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# *catena*-Poly[[[(acetato-$\kappa^2O,O'$)aquacadmium(II)]-$\mu$-L-threoninato-$\kappa^3N,O:O'$] monohydrate]

M. Abila Jeba Queen,[a]*‡ K. C. Bright[b] and S. Mary Delphine[a]

[a]Department of Physics, Holy Cross College (Autonomous), Nagercoil-629004, Tamil Nadu, India, and [b]Department of Physics, St. John's College, Anchal-691306, Kerala, India. *Correspondence e-mail: jeba.abi@gmail.com

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‡ Research scholar at Manonmaniam Sundaranar University, Abishekapatti, Tirunelveli, Tamil Nadu, India.

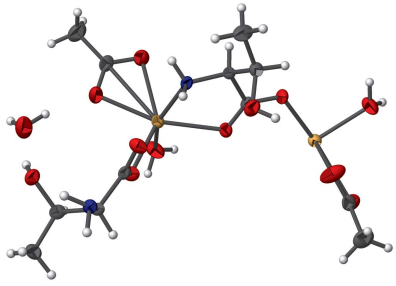
**Keywords:** crystal structure; L-threonine; cadmium acetate; hydrogen bonding.

**CCDC reference**: 1885062

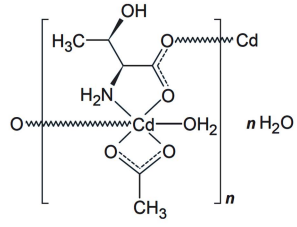
**Structural data**: full structural data are available from iucrdata.iucr.org

The title compound, $\{[Cd(C_2H_3O_2)(C_4H_8NO_3)(H_2O)]\cdot H_2O\}_n$, was synthesized from the reaction between L-threonine and cadmium acetate dihydrate. The complex consists of the $Cd^{II}$ metal ion bonded to bidentate threonine and acetate anions, and one water molecule. The carboxylate group of L-threonine bridges two metal cations related by the crystallographic screw axis parallel to [010], to form a one-dimensional polymeric structure in the crystal. The asymmetric unit is completed by one lattice water molecule, which is involved in hydrogen bonds.

**3D view**



**Chemical scheme**




## Structure description

L-threonine [IUPAC name: (2*S*,3*R*)-2-amino-3-hydroxybutanoic acid] has wide applications in industry, for example as an additive, or as a precursor for the biosynthesis of other chemicals (Dong *et al.*, 2012). On the other hand, cadmium acetate is used for glazing ceramics and pottery, in electroplating baths, in dyeing and printing textiles, and as an analytic reagent (Patnaik, 2003).

In the asymmetric unit of the title compound (Fig. 1) the Cd1—O1 bond length, 2.306 (4) Å, is in agreement with the distances reported in other cadmium acetate compounds (Vickers *et al.*, 2011). In the threonine ligand, C2—C3 [1.537 (7) Å] and C2—N1 [1.472 (6) Å] bond lengths are consistent with those reported for free L-threonine [1.532 (2) and 1.491 (2) Å, respectively; Janczak *et al.*, 1997; X-ray data at 12 K].

In the complex molecule, the $Cd^{II}$ ion is found to be in a six-coordination environment: the metal cation is coordinated by one carboxylate O atom and one amine N atom of the bidentate threonine ligand, two O atoms from the bidentate acetate ligand and one water molecule. Finally, one carboxylate O atom of the threonine ligand forms a bridge with a symmetry-related metal ion, completing the coordination sphere of the metal, and giving

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O5—H5···O7$^{i}$ | 0.82 | 1.90 | 2.701 (6) | 164 |
| N1—H1$A$···O4$^{ii}$ | 0.89 (3) | 2.21 (3) | 3.083 (5) | 170 (5) |
| N1—H1$B$···O3$^{iii}$ | 0.89 (3) | 2.28 (4) | 2.983 (5) | 136 (4) |
| O6—H6$D$···O5$^{i}$ | 0.89 (3) | 1.86 (3) | 2.753 (5) | 175 (6) |
| O6—H6$E$···O2$^{iv}$ | 0.88 (3) | 1.80 (3) | 2.676 (6) | 174 (7) |
| O7—H7$A$···O1 | 0.89 (3) | 1.84 (4) | 2.707 (6) | 163 (9) |
| O7—H7$B$···O6$^{v}$ | 0.88 (3) | 2.46 (5) | 3.290 (7) | 157 (9) |

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

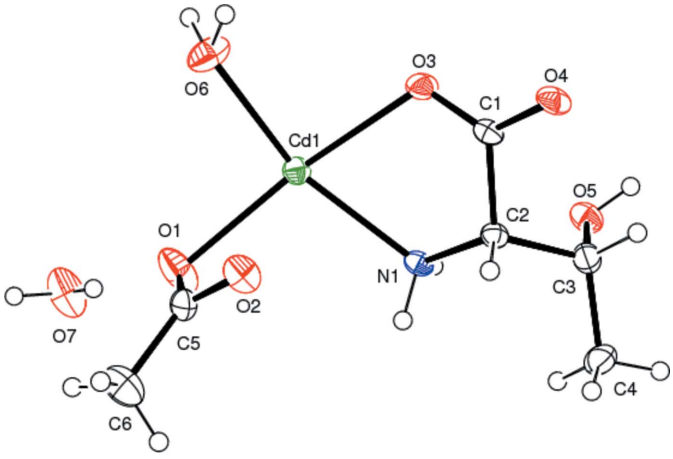



**Figure 1**
The asymmetric unit of the title complex, with displacement ellipsoids for non-H atoms at the 50% probability level.

a polymeric crystal structure along the [010] direction (Fig. 2). The O—Cd—O bond angles range from 53.95 (14) to 162.36 (14)°.

In the crystal structure, hydrogen bonds are formed, with all N—H and O—H groups from the L-threonine and water molecules serving as donor groups (Table 1), affording a layered supramolecular structure extending parallel to the [010] plane (Fig. 3).

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[Cd(C_2H_3O_2)(C_4H_8NO_3)(H_2O)]\cdot H_2O$ |
| $M_r$ | 325.59 |
| Crystal system, space group | Monoclinic, $P2_1$ |
| Temperature (K) | 293 |
| $a, b, c$ (Å) | 5.8199 (12), 8.8017 (16), 10.710 (2) |
| $\beta$ (°) | 91.916 (6) |
| $V$ (Å$^3$) | 548.30 (18) |
| $Z$ | 2 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 2.01 |
| Crystal size (mm) | 0.20 × 0.15 × 0.10 |
| | |
| Data collection | |
| Diffractometer | Bruker Kappa APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2004) |
| $T_{min}$, $T_{max}$ | 0.593, 0.746 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 4756, 2373, 2215 |
| $R_{int}$ | 0.027 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.639 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.021, 0.048, 1.06 |
| No. of reflections | 2373 |
| No. of parameters | 162 |
| No. of restraints | 7 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.29, −0.44 |
| Absolute structure | Flack $x$ determined using 960 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013) |
| Absolute structure parameter | −0.02 (2) |

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008).

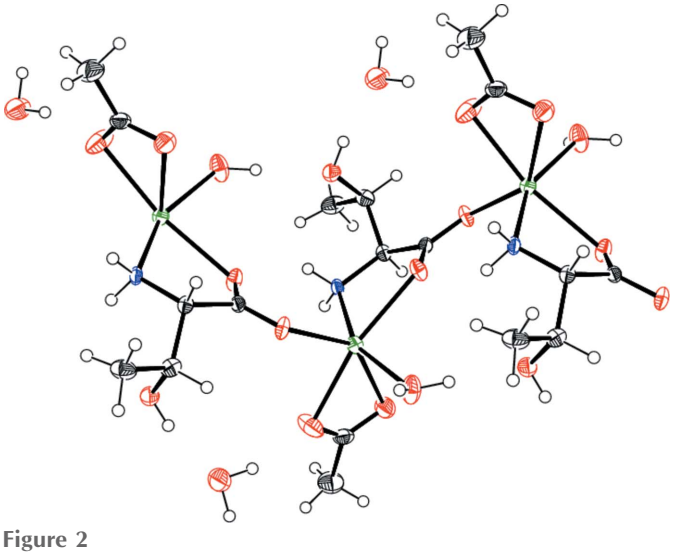


**Figure 2**
The polymeric structure of the title compound.

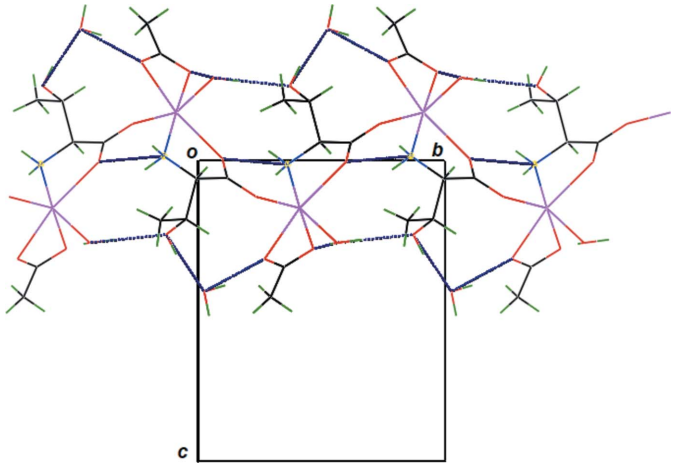



**Figure 3**
Packing diagram of the title complex viewed down the *a* axis, showing one polymeric chain forming hydrogen bonds (dashed blue lines) with lattice water molecules.

## Synthesis and crystallization

Crystals of the title compound were prepared by adding L-threonine to an aqueous solution of cadmium acetate dihydrate in a stoichiometric ratio. Good quality single crystals were grown by repeated crystallization of an aqueous solution of the complex, at room temperature, over several weeks.

## Refinement

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

## Acknowledgements

We are grateful to the SAIF, IIT Madras, for use of the X-ray data collection facility.

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# full crystallographic data

*IUCrData* (2018). **3**, x181770 [https://doi.org/10.1107/S2414314618017704]

## *catena*-Poly[[[(acetato-$\kappa^2O,O'$)aquacadmium(II)]-$\mu$-L-threoninato-$\kappa^3N,O:O'$] monohydrate]

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***catena*-Poly[[[(acetato-$\kappa^2O,O'$)aquacadmium(II)]-$\mu$-*L*-threoninato-$\kappa^3N,O:O'$] monohydrate]**

*Crystal data*

$[Cd(C_2H_3O_2)(C_4H_8NO_3)(H_2O)]\cdot H_2O$
$M_r$ = 325.59
Monoclinic, $P2_1$
$a$ = 5.8199 (12) Å
$b$ = 8.8017 (16) Å
$c$ = 10.710 (2) Å
$\beta$ = 91.916 (6)°
$V$ = 548.30 (18) Å$^3$
$Z$ = 2
$F(000)$ = 324
$D_x$ = 1.972 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2960 reflections
$\theta$ = 3.0–30.4°
$\mu$ = 2.01 mm$^{-1}$
$T$ = 293 K
Block, colourless
0.20 × 0.15 × 0.10 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
$T_{min}$ = 0.593, $T_{max}$ = 0.746
4756 measured reflections
2373 independent reflections
2215 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027
$\theta_{max}$ = 27.0°, $\theta_{min}$ = 3.0°
$h$ = −4→7
$k$ = −10→11
$l$ = −13→13

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.048
$S$ = 1.06
2373 reflections
162 parameters
7 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0151P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.43 e Å$^{-3}$
Absolute structure: Flack $x$ determined using 960 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.02 (2)

*Special details*

**Refinement**. The atomic positions of H atoms bonded to C atoms and hydroxyl atom O5 were calculated, and these H atoms were refined as riding to their parent atoms, with an isotropic displacement parameter calculated as $U_{iso}$ = 1.2–1.5$U_{eq}$(carrier atom). Water and amine H atoms were located in difference maps and refined freely. For these H atoms, N—H and O—H bond lengths were restrained to 0.90 (2) Å.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.1873 (8) | 0.6187 (5) | −0.0589 (4) | 0.0198 (10) |
| C2 | 0.3744 (8) | 0.4946 (5) | −0.0609 (4) | 0.0195 (10) |
| H2 | 0.5147 | 0.5378 | −0.0222 | 0.023* |
| C3 | 0.4290 (8) | 0.4515 (5) | −0.1958 (5) | 0.0259 (13) |
| H3 | 0.4545 | 0.5438 | −0.2446 | 0.031* |
| C4 | 0.6394 (9) | 0.3493 (7) | −0.2005 (5) | 0.0341 (13) |
| H4A | 0.6058 | 0.2529 | −0.1633 | 0.051* |
| H4B | 0.7657 | 0.3962 | −0.1552 | 0.051* |
| H4C | 0.6794 | 0.3344 | −0.2859 | 0.051* |
| C5 | 0.3471 (10) | 0.3480 (7) | 0.3548 (5) | 0.0285 (12) |
| C6 | 0.5144 (12) | 0.2946 (8) | 0.4545 (6) | 0.0476 (16) |
| H6A | 0.4398 | 0.2238 | 0.5080 | 0.071* |
| H6B | 0.5688 | 0.3799 | 0.5028 | 0.071* |
| H6C | 0.6420 | 0.2457 | 0.4166 | 0.071* |
| N1 | 0.3104 (7) | 0.3621 (4) | 0.0142 (4) | 0.0198 (9) |
| O1 | 0.1723 (8) | 0.2697 (5) | 0.3282 (4) | 0.0481 (12) |
| O2 | 0.3858 (7) | 0.4672 (5) | 0.2946 (4) | 0.0353 (10) |
| O3 | 0.0128 (6) | 0.5995 (4) | 0.0047 (4) | 0.0272 (8) |
| O4 | 0.2300 (6) | 0.7358 (4) | −0.1214 (3) | 0.0265 (8) |
| O5 | 0.2331 (6) | 0.3716 (3) | −0.2470 (3) | 0.0285 (9) |
| H5 | 0.1896 | 0.4121 | −0.3125 | 0.043* |
| O6 | −0.1803 (7) | 0.5625 (5) | 0.2746 (4) | 0.0394 (10) |
| O7 | −0.0219 (9) | 0.0255 (6) | 0.4365 (4) | 0.0514 (12) |
| Cd1 | 0.04345 (4) | 0.41168 (6) | 0.15898 (3) | 0.02231 (10) |
| H1A | 0.432 (6) | 0.316 (6) | 0.048 (4) | 0.022 (14)* |
| H1B | 0.253 (8) | 0.286 (4) | −0.031 (4) | 0.007 (12)* |
| H6D | −0.189 (11) | 0.663 (3) | 0.264 (6) | 0.05 (2)* |
| H6E | −0.326 (6) | 0.537 (8) | 0.278 (6) | 0.06 (2)* |
| H7A | 0.052 (16) | 0.110 (7) | 0.416 (8) | 0.10 (3)* |
| H7B | −0.009 (18) | 0.045 (10) | 0.517 (3) | 0.09 (3)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.023 (2) | 0.015 (2) | 0.021 (2) | 0.0010 (19) | −0.0055 (19) | −0.0012 (19) |
| C2 | 0.018 (2) | 0.017 (2) | 0.023 (2) | −0.0004 (19) | −0.0003 (19) | 0.002 (2) |
| C3 | 0.025 (2) | 0.029 (4) | 0.024 (2) | −0.0021 (18) | −0.0003 (18) | 0.0040 (19) |
| C4 | 0.028 (3) | 0.048 (3) | 0.027 (3) | 0.009 (2) | 0.003 (2) | −0.006 (2) |
| C5 | 0.034 (3) | 0.034 (3) | 0.018 (3) | 0.006 (2) | 0.001 (2) | −0.001 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6 | 0.049 (4) | 0.053 (4) | 0.039 (3) | 0.001 (3) | −0.015 (3) | 0.004 (3) |
| N1 | 0.023 (2) | 0.012 (2) | 0.024 (2) | 0.0013 (15) | −0.0024 (17) | 0.0017 (16) |
| O1 | 0.044 (2) | 0.053 (3) | 0.046 (2) | −0.020 (2) | −0.017 (2) | 0.025 (2) |
| O2 | 0.036 (2) | 0.033 (2) | 0.036 (2) | −0.0059 (17) | −0.006 (2) | 0.0043 (19) |
| O3 | 0.0255 (17) | 0.0204 (17) | 0.0359 (19) | 0.0047 (16) | 0.0052 (15) | 0.0076 (16) |
| O4 | 0.0274 (18) | 0.0158 (17) | 0.036 (2) | 0.0014 (14) | −0.0011 (16) | 0.0077 (15) |
| O5 | 0.0328 (17) | 0.025 (3) | 0.0270 (17) | 0.0011 (14) | −0.0069 (14) | −0.0011 (13) |
| O6 | 0.034 (2) | 0.027 (2) | 0.058 (3) | −0.0007 (18) | 0.017 (2) | −0.006 (2) |
| O7 | 0.069 (3) | 0.043 (3) | 0.041 (3) | −0.021 (2) | −0.014 (2) | 0.006 (2) |
| Cd1 | 0.02215 (14) | 0.02029 (16) | 0.02456 (16) | −0.0006 (2) | 0.00159 (10) | 0.0020 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—O3 | 1.252 (6) | C6—H6B | 0.9600 |
| C1—O4 | 1.259 (6) | C6—H6C | 0.9600 |
| C1—C2 | 1.543 (6) | N1—Cd1 | 2.274 (4) |
| C2—N1 | 1.472 (6) | N1—H1A | 0.89 (3) |
| C2—C3 | 1.537 (7) | N1—H1B | 0.89 (3) |
| C2—H2 | 0.9800 | O1—Cd1 | 2.306 (4) |
| C3—O5 | 1.432 (6) | O2—Cd1 | 2.475 (4) |
| C3—C4 | 1.521 (7) | O3—Cd1 | 2.340 (3) |
| C3—H3 | 0.9800 | O4—Cd1$^{i}$ | 2.247 (3) |
| C4—H4A | 0.9600 | O5—H5 | 0.8200 |
| C4—H4B | 0.9600 | O6—Cd1 | 2.258 (4) |
| C4—H4C | 0.9600 | O6—H6D | 0.89 (3) |
| C5—O1 | 1.254 (7) | O6—H6E | 0.88 (3) |
| C5—O2 | 1.255 (6) | O7—H7A | 0.89 (3) |
| C5—C6 | 1.497 (8) | O7—H7B | 0.88 (3) |
| C5—Cd1 | 2.755 (6) | Cd1—O4$^{ii}$ | 2.247 (3) |
| C6—H6A | 0.9600 | | |

| | | | |
|---|---|---|---|
| O3—C1—O4 | 125.3 (4) | Cd1—N1—H1A | 111 (3) |
| O3—C1—C2 | 119.9 (4) | C2—N1—H1B | 113 (3) |
| O4—C1—C2 | 114.8 (4) | Cd1—N1—H1B | 105 (3) |
| N1—C2—C3 | 112.4 (4) | H1A—N1—H1B | 99 (4) |
| N1—C2—C1 | 111.2 (4) | C5—O1—Cd1 | 96.9 (3) |
| C3—C2—C1 | 110.9 (4) | C5—O2—Cd1 | 88.9 (4) |
| N1—C2—H2 | 107.4 | C1—O3—Cd1 | 115.8 (3) |
| C3—C2—H2 | 107.4 | C1—O4—Cd1$^{i}$ | 120.6 (3) |
| C1—C2—H2 | 107.4 | C3—O5—H5 | 109.5 |
| O5—C3—C4 | 109.2 (4) | Cd1—O6—H6D | 123 (4) |
| O5—C3—C2 | 107.1 (4) | Cd1—O6—H6E | 117 (5) |
| C4—C3—C2 | 111.6 (4) | H6D—O6—H6E | 102 (6) |
| O5—C3—H3 | 109.6 | H7A—O7—H7B | 93 (8) |
| C4—C3—H3 | 109.6 | O4$^{ii}$—Cd1—O6 | 94.90 (13) |
| C2—C3—H3 | 109.6 | O4$^{ii}$—Cd1—N1 | 103.98 (13) |
| C3—C4—H4A | 109.5 | O6—Cd1—N1 | 155.03 (14) |
| C3—C4—H4B | 109.5 | O4$^{ii}$—Cd1—O1 | 88.69 (14) |

| | | | |
|---|---|---|---|
| H4A—C4—H4B | 109.5 | O6—Cd1—O1 | 93.77 (18) |
| C3—C4—H4C | 109.5 | N1—Cd1—O1 | 102.74 (15) |
| H4A—C4—H4C | 109.5 | O4$^{ii}$—Cd1—O3 | 108.86 (13) |
| H4B—C4—H4C | 109.5 | O6—Cd1—O3 | 86.58 (15) |
| O1—C5—O2 | 120.1 (5) | N1—Cd1—O3 | 72.03 (13) |
| O1—C5—C6 | 119.5 (5) | O1—Cd1—O3 | 162.36 (14) |
| O2—C5—C6 | 120.4 (6) | O4$^{ii}$—Cd1—O2 | 142.44 (13) |
| O1—C5—Cd1 | 56.2 (3) | O6—Cd1—O2 | 91.69 (16) |
| O2—C5—Cd1 | 64.0 (3) | N1—Cd1—O2 | 83.30 (14) |
| C6—C5—Cd1 | 173.0 (4) | O1—Cd1—O2 | 53.95 (14) |
| C5—C6—H6A | 109.5 | O3—Cd1—O2 | 108.42 (13) |
| C5—C6—H6B | 109.5 | O4$^{ii}$—Cd1—C5 | 115.40 (16) |
| H6A—C6—H6B | 109.5 | O6—Cd1—C5 | 93.96 (18) |
| C5—C6—H6C | 109.5 | N1—Cd1—C5 | 92.56 (15) |
| H6A—C6—H6C | 109.5 | O1—Cd1—C5 | 26.87 (15) |
| H6B—C6—H6C | 109.5 | O3—Cd1—C5 | 135.49 (16) |
| C2—N1—Cd1 | 114.3 (3) | O2—Cd1—C5 | 27.10 (14) |
| C2—N1—H1A | 112 (3) | | |

| | | | |
|---|---|---|---|
| O3—C1—C2—N1 | 1.9 (6) | C1—C2—N1—Cd1 | −21.0 (5) |
| O4—C1—C2—N1 | −179.9 (4) | O2—C5—O1—Cd1 | 3.6 (5) |
| O3—C1—C2—C3 | 127.8 (5) | C6—C5—O1—Cd1 | −173.5 (5) |
| O4—C1—C2—C3 | −54.1 (5) | O1—C5—O2—Cd1 | −3.3 (5) |
| N1—C2—C3—O5 | 55.2 (5) | C6—C5—O2—Cd1 | 173.8 (5) |
| C1—C2—C3—O5 | −70.0 (5) | O4—C1—O3—Cd1 | −160.1 (4) |
| N1—C2—C3—C4 | −64.3 (5) | C2—C1—O3—Cd1 | 17.8 (5) |
| C1—C2—C3—C4 | 170.5 (4) | O3—C1—O4—Cd1$^{i}$ | −12.8 (7) |
| C3—C2—N1—Cd1 | −146.0 (3) | C2—C1—O4—Cd1$^{i}$ | 169.2 (3) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O5—H5···O7$^{i}$ | 0.82 | 1.90 | 2.701 (6) | 164 |
| N1—H1*A*···O4$^{iii}$ | 0.89 (3) | 2.21 (3) | 3.083 (5) | 170 (5) |
| N1—H1*B*···O3$^{ii}$ | 0.89 (3) | 2.28 (4) | 2.983 (5) | 136 (4) |
| O6—H6*D*···O5$^{i}$ | 0.89 (3) | 1.86 (3) | 2.753 (5) | 175 (6) |
| O6—H6*E*···O2$^{iv}$ | 0.88 (3) | 1.80 (3) | 2.676 (6) | 174 (7) |
| O7—H7*A*···O1 | 0.89 (3) | 1.84 (4) | 2.707 (6) | 163 (9) |
| O7—H7*B*···O6$^{v}$ | 0.88 (3) | 2.46 (5) | 3.290 (7) | 157 (9) |

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