lithium salt of the ligand, prepared by adding 2 equiv. of $LiOH{\cdot}3H_2O$ in CD_3OD. ^{1}H NMR Li_2**L** (CD_3OD, 400 MHz, ppm): 0.76 (*d*, 3H, H^j) , 0.81 (*d*, 3H, H^i) , 1.36 (*m*, 1H, H^g) , 1.41 (*m*, 1H, $H^{g'}$), 1.67 (*m*, 1H, H^h) , 3.07 (*dd*, 1H, H^f) , 3.65 (*d*, 1H, H^e) , 3.94 (*d*, 1H, $H^{e'}$), 6.35 (*t*, 1H, H^c) , 6.45 (*d*, 1H, H^a) , 6.94 (*m*, 2H, $H^{b,d}$). *m*/*z* (ESI–MS, [Li**L**]$^-$); calculated: 242.22, found 242.02. IR (KBr, cm^{-1}) $\nu(COO)_{asym}$ 1600 (*s*), 1593 (*s*); ν $(COO)_{sym}$ 1393 (*m*), cm^{-1}.

Synthesis of [Cd(L)$_2$(phen)]·(H$_2$O)$_2$]

A methanolic solution of $Cd(NO_3)_2{\cdot}4H_2O$ (0.130 g, 0.421 mmol) was added under stirring to 20 ml of a methanolic solution of **L** (0.200 g, 0.843mmol) and NaOH (0.034 g, 0.843 mmol), followed by addition of phenanthroline monohydrate (0.076 g, 0.421mmol) in 5 ml of methanol. A clear solution was formed within half an hour under constant stirring. After 2 h, the solvent was evaporated to dryness. The residue was subsequently washed with methanol and diethyl ether, and finally dried under vacuum. Empirical formula $[Cd(\mathbf{L})_2(phen)]{\cdot}2H_2O$. Yield: 60%. $[Cd(\mathbf{L})_2(phen)]{\cdot}2H_2O$: IR (KBr, cm^{-1}) $\nu(COO)_{asym}$ 1594, $\nu(COO)_{sym}$ 1384, ν(phenolic, CO) 1257. ^{1}H NMR $[Cd(\mathbf{L})_2(phen)]{\cdot}2H_2O]$ (DMSO, 400 MHz. ppm): 0.6 (*s*, *broad*, 3H^J), 0.7 (*s*, *broad*, 3H^i), 1.3 (*s*, *broad*, 1H^g), 1.5 (*s*, *broad*, H$^{g'}$), 2.7 (*s*, *broad*, 1H^f), 2.9 (*s*, *broad*, 2H$^{e,e'}$), 6.6 (*s*, *broad*, 1H^d), 6.4 (*s*, *broad*, 1H^c), 6.6 (*s*, *broad*, 1H^b), 6.1 (*s*, *broad*,1H^a), 8.0 (*s*, *broad*, 2H^n), 8.1 (*s*, *broad*, 2H^m), 8.7 (*s*, *broad*, 2H^l), 9.1 (*s*, *broad*, 2H^k). ESI–Mass (-ve) at 829.18 (calculated 829.18). Suitable needle-shaped crystals for X-ray data collection were obtained by slow evaporation of a methanol: DMF (2:1 *v*:*v*) solution within a week.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Atoms O3, C3, C4 and C6 showed highly anisotropic displacement parameters and were modelled using the ISOR instruction in *SHELXL* (Sheldrick, 2015). The H atoms of the phenolic OH group were located from a difference-Fourier map and were constrained to ride on their parent atoms, with O—H = 0.82 Å and with U_{iso}(H) = 1.5U_{eq}(O). All C-bound H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C).

After unsuccessful attempts to model disordered solvent molecules, their contributions to the diffraction data were removed by using the SQUEEZE routine in *PLATON* (Spek, 2015). *PLATON* calculated a solvent-accessible void volume in the unit cell of 629 Å^3 (15.4% of the total cell volume), corresponding to 151 electrons (residual electron density after the last refinement cycle) per unit cell, or 37.75 electrons per one complex molecule. This number agrees with two water molecules. Although not modelled in the refined structure, the two water molecules are included in the formula and other crystallographic data.

Acknowledgements

The authors are grateful to the Department of Chemistry, Taras Shevchenko National University of Kyiv, 64, Vladimirska Str., Kiev, Ukraine, for financial support, and Dr Pratik Sen and Dr Manabendra Ray for valuable discussions.

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Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cd(C_{13}H_{18}NO_3)_2(C_{12}H_8N_2)]\cdot 2H_2O$
M_r	801.22
Crystal system, space group	Monoclinic, *I*2
Temperature (K)	293
a, *b*, *c* (Å)	18.0171 (6), 12.2561 (3), 18.8597 (9)
β (°)	101.582 (3)
V (Å^3)	4079.8 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.59
Crystal size (mm)	0.19 × 0.12 × 0.09
Data collection	
Diffractometer	Bruker SMART CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2011)
T_{min}, T_{max}	0.867, 0.942
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22798, 7944, 6342
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.076, 0.99
No. of reflections	7944
No. of parameters	444
No. of restraints	37
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.18
Absolute structure	Refined as an inversion twin
Absolute structure parameter	−0.03 (3)

Computer programs: *SMART* and *SAINT* (Bruker, 2011), *SHELXTL* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008).

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supporting information

Acta Cryst. (2018). E**74**, 1565-1568 [https://doi.org/10.1107/S2056989018013877]

Crystal structure of bis[(*S*)-2-(2-hydroxybenzylamino)-4-methylpentanoato-κ^2N,O^1](1,10-phenanthroline-κ^2N,N')cadmium dihydrate

Md. Serajul Haque Faizi, Necmi Dege, James Pogrebetsky and Turganbay S. Iskenderov

Computing details

Data collection: *SMART* (Bruker, 2011); cell refinement: *SAINT* (Bruker, 2011); data reduction: *SAINT* (Bruker, 2011); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Bis[(*S*)-2-(2-hydroxybenzylamino)-4-methylpentanoato-κ^2N,O^1](1,10-phenanthroline-κ^2N,N')cadmium dihydrate

Crystal data

$[Cd(C_{13}H_{18}NO_3)_2(C_{12}H_8N_2)]\cdot 2H_2O$
M_r = 801.22
Monoclinic, *I*2
a = 18.0171 (6) Å
b = 12.2561 (3) Å
c = 18.8597 (9) Å
β = 101.582 (3)°
V = 4079.8 (3) Å^3
Z = 4
F(000) = 1584
D_x = 1.304 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 2245 reflections
θ = 1.8–26.0°
μ = 0.59 mm^{-1}
T = 293 K
Needle, colorless
0.19 × 0.12 × 0.09 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube, x-ray
Graphite monochromator
phi and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2011)
T_{min} = 0.867, T_{max} = 0.942
22798 measured reflections
7944 independent reflections
6342 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 26.0°, θ_{min} = 1.8°
h = −22→21
k = −15→15
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.076
S = 0.99
7944 reflections
444 parameters
37 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0365P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.036
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: −0.03 (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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.500000	0.69148 (3)	0.500000	0.05478 (18)
C1	0.3532 (4)	0.5367 (7)	0.4350 (4)	0.094 (2)
H1	0.328791	0.603070	0.423336	0.113*
C2	0.3123 (6)	0.4396 (10)	0.4188 (6)	0.136 (4)
H2	0.261275	0.441306	0.396832	0.163*
C3	0.3476 (8)	0.3454 (10)	0.4352 (6)	0.142 (4)
H3	0.320426	0.281053	0.424184	0.171*
C4	0.4239 (6)	0.3391 (6)	0.4682 (4)	0.106 (2)
C5	0.4604 (3)	0.4394 (4)	0.4823 (3)	0.0693 (15)
C6	0.4641 (6)	0.2410 (6)	0.4860 (6)	0.146 (6)
H6	0.438503	0.174909	0.477383	0.176*
C7	0.3702 (3)	0.8567 (5)	0.5040 (3)	0.0707 (15)
C8	0.4129 (4)	0.8566 (6)	0.5827 (4)	0.0677 (19)
H8	0.376062	0.862966	0.614269	0.081*
C9	0.4657 (4)	0.9528 (5)	0.5960 (3)	0.0820 (18)
H9A	0.436890	1.017813	0.578965	0.098*
H9B	0.503823	0.943726	0.566820	0.098*
C10	0.5066 (6)	0.9725 (7)	0.6751 (4)	0.121 (3)
H10	0.533040	0.904880	0.692573	0.145*
C11	0.5670 (6)	1.0626 (7)	0.6790 (5)	0.152 (4)
H11A	0.600500	1.044664	0.646987	0.228*
H11B	0.542692	1.131051	0.664725	0.228*
H11C	0.595593	1.068085	0.727635	0.228*
C12	0.4540 (7)	0.9980 (11)	0.7240 (6)	0.208 (6)
H12A	0.416817	0.941072	0.720849	0.313*
H12B	0.481962	1.003153	0.772901	0.313*
H12C	0.429061	1.066120	0.709991	0.313*
C13	0.4116 (3)	0.6711 (5)	0.6333 (4)	0.0833 (18)
H13A	0.365937	0.653468	0.598276	0.100*
H13B	0.396256	0.704215	0.674837	0.100*
C14	0.4537 (3)	0.5672 (5)	0.6570 (3)	0.0637 (14)
C15	0.4194 (4)	0.4692 (7)	0.6421 (3)	0.0750 (16)
H15	0.370191	0.467626	0.614955	0.090*
C16	0.4535 (5)	0.3729 (6)	0.6649 (4)	0.089 (2)
H16	0.428382	0.307134	0.653054	0.106*
C17	0.5248 (5)	0.3745 (6)	0.7052 (4)	0.096 (2)
H17	0.548436	0.309439	0.722026	0.116*
C18	0.5618 (4)	0.4705 (7)	0.7211 (4)	0.099 (2)

H18	0.611238	0.471017	0.747584	0.119*
C19	0.5264 (4)	0.5667 (5)	0.6981 (3)	0.0790 (17)
N1	0.4256 (3)	0.5362 (4)	0.4664 (2)	0.0674 (12)
N2	0.4565 (2)	0.7519 (3)	0.6006 (2)	0.0576 (10)
H2A	0.501263	0.769513	0.637666	0.069*
O1	0.3930 (2)	0.7999 (3)	0.4576 (2)	0.0728 (10)
O2	0.3145 (3)	0.9197 (4)	0.4897 (3)	0.1030 (15)
O3	0.5641 (3)	0.6627 (4)	0.7132 (3)	0.130 (2)
H3A	0.542946	0.699788	0.739444	0.194*
Cd2	0.500000	0.46530 (4)	1.000000	0.05859 (18)
C20	0.5982 (4)	0.3122 (7)	0.9104 (4)	0.076 (2)
H20	0.614551	0.379213	0.896042	0.091*
C21	0.6251 (4)	0.2141 (7)	0.8843 (4)	0.094 (2)
H21	0.659847	0.216857	0.853995	0.113*
C22	0.6000 (4)	0.1167 (7)	0.9037 (4)	0.098 (2)
H22	0.615858	0.052420	0.885145	0.118*
C23	0.5505 (3)	0.1129 (5)	0.9514 (4)	0.0829 (19)
C24	0.5265 (3)	0.2132 (4)	0.9755 (3)	0.0661 (14)
C25	0.5235 (4)	0.0111 (5)	0.9773 (5)	0.104 (3)
H25	0.539693	−0.055026	0.961602	0.124*
C26	0.5314 (4)	0.6410 (6)	0.8935 (4)	0.0804 (18)
C27	0.4446 (3)	0.6360 (4)	0.8759 (3)	0.0664 (14)
H27	0.428202	0.641918	0.823245	0.080*
C28	0.4105 (4)	0.7320 (5)	0.9101 (3)	0.0778 (16)
H28A	0.424075	0.724288	0.962241	0.093*
H28B	0.434021	0.798545	0.897435	0.093*
C29	0.3254 (5)	0.7458 (6)	0.8891 (5)	0.098 (2)
H29	0.301566	0.675093	0.894081	0.117*
C30	0.3004 (6)	0.7846 (11)	0.8102 (6)	0.195 (5)
H30A	0.317410	0.733412	0.778404	0.293*
H30B	0.246106	0.789565	0.798264	0.293*
H30C	0.321961	0.854958	0.804816	0.293*
C31	0.2988 (6)	0.8255 (8)	0.9385 (7)	0.164 (4)
H31A	0.244850	0.833614	0.924712	0.246*
H31B	0.311856	0.799333	0.987370	0.246*
H31C	0.322687	0.894820	0.935077	0.246*
C32	0.3922 (3)	0.4556 (4)	0.8372 (3)	0.0645 (13)
H32A	0.435248	0.441562	0.814871	0.077*
H32B	0.353162	0.490151	0.801309	0.077*
C33	0.3628 (3)	0.3497 (4)	0.8590 (3)	0.0593 (12)
C34	0.3872 (3)	0.2514 (5)	0.8345 (3)	0.0728 (15)
H34	0.423115	0.252114	0.805316	0.087*
C35	0.3586 (4)	0.1516 (5)	0.8532 (4)	0.0872 (19)
H35	0.374557	0.086691	0.835592	0.105*
C36	0.3074 (4)	0.1500 (5)	0.8971 (4)	0.0847 (19)
H36	0.288831	0.083470	0.909771	0.102*
C37	0.2824 (3)	0.2463 (5)	0.9235 (4)	0.0759 (16)
H37	0.249014	0.244196	0.955244	0.091*

C38	0.3078 (3)	0.3458 (4)	0.9020 (3)	0.0606 (13)
N3	0.5503 (2)	0.3089 (4)	0.9548 (2)	0.0644 (11)
N4	0.4156 (2)	0.5315 (3)	0.8985 (2)	0.0529 (9)
H4	0.369103	0.549857	0.915387	0.063*
O4	0.5687 (2)	0.5731 (4)	0.9349 (2)	0.0770 (11)
O5	0.5606 (4)	0.7171 (7)	0.8649 (4)	0.164 (4)
O6	0.2817 (2)	0.4428 (3)	0.9223 (2)	0.0803 (11)
H6A	0.250728	0.431603	0.947898	0.120*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0543 (4)	0.0500 (4)	0.0664 (4)	0.000	0.0272 (3)	0.000
C1	0.072 (4)	0.118 (6)	0.096 (5)	−0.017 (4)	0.024 (4)	−0.012 (4)
C2	0.101 (7)	0.160 (10)	0.143 (8)	−0.066 (7)	0.015 (6)	−0.024 (8)
C3	0.197 (12)	0.117 (8)	0.126 (8)	−0.089 (9)	0.064 (8)	−0.035 (7)
C4	0.171 (8)	0.073 (5)	0.082 (5)	−0.042 (5)	0.048 (5)	−0.010 (4)
C5	0.105 (4)	0.051 (3)	0.058 (3)	−0.009 (3)	0.031 (3)	−0.002 (2)
C6	0.303 (19)	0.057 (4)	0.105 (9)	−0.026 (6)	0.101 (11)	−0.008 (5)
C7	0.072 (4)	0.066 (3)	0.085 (4)	0.019 (3)	0.043 (3)	0.027 (3)
C8	0.085 (4)	0.051 (4)	0.078 (5)	0.007 (3)	0.044 (4)	0.012 (3)
C9	0.121 (5)	0.056 (4)	0.080 (4)	0.017 (3)	0.047 (4)	0.009 (3)
C10	0.184 (8)	0.091 (5)	0.095 (5)	−0.019 (6)	0.045 (5)	−0.015 (5)
C11	0.220 (11)	0.090 (6)	0.136 (8)	−0.023 (7)	0.012 (7)	−0.021 (6)
C12	0.244 (13)	0.261 (15)	0.145 (9)	−0.056 (11)	0.097 (10)	−0.084 (9)
C13	0.093 (4)	0.070 (4)	0.103 (5)	0.014 (3)	0.056 (4)	0.029 (3)
C14	0.074 (4)	0.067 (4)	0.057 (3)	0.012 (3)	0.029 (3)	0.015 (3)
C15	0.083 (4)	0.080 (4)	0.062 (3)	−0.012 (4)	0.016 (3)	0.015 (4)
C16	0.141 (7)	0.063 (4)	0.069 (4)	−0.006 (4)	0.036 (4)	0.008 (3)
C17	0.144 (7)	0.075 (5)	0.077 (5)	0.031 (5)	0.037 (5)	0.021 (4)
C18	0.106 (5)	0.107 (6)	0.079 (4)	0.010 (5)	0.002 (4)	0.030 (4)
C19	0.117 (5)	0.062 (4)	0.054 (3)	−0.008 (4)	0.006 (3)	0.013 (3)
N1	0.072 (3)	0.070 (3)	0.064 (3)	−0.019 (2)	0.022 (2)	−0.003 (2)
N2	0.067 (3)	0.052 (2)	0.061 (2)	0.007 (2)	0.033 (2)	0.011 (2)
O1	0.073 (2)	0.078 (3)	0.074 (2)	0.0225 (19)	0.029 (2)	0.006 (2)
O2	0.099 (3)	0.117 (3)	0.106 (3)	0.057 (3)	0.052 (3)	0.039 (3)
O3	0.182 (5)	0.094 (4)	0.090 (3)	−0.043 (3)	−0.027 (3)	0.017 (3)
Cd2	0.0580 (4)	0.0627 (4)	0.0563 (4)	0.000	0.0145 (3)	0.000
C20	0.075 (4)	0.082 (5)	0.071 (4)	0.008 (4)	0.011 (3)	−0.012 (4)
C21	0.086 (4)	0.112 (6)	0.088 (5)	0.018 (4)	0.025 (3)	−0.026 (4)
C22	0.089 (5)	0.088 (6)	0.109 (6)	0.022 (4)	−0.002 (4)	−0.034 (4)
C23	0.064 (4)	0.081 (5)	0.092 (5)	0.015 (3)	−0.013 (3)	−0.018 (4)
C24	0.053 (3)	0.064 (4)	0.073 (4)	0.003 (2)	−0.007 (2)	−0.006 (3)
C25	0.099 (7)	0.054 (4)	0.141 (8)	0.006 (3)	−0.018 (4)	−0.011 (4)
C26	0.085 (5)	0.091 (5)	0.070 (4)	−0.035 (4)	0.028 (4)	−0.007 (4)
C27	0.086 (4)	0.066 (3)	0.046 (3)	−0.020 (3)	0.011 (3)	0.008 (2)
C28	0.104 (5)	0.055 (3)	0.068 (4)	−0.013 (3)	0.001 (3)	0.009 (3)
C29	0.110 (6)	0.056 (4)	0.119 (6)	0.007 (4)	0.005 (5)	0.005 (4)

C30	0.150 (9)	0.275 (15)	0.136 (9)	0.038 (9)	−0.033 (7)	0.031 (9)
C31	0.180 (10)	0.124 (8)	0.189 (11)	0.073 (7)	0.038 (8)	0.017 (7)
C32	0.071 (3)	0.068 (3)	0.053 (3)	−0.010 (3)	0.009 (2)	−0.003 (3)
C33	0.055 (3)	0.054 (3)	0.065 (3)	−0.011 (2)	0.001 (2)	−0.009 (2)
C34	0.069 (3)	0.070 (4)	0.076 (4)	0.002 (3)	0.006 (3)	−0.016 (3)
C35	0.088 (5)	0.057 (4)	0.113 (5)	−0.004 (3)	0.010 (4)	−0.018 (3)
C36	0.067 (4)	0.055 (4)	0.126 (6)	−0.008 (3)	0.006 (4)	0.005 (4)
C37	0.054 (3)	0.072 (4)	0.101 (5)	−0.011 (3)	0.014 (3)	0.009 (4)
C38	0.058 (3)	0.053 (3)	0.070 (3)	−0.011 (2)	0.011 (3)	−0.009 (3)
N3	0.055 (3)	0.072 (3)	0.064 (3)	−0.001 (2)	0.008 (2)	−0.009 (2)
N4	0.058 (2)	0.052 (2)	0.050 (2)	−0.0103 (18)	0.0133 (18)	−0.0006 (18)
O4	0.061 (2)	0.091 (3)	0.083 (3)	−0.013 (2)	0.026 (2)	−0.005 (2)
O5	0.157 (5)	0.182 (8)	0.148 (5)	−0.098 (6)	0.021 (4)	0.078 (6)
O6	0.071 (2)	0.059 (2)	0.124 (3)	−0.0123 (18)	0.049 (2)	−0.011 (2)

Geometric parameters (Å, º)

Cd1—N2^{i}	2.315 (4)	Cd2—O4^{ii}	2.322 (4)
Cd1—N2	2.315 (4)	Cd2—O4	2.322 (4)
Cd1—N1^{i}	2.341 (4)	Cd2—N4^{ii}	2.339 (4)
Cd1—N1	2.341 (4)	Cd2—N4	2.339 (4)
Cd1—O1^{i}	2.346 (3)	Cd2—N3	2.351 (5)
Cd1—O1	2.346 (3)	Cd2—N3^{ii}	2.352 (5)
C1—N1	1.320 (8)	C20—N3	1.321 (8)
C1—C2	1.400 (12)	C20—C21	1.420 (10)
C1—H1	0.9300	C20—H20	0.9300
C2—C3	1.324 (15)	C21—C22	1.353 (10)
C2—H2	0.9300	C21—H21	0.9300
C3—C4	1.393 (15)	C22—C23	1.388 (10)
C3—H3	0.9300	C22—H22	0.9300
C4—C5	1.393 (9)	C23—C24	1.408 (8)
C4—C6	1.408 (12)	C23—C25	1.459 (9)
C5—N1	1.347 (7)	C24—N3	1.333 (7)
C5—C5^{i}	1.449 (12)	C24—C24^{ii}	1.458 (12)
C6—C6^{i}	1.30 (2)	C25—C25^{ii}	1.318 (16)
C6—H6	0.9300	C25—H25	0.9300
C7—O1	1.251 (6)	C26—O4	1.242 (8)
C7—O2	1.252 (6)	C26—O5	1.246 (8)
C7—C8	1.529 (9)	C26—C27	1.533 (8)
C8—C9	1.503 (10)	C27—N4	1.477 (6)
C8—N2	1.506 (8)	C27—C28	1.529 (8)
C8—H8	0.9800	C27—H27	0.9800
C9—C10	1.544 (10)	C28—C29	1.514 (10)
C9—H9A	0.9700	C28—H28A	0.9700
C9—H9B	0.9700	C28—H28B	0.9700
C10—C12	1.482 (12)	C29—C31	1.494 (13)
C10—C11	1.543 (11)	C29—C30	1.540 (13)
C10—H10	0.9800	C29—H29	0.9800

C11—H11A	0.9600	C30—H30A	0.9600
C11—H11B	0.9600	C30—H30B	0.9600
C11—H11C	0.9600	C30—H30C	0.9600
C12—H12A	0.9600	C31—H31A	0.9600
C12—H12B	0.9600	C31—H31B	0.9600
C12—H12C	0.9600	C31—H31C	0.9600
C13—N2	1.489 (6)	C32—N4	1.477 (6)
C13—C14	1.504 (7)	C32—C33	1.491 (7)
C13—H13A	0.9700	C32—H32A	0.9700
C13—H13B	0.9700	C32—H32B	0.9700
C14—C15	1.355 (10)	C33—C34	1.393 (7)
C14—C19	1.380 (8)	C33—C38	1.402 (7)
C15—C16	1.360 (10)	C34—C35	1.400 (8)
C15—H15	0.9300	C34—H34	0.9300
C16—C17	1.354 (9)	C35—C36	1.358 (10)
C16—H16	0.9300	C35—H35	0.9300
C17—C18	1.356 (10)	C36—C37	1.391 (9)
C17—H17	0.9300	C36—H36	0.9300
C18—C19	1.369 (9)	C37—C38	1.391 (8)
C18—H18	0.9300	C37—H37	0.9300
C19—O3	1.359 (7)	C38—O6	1.360 (6)
N2—H2A	0.9800	N4—H4	0.9800
O3—H3A	0.8200	O6—H6A	0.8200

N2^{i}—Cd1—N2	142.70 (19)	O4^{ii}—Cd2—O4	110.6 (2)
N2^{i}—Cd1—N1^{i}	102.22 (15)	O4^{ii}—Cd2—N4^{ii}	72.40 (14)
N2—Cd1—N1^{i}	107.96 (14)	O4—Cd2—N4^{ii}	84.68 (14)
N2^{i}—Cd1—N1	107.96 (14)	O4^{ii}—Cd2—N4	84.68 (14)
N2—Cd1—N1	102.22 (15)	O4—Cd2—N4	72.40 (14)
N1^{i}—Cd1—N1	71.2 (2)	N4^{ii}—Cd2—N4	139.38 (18)
N2^{i}—Cd1—O1^{i}	73.01 (13)	O4^{ii}—Cd2—N3	160.06 (16)
N2—Cd1—O1^{i}	85.98 (14)	O4—Cd2—N3	89.30 (16)
N1^{i}—Cd1—O1^{i}	88.94 (16)	N4^{ii}—Cd2—N3	110.19 (13)
N1—Cd1—O1^{i}	159.98 (16)	N4—Cd2—N3	102.76 (14)
N2^{i}—Cd1—O1	85.98 (14)	O4^{ii}—Cd2—N3^{ii}	89.30 (17)
N2—Cd1—O1	73.01 (13)	O4—Cd2—N3^{ii}	160.06 (16)
N1^{i}—Cd1—O1	159.98 (16)	N4^{ii}—Cd2—N3^{ii}	102.76 (14)
N1—Cd1—O1	88.94 (16)	N4—Cd2—N3^{ii}	110.18 (13)
O1^{i}—Cd1—O1	111.0 (2)	N3—Cd2—N3^{ii}	70.8 (2)
N1—C1—C2	121.5 (8)	N3—C20—C21	120.3 (8)
N1—C1—H1	119.2	N3—C20—H20	119.8
C2—C1—H1	119.2	C21—C20—H20	119.8
C3—C2—C1	118.9 (10)	C22—C21—C20	119.9 (7)
C3—C2—H2	120.6	C22—C21—H21	120.0
C1—C2—H2	120.6	C20—C21—H21	120.0
C2—C3—C4	122.5 (9)	C21—C22—C23	119.8 (6)
C2—C3—H3	118.7	C21—C22—H22	120.1
C4—C3—H3	118.7	C23—C22—H22	120.1

C3—C4—C5	114.9 (8)	C22—C23—C24	117.3 (7)
C3—C4—C6	124.6 (9)	C22—C23—C25	123.2 (7)
C5—C4—C6	120.5 (9)	C24—C23—C25	119.6 (7)
N1—C5—C4	123.6 (7)	N3—C24—C23	122.5 (6)
N1—C5—C5^{i}	118.3 (3)	N3—C24—C24^{ii}	118.3 (3)
C4—C5—C5^{i}	118.1 (5)	C23—C24—C24^{ii}	119.2 (4)
C6^{i}—C6—C4	121.3 (6)	C25^{ii}—C25—C23	121.2 (4)
C6^{i}—C6—H6	119.3	C25^{ii}—C25—H25	119.4
C4—C6—H6	119.3	C23—C25—H25	119.4
O1—C7—O2	123.6 (6)	O4—C26—O5	123.5 (7)
O1—C7—C8	120.5 (5)	O4—C26—C27	120.6 (5)
O2—C7—C8	115.9 (6)	O5—C26—C27	115.9 (7)
C9—C8—N2	110.3 (5)	N4—C27—C28	110.5 (4)
C9—C8—C7	109.8 (5)	N4—C27—C26	112.2 (5)
N2—C8—C7	110.9 (5)	C28—C27—C26	110.8 (5)
C9—C8—H8	108.6	N4—C27—H27	107.7
N2—C8—H8	108.6	C28—C27—H27	107.7
C7—C8—H8	108.6	C26—C27—H27	107.7
C8—C9—C10	116.6 (6)	C29—C28—C27	116.6 (5)
C8—C9—H9A	108.1	C29—C28—H28A	108.2
C10—C9—H9A	108.1	C27—C28—H28A	108.2
C8—C9—H9B	108.1	C29—C28—H28B	108.2
C10—C9—H9B	108.1	C27—C28—H28B	108.2
H9A—C9—H9B	107.3	H28A—C28—H28B	107.3
C12—C10—C11	110.7 (8)	C31—C29—C28	110.2 (7)
C12—C10—C9	113.2 (9)	C31—C29—C30	109.4 (8)
C11—C10—C9	110.7 (7)	C28—C29—C30	111.8 (8)
C12—C10—H10	107.3	C31—C29—H29	108.5
C11—C10—H10	107.3	C28—C29—H29	108.5
C9—C10—H10	107.3	C30—C29—H29	108.5
C10—C11—H11A	109.5	C29—C30—H30A	109.5
C10—C11—H11B	109.5	C29—C30—H30B	109.5
H11A—C11—H11B	109.5	H30A—C30—H30B	109.5
C10—C11—H11C	109.5	C29—C30—H30C	109.5
H11A—C11—H11C	109.5	H30A—C30—H30C	109.5
H11B—C11—H11C	109.5	H30B—C30—H30C	109.5
C10—C12—H12A	109.5	C29—C31—H31A	109.5
C10—C12—H12B	109.5	C29—C31—H31B	109.5
H12A—C12—H12B	109.5	H31A—C31—H31B	109.5
C10—C12—H12C	109.5	C29—C31—H31C	109.5
H12A—C12—H12C	109.5	H31A—C31—H31C	109.5
H12B—C12—H12C	109.5	H31B—C31—H31C	109.5
N2—C13—C14	113.7 (4)	N4—C32—C33	113.2 (4)
N2—C13—H13A	108.8	N4—C32—H32A	108.9
C14—C13—H13A	108.8	C33—C32—H32A	108.9
N2—C13—H13B	108.8	N4—C32—H32B	108.9
C14—C13—H13B	108.8	C33—C32—H32B	108.9
H13A—C13—H13B	107.7	H32A—C32—H32B	107.7

C15—C14—C19	117.1 (5)	C34—C33—C38	118.0 (5)
C15—C14—C13	120.4 (6)	C34—C33—C32	120.5 (5)
C19—C14—C13	122.4 (6)	C38—C33—C32	121.4 (5)
C14—C15—C16	123.0 (6)	C33—C34—C35	121.0 (6)
C14—C15—H15	118.5	C33—C34—H34	119.5
C16—C15—H15	118.5	C35—C34—H34	119.5
C17—C16—C15	118.9 (7)	C36—C35—C34	119.8 (6)
C17—C16—H16	120.6	C36—C35—H35	120.1
C15—C16—H16	120.6	C34—C35—H35	120.1
C16—C17—C18	120.4 (6)	C35—C36—C37	120.9 (6)
C16—C17—H17	119.8	C35—C36—H36	119.5
C18—C17—H17	119.8	C37—C36—H36	119.5
C17—C18—C19	120.0 (6)	C36—C37—C38	119.4 (6)
C17—C18—H18	120.0	C36—C37—H37	120.3
C19—C18—H18	120.0	C38—C37—H37	120.3
O3—C19—C18	119.8 (6)	O6—C38—C37	122.1 (5)
O3—C19—C14	119.4 (6)	O6—C38—C33	117.2 (5)
C18—C19—C14	120.7 (6)	C37—C38—C33	120.7 (5)
C1—N1—C5	118.6 (5)	C20—N3—C24	120.1 (6)
C1—N1—Cd1	125.3 (5)	C20—N3—Cd2	123.6 (5)
C5—N1—Cd1	116.1 (4)	C24—N3—Cd2	116.3 (4)
C13—N2—C8	110.9 (4)	C32—N4—C27	112.5 (4)
C13—N2—Cd1	115.4 (3)	C32—N4—Cd2	117.3 (3)
C8—N2—Cd1	109.6 (3)	C27—N4—Cd2	109.1 (3)
C13—N2—H2A	106.8	C32—N4—H4	105.7
C8—N2—H2A	106.8	C27—N4—H4	105.7
Cd1—N2—H2A	106.8	Cd2—N4—H4	105.7
C7—O1—Cd1	116.1 (4)	C26—O4—Cd2	115.8 (4)
C19—O3—H3A	109.5	C38—O6—H6A	109.5

N1—C1—C2—C3	−0.4 (15)	N3—C20—C21—C22	1.6 (10)
C1—C2—C3—C4	0.2 (17)	C20—C21—C22—C23	−2.7 (10)
C2—C3—C4—C5	−0.4 (15)	C21—C22—C23—C24	2.3 (9)
C2—C3—C4—C6	−179.3 (11)	C21—C22—C23—C25	−177.3 (7)
C3—C4—C5—N1	0.7 (10)	C22—C23—C24—N3	−0.8 (8)
C6—C4—C5—N1	179.6 (8)	C25—C23—C24—N3	178.7 (6)
C3—C4—C5—C5^{i}	179.1 (7)	C22—C23—C24—C24^{ii}	178.9 (6)
C6—C4—C5—C5^{i}	−2.0 (11)	C25—C23—C24—C24^{ii}	−1.5 (9)
C3—C4—C6—C6^{i}	177.1 (14)	C22—C23—C25—C25^{ii}	180.0 (9)
C5—C4—C6—C6^{i}	−2 (2)	C24—C23—C25—C25^{ii}	0.4 (13)
O1—C7—C8—C9	96.8 (7)	O4—C26—C27—N4	−13.5 (8)
O2—C7—C8—C9	−80.3 (7)	O5—C26—C27—N4	167.5 (6)
O1—C7—C8—N2	−25.4 (8)	O4—C26—C27—C28	110.5 (6)
O2—C7—C8—N2	157.5 (5)	O5—C26—C27—C28	−68.5 (8)
N2—C8—C9—C10	−64.3 (8)	N4—C27—C28—C29	−62.8 (6)
C7—C8—C9—C10	173.2 (6)	C26—C27—C28—C29	172.3 (5)
C8—C9—C10—C12	−63.4 (10)	C27—C28—C29—C31	167.2 (7)
C8—C9—C10—C11	171.6 (7)	C27—C28—C29—C30	−71.0 (9)

N2—C13—C14—C15	−135.5 (6)	N4—C32—C33—C34	−133.4 (5)
N2—C13—C14—C19	48.4 (8)	N4—C32—C33—C38	49.2 (6)
C19—C14—C15—C16	−0.7 (9)	C38—C33—C34—C35	−1.0 (8)
C13—C14—C15—C16	−177.0 (6)	C32—C33—C34—C35	−178.4 (5)
C14—C15—C16—C17	0.8 (10)	C33—C34—C35—C36	−1.4 (9)
C15—C16—C17—C18	−1.4 (11)	C34—C35—C36—C37	0.5 (10)
C16—C17—C18—C19	1.8 (11)	C35—C36—C37—C38	2.8 (10)
C17—C18—C19—O3	−179.0 (7)	C36—C37—C38—O6	175.8 (5)
C17—C18—C19—C14	−1.7 (10)	C36—C37—C38—C33	−5.3 (8)
C15—C14—C19—O3	178.5 (5)	C34—C33—C38—O6	−176.6 (4)
C13—C14—C19—O3	−5.3 (9)	C32—C33—C38—O6	0.7 (7)
C15—C14—C19—C18	1.1 (9)	C34—C33—C38—C37	4.4 (8)
C13—C14—C19—C18	177.4 (5)	C32—C33—C38—C37	−178.3 (5)
C2—C1—N1—C5	0.7 (10)	C21—C20—N3—C24	−0.2 (9)
C2—C1—N1—Cd1	−178.0 (6)	C21—C20—N3—Cd2	−178.8 (5)
C4—C5—N1—C1	−0.9 (8)	C23—C24—N3—C20	−0.2 (8)
C5^{i}—C5—N1—C1	−179.3 (6)	C24^{ii}—C24—N3—C20	−179.9 (6)
C4—C5—N1—Cd1	177.9 (5)	C23—C24—N3—Cd2	178.6 (4)
C5^{i}—C5—N1—Cd1	−0.5 (7)	C24^{ii}—C24—N3—Cd2	−1.2 (7)
C14—C13—N2—C8	−176.2 (5)	C33—C32—N4—C27	179.9 (4)
C14—C13—N2—Cd1	58.4 (6)	C33—C32—N4—Cd2	52.3 (5)
C9—C8—N2—C13	143.7 (5)	C28—C27—N4—C32	134.3 (5)
C7—C8—N2—C13	−94.4 (6)	C26—C27—N4—C32	−101.4 (5)
C9—C8—N2—Cd1	−87.7 (5)	C28—C27—N4—Cd2	−93.8 (4)
C7—C8—N2—Cd1	34.2 (6)	C26—C27—N4—Cd2	30.4 (5)
O2—C7—O1—Cd1	179.1 (5)	O5—C26—O4—Cd2	166.8 (6)
C8—C7—O1—Cd1	2.2 (7)	C27—C26—O4—Cd2	−12.1 (8)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6*A*···O2^{iii}	0.82	1.83	2.645 (5)	174
N4—H4···O6	0.98	2.07	2.763 (5)	126
N2—H2*A*···O3	0.98	2.09	2.795 (6)	127
O3—H3*A*···O5	0.82	2.33	2.951 (9)	133
C28—H28*A*···O4^{ii}	0.97	2.67	3.470 (7)	141

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