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Poly[[hexaaquabis(μ_3-pyrimidine-4,6-dicarboxylato)dicalcium] dihydrate]

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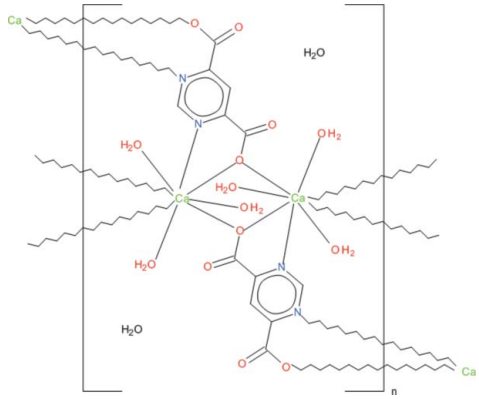
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.107; data-to-parameter ratio = 16.5.

The polymeric structure of the title compound, {[$Ca_2(C_6H_2N_2O_4)_2(H_2O)_6$]·$2H_2O$}$_n$, is built up of molecular layers composed of Ca^{II} ions bridged by both ligand N and O atoms with one of the O atoms being bis-monodentate. Two adjacent Ca^{II} ions are bridged by these O atoms, forming a centrosymmetric dimer which is the building unit of the structure. The dimers are nodes of a cross-linked molecular layer parallel to (101). The Ca^{II} ion is coordinated by two bidentate ligands, one monodentate ligand and three water molecules in the form of a distorted polyhedron with a coordination number of eight. Solvate water molecules located between adjacent layers participate as donors and acceptors in a system of hydrogen bonds in which coordinating water molecules also act as donors and non-coordinating carboxylate O atoms act as acceptors.

Related literature

For the crystal structures of Ca^{II} complexes with pyrazine-2,6-dicarboxylate and water ligands, see: Starosta *et al.* (2003, 2004). The crystal structure of pyrimidine-4,6-dicarboxylic acid dihydrate was reported by Beobide *et al.* (2007).



Experimental

Crystal data

$[Ca_2(C_6H_2N_2O_4)_2(H_2O)_6]\cdot 2H_2O$
M_r = 278.24
Monoclinic, $P2_1/n$
a = 7.7053 (15) Å
b = 11.432 (2) Å
c = 11.916 (2) Å
β = 92.16 (3)°
V = 1048.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.64 mm^{-1}
T = 293 K
0.10 × 0.04 × 0.03 mm

Data collection

Kuma KM-4 four-circle diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2008)
T_{min} = 0.968, T_{max} = 0.982
3274 measured reflections
3065 independent reflections
1709 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
3 standard reflections every 200 reflections
intensity decay: 2.9%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.107
S = 1.01
3065 reflections
186 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ca1—O5	2.398 (2)	Ca1—O6	2.502 (2)
Ca1—O7	2.420 (2)	Ca1—O1	2.5061 (17)
Ca1—O3^{i}	2.4361 (17)	Ca1—N1	2.563 (2)
Ca1—O1^{ii}	2.4823 (16)	Ca1—N3^{i}	2.6133 (19)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H72···O2^{iii}	0.80 (6)	2.34 (6)	3.048 (3)	149 (6)
O6—H61···O2^{ii}	0.85 (5)	1.88 (5)	2.698 (3)	163 (5)
O8—H81···O3^{iv}	0.76 (4)	2.04 (4)	2.793 (3)	170 (4)
O8—H82···O6^{v}	0.77 (5)	2.09 (5)	2.818 (3)	157 (5)
O5—H52···O8^{vi}	0.87 (4)	1.94 (4)	2.798 (3)	169 (4)
O6—H62···O4^{iii}	0.77 (4)	1.96 (4)	2.719 (2)	167 (4)
O7—H71···O4^{vii}	0.79 (4)	2.16 (4)	2.902 (3)	158 (3)
O5—H51···O8^{iv}	0.78 (4)	2.04 (4)	2.816 (3)	176 (4)

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

Data collection: *KM-4 Software* (Kuma, 1996); cell refinement: *KM-4 Software*; data reduction: *DATAPROC* (Kuma, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QM2088).

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Starosta, W., Ptasiewicz-Bąk, H. & Leciejewicz, J. (2004). *J. Coord. Chem.* **57**, 167–173.

supporting information

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Poly[[hexaaquabis(μ_3-pyrimidine-4,6-dicarboxylato)dicalcium] dihydrate]

Wojciech Starosta and Janusz Leciejewicz

S1. Comment

The asymmetric unit of the title compound contains one Ca^{II} ion, one fully deprotonated pyrimidine-4,6-diarboxylate ligand molecule, three water molecules coordinated to the metal ion and one solvation water molecule. The ligand molecule acts in μ_3 mode and bridges Ca^{II} ions using monodentate N and O atoms and another O atom which is bidentate. One of the O atoms in the carboxylate groups remains uncoordinated. Ca1 and $Ca1^{ii}$ ions are related by an inversion centre and bridged by bidentate carboxylato O1 and $O1^{ii}$ atoms to form a dimeric moiety (Fig.1). Due to the bridging action of the ligands the dimers are the nodes of a cross-linked two dimensional molecular network. The structure of the title compound can be thus visualized as built of molecular layers parallel to the crystal (101) plane (Fig.2). Solvation water molecules are located between adjacent layers. The Ca^{II} ion has a distorted eight coordinate geometry. The observed Ca—N and Ca—O bond distances are typical (Table 1). The pyrimidine ring is planar with an r.m.s. of 0.0079 (2) Å; carboxylate groups C7/O1/O2 and C8/O3/O4 make dihedral angles with the plane of 9.7 (1)° and 8.9 (1)°, respectively. Bond distances and bond angles within the pyrimidine ring do not differ from those reported for the parent acid (Beobide, *et al.*, 2007). In a system of hydrogen bonds, which is responsible for structure stability, solvation and coordinated water molecules act as donors and as acceptors and coordination inactive carboxylato O atoms act as acceptors (Table 2). Centro-symmetric dimeric units in which two Ca^{II}ions are bridged by ligand bidentate carboxylato O atoms have been also observed in the structures of complexes with pyrazine-2,6-dicarboxylate and water ligands. In all, dimeric units bridged by pairs of coordinated aqua O atoms form "ladder" type molecular ribbons (Starosta, *et al.*, 2003, 2004).

S2. Experimental

An aqueous solution containing 1 mmol of calcium acetate hydrate and 1 mmol of pyrimidine-4,6-diarboxylic acid dihydrate was refluxed with constant stirring for 6 h. After cooling to room temperature, the solution was left to evaporate. Well formed single-crystal blocks appeared overnight at the bottom of the reaction pot. They were separated from the mother liquid, washed with cold water and dried in air.

S3. Refinement

Hydrogen atoms attached to water molecules were located in a difference map and refined isotropically, while two H atoms attached to pyrimidine C atoms were located at a calculated positions and treated as riding on the parent atoms with C—H=0.93 Å and

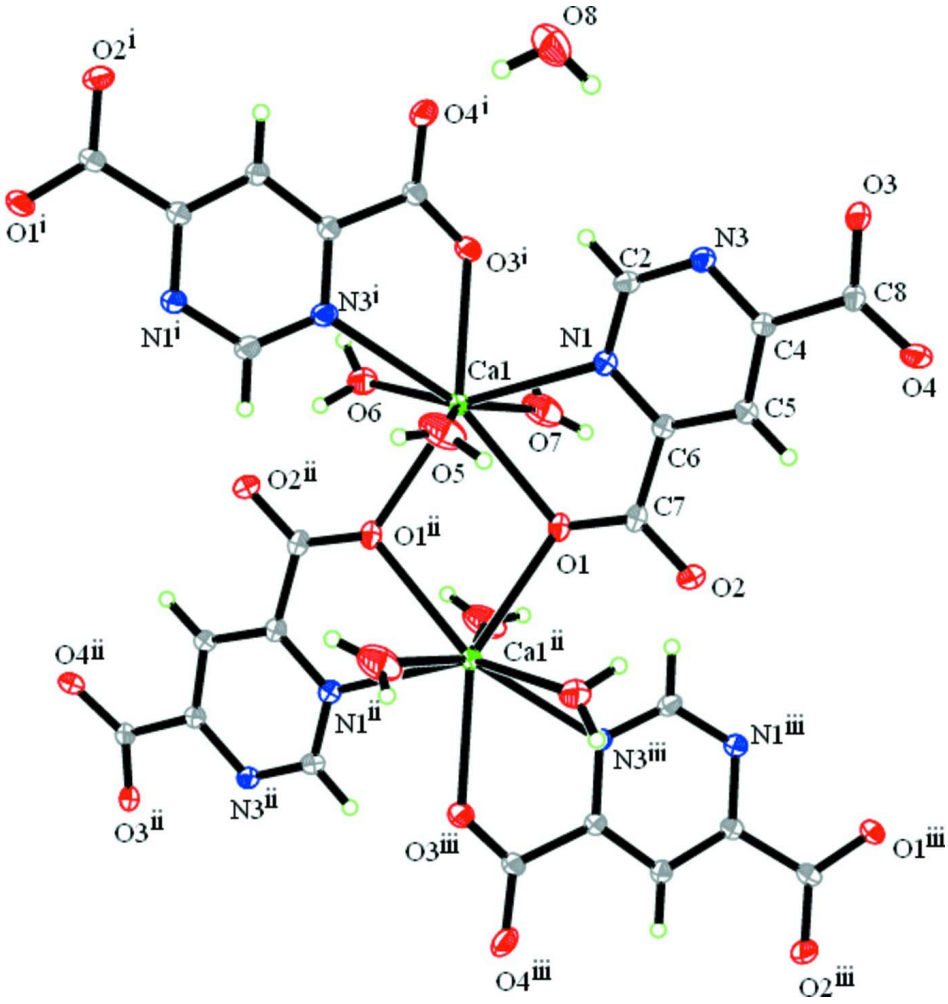

Figure 1

A fragment of the molecular layer showing a dimeric moiety with atom labelling scheme and 50% probability displacement ellipsoids. Symmetry code: [i] -*x* + 1/2, *y* - 1/2, -*z* + 3/2; [ii] -*x*, -*y*,-*z* + 1; [iii] *x* - 1/2, -*y* + 1/2, *z* + 1/2.

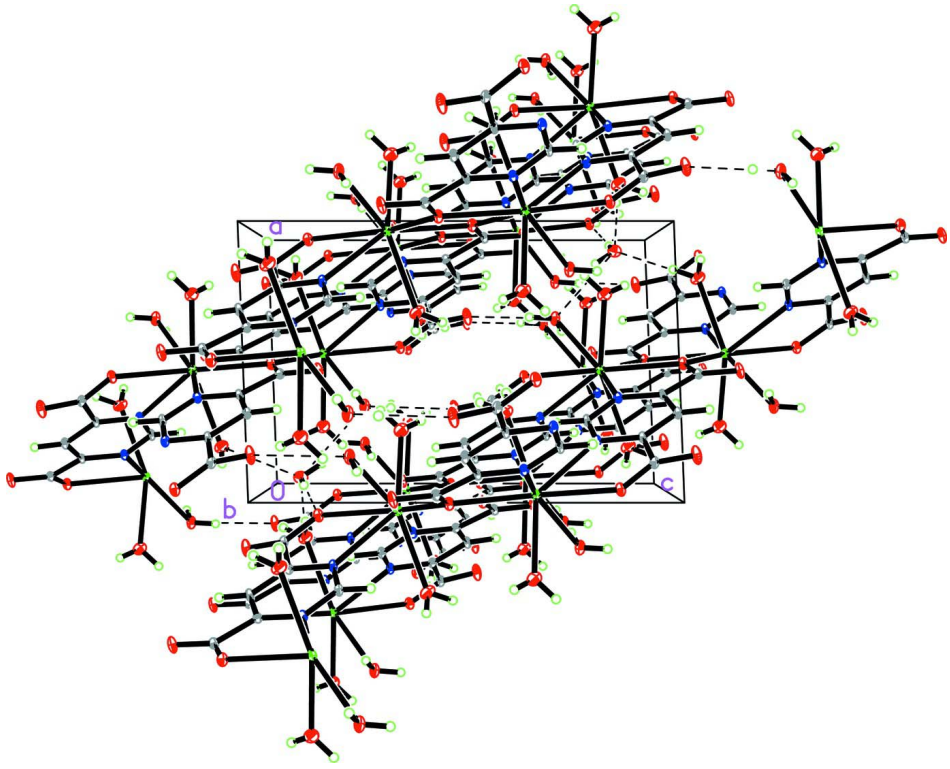

Figure 2

The alignment of molecular layers in the structure of a Ca^{II} complex with pyrimidine-4,6-carboxylate and water ligands viewed along [010].

Poly[[hexaaquabis(μ_3-pyrimidine-4,6-dicarboxylato)dicalcium] dihydrate]

Crystal data

$[Ca_2(C_6H_2N_2O_4)_2(H_2O)_6]\cdot 2H_2O$
$M_r = 278.24$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.7053$ (15) Å
$b = 11.432$ (2) Å
$c = 11.916$ (2) Å
$\beta = 92.16$ (3)°
$V = 1048.9$ (4) Å^3
$Z = 4$
$F(000) = 576$
$D_x = 1.762$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 6$–15°
$\mu = 0.64$ mm^{-1}
$T = 293$ K
Blocks, colourless
0.10 × 0.04 × 0.03 mm

Data collection

Kuma KM-4 four-circle diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
profile data from $\omega/2\theta$ scans
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2008)
$T_{min} = 0.968$, $T_{max} = 0.982$
3274 measured reflections
3065 independent reflections
1709 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 30.1°$, $\theta_{min} = 2.5°$
$h = 0\rightarrow 10$
$k = -16\rightarrow 0$
$l = -16\rightarrow 16$
3 standard reflections every 200 reflections
intensity decay: 2.9%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.107$
$S = 1.01$
3065 reflections
186 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0572P)^2 + 0.0532P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.
Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ca1	0.03092 (6)	0.05117 (4)	0.65920 (3)	0.01409 (11)
O1	0.0060 (2)	0.12495 (14)	0.46120 (13)	0.0195 (3)
O2	0.0320 (3)	0.27178 (16)	0.33877 (13)	0.0261 (4)
N1	0.1313 (3)	0.26241 (16)	0.63011 (14)	0.0163 (4)
C6	0.1190 (3)	0.30679 (18)	0.52650 (17)	0.0148 (4)
C5	0.1834 (3)	0.41685 (18)	0.50185 (18)	0.0174 (4)
H5	0.1705	0.4487	0.4302	0.021*
C7	0.0438 (3)	0.22887 (19)	0.43434 (18)	0.0165 (4)
O4	0.3231 (3)	0.64500 (15)	0.48018 (14)	0.0313 (5)
O7	−0.2529 (3)	0.14194 (19)	0.6459 (2)	0.0342 (5)
O6	−0.1678 (3)	−0.08219 (17)	0.76038 (16)	0.0267 (4)
N3	0.2839 (3)	0.43217 (16)	0.69222 (14)	0.0169 (4)
O5	0.3228 (3)	0.0407 (2)	0.59679 (18)	0.0348 (5)
C2	0.2132 (3)	0.32771 (19)	0.70832 (18)	0.0180 (4)
H2	0.2216	0.2974	0.7807	0.022*
C4	0.2679 (3)	0.47703 (19)	0.58880 (17)	0.0152 (4)
C8	0.3517 (3)	0.59611 (18)	0.57191 (18)	0.0170 (4)
O8	0.9331 (3)	0.35726 (19)	0.89833 (19)	0.0303 (4)
H51	0.390 (5)	−0.010 (4)	0.601 (3)	0.047 (11)*
O3	0.4436 (2)	0.63449 (14)	0.65273 (13)	0.0199 (3)
H71	−0.285 (4)	0.187 (3)	0.600 (3)	0.031 (9)*
H62	−0.174 (5)	−0.090 (3)	0.824 (3)	0.038 (10)*
H52	0.358 (5)	0.081 (4)	0.540 (3)	0.055 (12)*
H82	0.882 (6)	0.384 (5)	0.847 (4)	0.076 (16)*

H81	0.957 (5)	0.293 (3)	0.888 (3)	0.036 (9)*
H61	−0.120 (6)	−0.146 (4)	0.743 (4)	0.081 (16)*
H72	−0.324 (8)	0.138 (5)	0.693 (5)	0.10 (2)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.0198 (2)	0.01036 (17)	0.01203 (17)	−0.00052 (18)	−0.00070 (13)	−0.00012 (16)
O1	0.0290 (9)	0.0126 (7)	0.0168 (7)	−0.0043 (6)	−0.0002 (6)	−0.0028 (6)
O2	0.0448 (10)	0.0193 (8)	0.0135 (7)	−0.0052 (8)	−0.0076 (7)	0.0006 (6)
N1	0.0223 (9)	0.0135 (8)	0.0131 (8)	−0.0017 (7)	−0.0013 (7)	−0.0006 (7)
C6	0.0180 (10)	0.0128 (9)	0.0135 (9)	−0.0005 (8)	−0.0010 (8)	−0.0012 (7)
C5	0.0266 (11)	0.0124 (9)	0.0130 (8)	−0.0024 (8)	−0.0019 (8)	0.0011 (7)
C7	0.0205 (10)	0.0135 (9)	0.0155 (9)	−0.0016 (8)	−0.0009 (8)	−0.0038 (8)
O4	0.0595 (14)	0.0183 (8)	0.0154 (8)	−0.0108 (9)	−0.0070 (8)	0.0064 (6)
O7	0.0323 (11)	0.0327 (11)	0.0378 (11)	0.0116 (9)	0.0063 (9)	0.0124 (9)
O6	0.0394 (11)	0.0236 (9)	0.0172 (8)	−0.0052 (8)	0.0030 (8)	0.0011 (7)
N3	0.0241 (9)	0.0149 (9)	0.0117 (7)	−0.0054 (7)	0.0003 (7)	0.0005 (6)
O5	0.0301 (10)	0.0360 (12)	0.0389 (11)	0.0114 (9)	0.0109 (8)	0.0158 (9)
C2	0.0264 (12)	0.0164 (10)	0.0112 (8)	−0.0030 (9)	−0.0013 (8)	0.0013 (8)
C4	0.0206 (10)	0.0123 (9)	0.0125 (9)	−0.0006 (8)	0.0001 (8)	−0.0001 (7)
C8	0.0257 (12)	0.0116 (9)	0.0136 (9)	−0.0029 (9)	0.0013 (8)	−0.0012 (7)
O8	0.0296 (10)	0.0219 (10)	0.0392 (11)	0.0042 (8)	0.0005 (8)	−0.0076 (8)
O3	0.0298 (9)	0.0132 (7)	0.0164 (7)	−0.0064 (7)	−0.0026 (6)	−0.0015 (6)

Geometric parameters (Å, º)

Ca1—O5	2.398 (2)	C5—H5	0.9300
Ca1—O7	2.420 (2)	O4—C8	1.240 (3)
Ca1—O3^{i}	2.4361 (17)	O7—H71	0.79 (4)
Ca1—O1^{ii}	2.4823 (16)	O7—H72	0.80 (6)
Ca1—O6	2.502 (2)	O6—H62	0.77 (4)
Ca1—O1	2.5061 (17)	O6—H61	0.85 (5)
Ca1—N1	2.563 (2)	N3—C2	1.330 (3)
Ca1—N3^{i}	2.6133 (19)	N3—C4	1.336 (3)
Ca1—Ca1^{ii}	3.9817 (11)	N3—Ca1^{iii}	2.6133 (19)
Ca1—H61	2.74 (5)	O5—H51	0.78 (4)
O1—C7	1.267 (3)	O5—H52	0.87 (4)
O1—Ca1^{ii}	2.4823 (16)	C2—H2	0.9300
O2—C7	1.240 (3)	C4—C8	1.523 (3)
N1—C2	1.334 (3)	C8—O3	1.253 (3)
N1—C6	1.335 (3)	O8—H82	0.77 (5)
C6—C5	1.388 (3)	O8—H81	0.76 (4)
C6—C7	1.512 (3)	O3—Ca1^{iii}	2.4361 (17)
C5—C4	1.385 (3)		
O5—Ca1—O7	148.95 (7)	N1—Ca1—H61	163.4 (11)
O5—Ca1—O3^{i}	105.11 (8)	N3^{i}—Ca1—H61	63.5 (11)

O7—Ca1—O3^{i}	86.21 (7)	Ca1^{ii}—Ca1—H61	93.9 (11)
O5—Ca1—O1^{ii}	82.45 (7)	C7—O1—Ca1^{ii}	129.56 (14)
O7—Ca1—O1^{ii}	103.09 (7)	C7—O1—Ca1	122.89 (13)
O3^{i}—Ca1—O1^{ii}	148.46 (6)	Ca1^{ii}—O1—Ca1	105.91 (6)
O5—Ca1—O6	135.80 (7)	C2—N1—C6	116.67 (19)
O7—Ca1—O6	74.03 (7)	C2—N1—Ca1	124.75 (14)
O3^{i}—Ca1—O6	79.90 (6)	C6—N1—Ca1	118.15 (14)
O1^{ii}—Ca1—O6	74.06 (6)	N1—C6—C5	121.77 (19)
O5—Ca1—O1	76.37 (7)	N1—C6—C7	117.37 (19)
O7—Ca1—O1	75.95 (7)	C5—C6—C7	120.70 (19)
O3^{i}—Ca1—O1	137.32 (5)	C4—C5—C6	116.97 (19)
O1^{ii}—Ca1—O1	74.09 (6)	C4—C5—H5	121.5
O6—Ca1—O1	129.21 (6)	C6—C5—H5	121.5
O5—Ca1—N1	73.37 (7)	O2—C7—O1	126.4 (2)
O7—Ca1—N1	82.17 (7)	O2—C7—C6	116.52 (19)
O3^{i}—Ca1—N1	75.03 (6)	O1—C7—C6	117.02 (19)
O1^{ii}—Ca1—N1	135.61 (6)	Ca1—O7—H71	126 (2)
O6—Ca1—N1	146.35 (7)	Ca1—O7—H72	125 (4)
O1—Ca1—N1	64.43 (5)	H71—O7—H72	109 (5)
O5—Ca1—N3^{i}	71.93 (7)	Ca1—O6—H62	127 (3)
O7—Ca1—N3^{i}	137.41 (7)	Ca1—O6—H61	97 (3)
O3^{i}—Ca1—N3^{i}	63.72 (6)	H62—O6—H61	101 (4)
O1^{ii}—Ca1—N3^{i}	90.98 (6)	C2—N3—C4	116.97 (18)
O6—Ca1—N3^{i}	71.62 (7)	C2—N3—Ca1^{iii}	125.87 (14)
O1—Ca1—N3^{i}	146.45 (6)	C4—N3—Ca1^{iii}	117.02 (14)
N1—Ca1—N3^{i}	114.97 (6)	Ca1—O5—H51	131 (3)
O5—Ca1—Ca1^{ii}	76.69 (6)	Ca1—O5—H52	122 (3)
O7—Ca1—Ca1^{ii}	89.33 (6)	H51—O5—H52	103 (4)
O3^{i}—Ca1—Ca1^{ii}	173.73 (4)	N3—C2—N1	126.0 (2)
O1^{ii}—Ca1—Ca1^{ii}	37.25 (4)	N3—C2—H2	117.0
O6—Ca1—Ca1^{ii}	103.10 (5)	N1—C2—H2	117.0
O1—Ca1—Ca1^{ii}	36.84 (4)	N3—C4—C5	121.6 (2)
N1—Ca1—Ca1^{ii}	100.01 (4)	N3—C4—C8	116.09 (18)
N3^{i}—Ca1—Ca1^{ii}	122.36 (5)	C5—C4—C8	122.31 (18)
O5—Ca1—H61	119.2 (10)	O4—C8—O3	126.6 (2)
O7—Ca1—H61	88.9 (10)	O4—C8—C4	117.21 (19)
O3^{i}—Ca1—H61	90.5 (11)	O3—C8—C4	116.20 (18)
O1^{ii}—Ca1—H61	60.1 (11)	H82—O8—H81	112 (4)
O6—Ca1—H61	17.9 (10)	C8—O3—Ca1^{iii}	126.43 (14)
O1—Ca1—H61	126.9 (11)		

Symmetry codes: (i) $-x+1/2, y-1/2, -z+3/2$; (ii) $-x, -y, -z+1$; (iii) $-x+1/2, y+1/2, -z+3/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H72···O2^{iv}	0.80 (6)	2.34 (6)	3.048 (3)	149 (6)
O6—H61···O2^{ii}	0.85 (5)	1.88 (5)	2.698 (3)	163 (5)

O8—H81···O3^{v}	0.76 (4)	2.04 (4)	2.793 (3)	170 (4)
O8—H82···O6^{iii}	0.77 (5)	2.09 (5)	2.818 (3)	157 (5)
O5—H52···O8^{vi}	0.87 (4)	1.94 (4)	2.798 (3)	169 (4)
O6—H62···O4^{iv}	0.77 (4)	1.96 (4)	2.719 (2)	167 (4)
O7—H71···O4^{vii}	0.79 (4)	2.16 (4)	2.902 (3)	158 (3)
O5—H51···O8^{v}	0.78 (4)	2.04 (4)	2.816 (3)	176 (4)

Symmetry codes: (ii) $-x, -y, -z+1$; (iii) $-x+1/2, y+1/2, -z+3/2$; (iv) $x-1/2, -y+1/2, z+1/2$; (v) $-x+3/2, y-1/2, -z+3/2$; (vi) $x-1/2, -y+1/2, z-1/2$; (vii) $-x, -y+1, -z+1$.