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 Poly[*trans*-diaquabis[μ -3-(3-pyridyl)-propionato- κ^2N,O]cadmium(II)]

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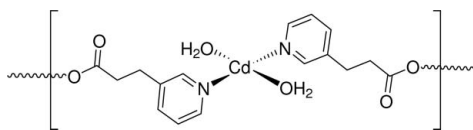
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.002$ Å; R factor = 0.016; wR factor = 0.042; data-to-parameter ratio = 13.6.

The title compound $[Cd(L)_2(H_2O)_2]_n$ ($L = 3$ -pyridine-propionic acid, $C_8H_8NO_2$), is a two-dimensional coordination polymer in which the Cd^{II} ion lies on an inversion center and is coordinated in a slightly distorted octahedral environment. The aqua H atoms are involved in intermolecular $O-H \cdots O$ hydrogen bonds, which extend the two-dimensional structure to a three-dimensional architecture. The $Cd \cdots Cd$ separation within a layer is 9.0031 (1) Å.

Related literature

For the isostructural zinc analog, see: Wang *et al.* (2006) and for the cobalt and nickel analogs, see: Martin *et al.* (2007). For background information on coordination polymers, see: Batten *et al.* (2009); Lu (2003); Perry *et al.* (2009); Robin & Fromm (2006). For coordination polymers based on pyridine carboxylates, see: Huh & Lee (2006, 2007, 2008); Kim *et al.* (2007); Min *et al.* (2001, 2002); Min & Lee (2002).



Experimental

Crystal data

 $[Cd(C_8H_8NO_2)_2(H_2O)_2]$
 $M_r = 448.74$

 Monoclinic, $P2_1/n$
 $a = 9.6934$ (4) Å

 $b = 8.9082$ (4) Å

 $c = 10.1199$ (5) Å

 $\beta = 104.309$ (2)°

 $V = 846.75$ (7) Å³
 $Z = 2$

 Mo $K\alpha$ radiation

 $\mu = 1.33$ mm⁻¹
 $T = 296$ K

 $0.42 \times 0.38 \times 0.28$ mm

Data collection

Bruker SMART CCD diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

 $T_{min} = 0.606$, $T_{max} = 0.708$

 12941 measured reflections
 2113 independent reflections

 1911 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.021$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.016$
 $wR(F^2) = 0.042$
 $S = 1.05$

2113 reflections

155 parameters

All H-atom parameters refined

 $\Delta\rho_{max} = 0.30$ e Å⁻³
 $\Delta\rho_{min} = -0.22$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cd1—O3 ⁱ	2.2704 (9)	Cd1—N1	2.3374 (10)
Cd1—O1	2.3306 (11)		
O3 ⁱ —Cd1—O1	86.35 (4)	O1—Cd1—N1	89.58 (4)
O3 ⁱ —Cd1—N1 ⁱⁱ	91.31 (4)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H01B \cdots O2 ⁱⁱⁱ	0.83 (3)	2.01 (3)	2.8361 (16)	174 (2)
O1—H01A \cdots O2 ^{iv}	0.88 (2)	1.94 (2)	2.7546 (17)	155 (2)

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

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL software used to prepare material for publication: SHELXTL.

This work was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (No. 2009-007996).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2993).

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Poly[*trans*-diaquabis[μ -3-(3-pyridyl)propionato- κ^2 N,O]cadmium(II)]

Young Ok Jang and Soon W. Lee

S1. Comment

Coordination polymers have gained attention due to their desirable properties applicable to size-selective adsorption, gas storage, host–guest recognition, catalysis, and photoluminescence (Batten *et al.*, 2009; Perry IV *et al.*, 2009; Robin & Fromm, 2006). We have been continually interested in the preparation, structures, and properties of coordination polymers based on the linking ligands of pyridine carboxylate derivatives, in which the carboxylate groups are directly attached to the pyridine ring (Huh & Lee, 2006; Huh & Lee, 2007; Huh & Lee, 2008; Kim *et al.*, 2007; Min *et al.*, 2001; Min *et al.*, 2002; Min & Lee, 2002).

Linking ligands containing both N-donors and O-donors are frequently used for the construction of coordination polymers (Lu, 2003). In particular, silver, copper, zinc, cobalt, and nickel coordination polymers containing 3-pyridinepropionic acid as a linking ligand have been reported (Wang *et al.*, 2006; Martin *et al.*, 2007). This ligand has an ethylene (–CH₂–CH₂–) spacer between the pyridyl and carboxylate groups and therefore is flexible. As an extension of our study, we investigated the preparation of cadmium coordination polymers by employing this ligand.

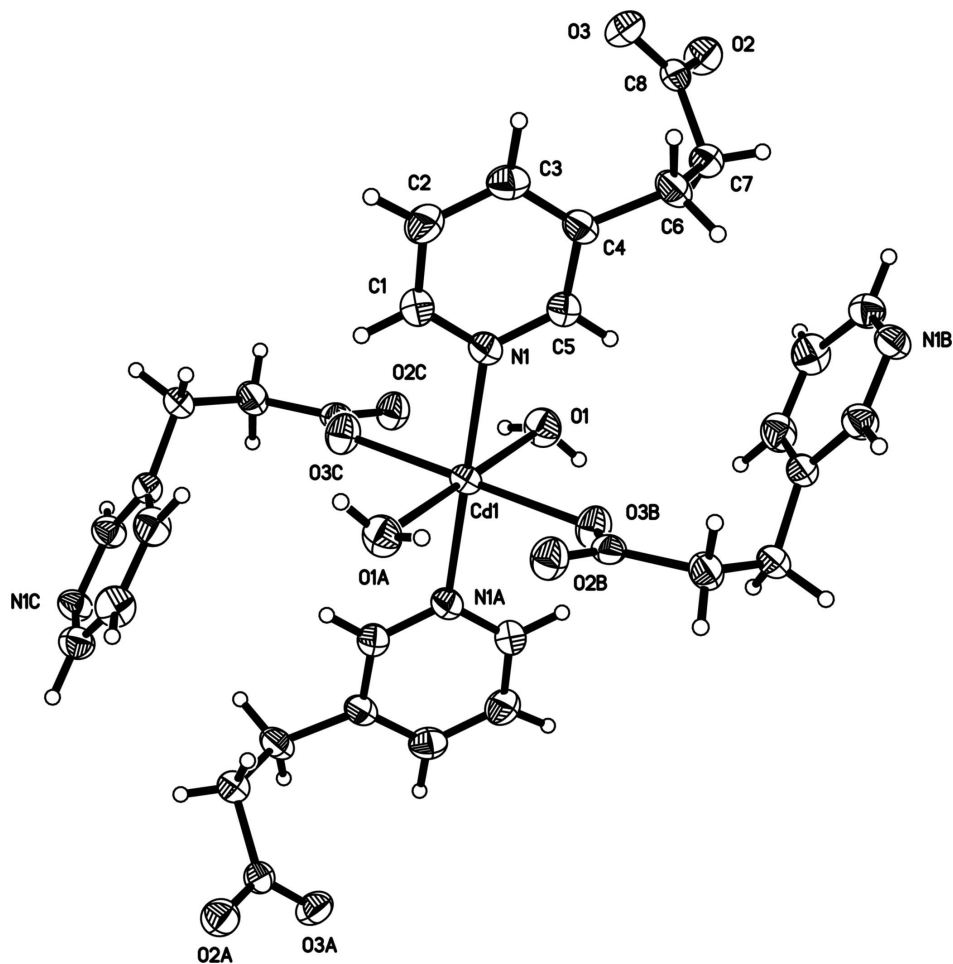
The title compound is isostructural with the zinc (Wang *et al.*, 2006), cobalt, and nickel (Martin *et al.*, 2007) analogs with the empirical formula [Cd(L)₂(H₂O)₂] (L = 3-pyridinepropionic acid). The local coordination environment around the Cd atom and the atom-numbering scheme is shown in Fig. 1. The asymmetric unit consists of one half Cd^{II} ion, one L ligand, and one aqua ligand. The Cd^{II} ion lies on a crystallographic inversion center, and the remaining atoms occupy general positions. The coordination environment of the Cd^{II} ion is slightly-distorted octahedral. The monomer units [Cd(L)₂(H₂O)₂] are linked by covalent bonds (Cd–N and Cd–O) to form a 2-D layer approximately in the (101) plane (Fig. 2) and then extended into a 3-D architecture by hydrogen bonding. Two carboxylate O atoms (O2 and O3) act differently. Whereas O2 acts as a H-bond acceptor to the aqua ligands in the neighboring units, O3 is coordinated to the Cd metal to contribute to the formation of the 2-D layer, in which the Cd^{II}–Cd^{II} separation is 9.0031 (1) Å.

S2. Experimental

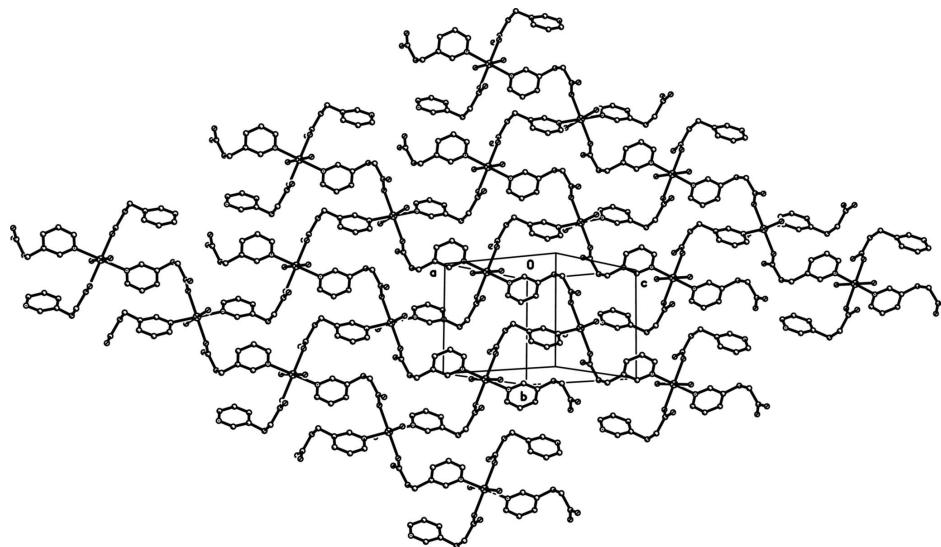
A mixture of 3-pyridinepropionic acid (0.98 g, 6.5 mmol), [Cd(NO₃)₂]₆(H₂O) (1 g, 3.2 mmol), NaOH (6.5 mmol), and H₂O (6 ml) was heated at 453 K for 2 days in a 23 ml Teflon-lined stainless-steel autoclave and then cooled slowly to room temperature to obtain pale yellow crystals. The product was collected by filtration, washed with H₂O (3 × 10 ml) and ethanol (5 × 10 ml), and then air-dried. (1.18 g, 2.6 mmol, 82%). mp: 538–540 K. IR (KBr, cm⁻¹): 3199 (*s*), 2173 (*w*), 1606 (*s*), 1302 (*w*), 1247 (*w*), 1201 (*w*), 1117 (*m*), 1047 (*m*), 961 (*s*), 607 (*s*)

S3. Refinement

All H atoms were located and refined isotropically.

**Figure 1**

Local coordination environment around the Cd metal in the title compound showing 50% probability displacement ellipsoids (symmetry codes: (A) $-x + 1, -y, -z$, (B) $-x + 1/2, y - 1/2, -z + 1/2$, (C) $x + 1/2, -y + 1/2, z - 1/2$).

**Figure 2**

Packing diagram of the title compound, showing a two-dimensional network.

Poly[*trans*-diaquabis[μ -3-(3-pyridyl)propionato- κ^2 N,O]cadmium(II)]

Crystal data

[Cd(C₈H₈NO₂)₂(H₂O)₂]

$M_r = 448.74$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 9.6934 (4) \text{ \AA}$

$b = 8.9082 (4) \text{ \AA}$

$c = 10.1199 (5) \text{ \AA}$

$\beta = 104.309 (2)^\circ$

$V = 846.75 (7) \text{ \AA}^3$

$Z = 2$

$F(000) = 452$

$D_x = 1.760 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 8598 reflections

$\theta = 2.6\text{--}28.4^\circ$

$\mu = 1.33 \text{ mm}^{-1}$

$T = 296 \text{ K}$

Block, colourless

$0.42 \times 0.38 \times 0.28 \text{ mm}$

Data collection

Bruker SMART CCD

diffractometer

Radiation source: sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.606$, $T_{\max} = 0.708$

12941 measured reflections

2113 independent reflections

1911 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.021$

$\theta_{\max} = 28.4^\circ$, $\theta_{\min} = 3.1^\circ$

$h = -12 \rightarrow 12$

$k = -11 \rightarrow 11$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.016$

$wR(F^2) = 0.042$

$S = 1.05$

2113 reflections

155 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

All H-atom parameters refined

$$w = 1/[\sigma^2(F_o^2) + (0.0233P)^2 + 0.1949P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.30 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$$

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. 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.5000	0.0000	0.0000	0.02437 (5)
N1	0.28876 (11)	0.07564 (12)	0.05233 (11)	0.0301 (2)
O1	0.61972 (13)	0.02896 (15)	0.22844 (12)	0.0382 (2)
O2	0.21558 (10)	0.21211 (11)	0.63186 (10)	0.0359 (2)
O3	0.04577 (10)	0.26152 (10)	0.44405 (10)	0.0352 (2)
C1	0.20346 (15)	0.17483 (15)	-0.02640 (14)	0.0329 (3)
C2	0.07951 (16)	0.22538 (17)	0.00161 (16)	0.0379 (3)
C3	0.04061 (15)	0.16952 (16)	0.11451 (15)	0.0357 (3)
C4	0.12544 (13)	0.06336 (15)	0.19621 (13)	0.0284 (3)
C5	0.24972 (16)	0.02120 (15)	0.16092 (16)	0.0303 (3)
C6	0.08326 (19)	-0.01072 (15)	0.31409 (17)	0.0345 (3)
C7	0.17242 (17)	0.03087 (17)	0.45527 (15)	0.0325 (3)
C8	0.14245 (13)	0.18100 (13)	0.51422 (13)	0.0260 (2)
H1	0.2335 (18)	0.208 (2)	-0.1008 (18)	0.042 (4)*
H2	0.0224 (18)	0.296 (2)	-0.0590 (18)	0.043 (4)*
H3	-0.0467 (19)	0.199 (2)	0.1376 (18)	0.050 (5)*
H5	0.314 (2)	-0.048 (2)	0.2165 (19)	0.044 (5)*
H6A	-0.022 (2)	0.0146 (17)	0.302 (2)	0.045 (6)*
H6B	0.0908 (17)	-0.1217 (19)	0.3076 (17)	0.039 (4)*
H7A	0.274 (3)	0.037 (3)	0.460 (2)	0.059 (6)*
H7B	0.158 (2)	-0.041 (2)	0.525 (2)	0.045 (5)*
HO1A	0.673 (2)	0.105 (3)	0.217 (2)	0.066 (7)*
HO1B	0.672 (3)	-0.041 (3)	0.266 (3)	0.065 (7)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02423 (8)	0.02733 (8)	0.02284 (8)	-0.00074 (4)	0.00826 (5)	-0.00185 (4)
N1	0.0303 (5)	0.0323 (6)	0.0310 (6)	0.0030 (4)	0.0137 (4)	0.0022 (4)
O1	0.0427 (6)	0.0401 (6)	0.0278 (5)	-0.0014 (5)	0.0011 (5)	-0.0019 (4)
O2	0.0375 (5)	0.0343 (5)	0.0338 (5)	0.0007 (4)	0.0047 (4)	-0.0022 (4)
O3	0.0369 (5)	0.0296 (5)	0.0372 (5)	0.0071 (4)	0.0055 (4)	-0.0010 (4)

C1	0.0388 (7)	0.0314 (6)	0.0303 (7)	0.0007 (5)	0.0120 (6)	0.0035 (5)
C2	0.0378 (7)	0.0357 (7)	0.0387 (8)	0.0090 (6)	0.0064 (6)	0.0053 (6)
C3	0.0293 (6)	0.0380 (7)	0.0413 (8)	0.0047 (5)	0.0119 (6)	-0.0040 (6)
C4	0.0309 (6)	0.0288 (6)	0.0281 (6)	-0.0039 (5)	0.0120 (5)	-0.0049 (5)
C5	0.0317 (7)	0.0316 (7)	0.0295 (7)	0.0043 (5)	0.0114 (6)	0.0036 (5)
C6	0.0407 (8)	0.0357 (8)	0.0318 (8)	-0.0082 (5)	0.0178 (6)	-0.0043 (5)
C7	0.0385 (8)	0.0323 (6)	0.0286 (7)	0.0063 (6)	0.0120 (6)	0.0010 (5)
C8	0.0265 (6)	0.0252 (6)	0.0294 (6)	-0.0013 (4)	0.0126 (5)	0.0024 (5)

Geometric parameters (Å, °)

Cd1—O3 ⁱ	2.2704 (9)	C1—H1	0.919 (18)
Cd1—O3 ⁱⁱ	2.2705 (9)	C2—C3	1.381 (2)
Cd1—O1	2.3306 (11)	C2—H2	0.954 (17)
Cd1—O1 ⁱⁱⁱ	2.3306 (11)	C3—C4	1.385 (2)
Cd1—N1 ⁱⁱⁱ	2.3374 (10)	C3—H3	0.969 (18)
Cd1—N1	2.3374 (10)	C4—C5	1.3902 (18)
N1—C1	1.3318 (17)	C4—C6	1.5055 (19)
N1—C5	1.3385 (18)	C5—H5	0.96 (2)
O1—HO1A	0.88 (2)	C6—C7	1.522 (2)
O1—HO1B	0.83 (3)	C6—H6A	1.03 (2)
O2—C8	1.2568 (15)	C6—H6B	0.995 (17)
O3—C8	1.2522 (15)	C7—C8	1.5213 (19)
O3—Cd1 ^{iv}	2.2705 (9)	C7—H7A	0.98 (2)
C1—C2	1.3766 (19)	C7—H7B	0.99 (2)
O3 ⁱ —Cd1—O3 ⁱⁱ	180.0	C1—C2—H2	118.7 (11)
O3 ⁱ —Cd1—O1	86.35 (4)	C3—C2—H2	122.4 (11)
O3 ⁱⁱ —Cd1—O1	93.65 (4)	C2—C3—C4	119.78 (12)
O3 ⁱ —Cd1—O1 ⁱⁱⁱ	93.65 (4)	C2—C3—H3	122.3 (11)
O3 ⁱⁱ —Cd1—O1 ⁱⁱⁱ	86.35 (4)	C4—C3—H3	117.9 (11)
O1—Cd1—O1 ⁱⁱⁱ	180.00 (3)	C3—C4—C5	117.09 (12)
O3 ⁱ —Cd1—N1 ⁱⁱⁱ	91.31 (4)	C3—C4—C6	122.34 (12)
O3 ⁱⁱ —Cd1—N1 ⁱⁱⁱ	88.69 (4)	C5—C4—C6	120.49 (13)
O1—Cd1—N1 ⁱⁱⁱ	90.42 (4)	N1—C5—C4	123.49 (13)
O1 ⁱⁱⁱ —Cd1—N1 ⁱⁱⁱ	89.58 (4)	N1—C5—H5	116.2 (11)
O3 ⁱ —Cd1—N1	88.69 (4)	C4—C5—H5	120.3 (11)
O3 ⁱⁱ —Cd1—N1	91.31 (4)	C4—C6—C7	115.77 (12)
O1—Cd1—N1	89.58 (4)	C4—C6—H6A	105.5 (12)
O1 ⁱⁱⁱ —Cd1—N1	90.42 (4)	C7—C6—H6A	112.2 (13)
N1 ⁱⁱⁱ —Cd1—N1	180.00 (5)	C4—C6—H6B	110.2 (10)
C1—N1—C5	118.16 (11)	C7—C6—H6B	105.7 (9)
C1—N1—Cd1	120.32 (9)	H6A—C6—H6B	107.3 (13)
C5—N1—Cd1	121.52 (9)	C8—C7—C6	117.58 (12)
Cd1—O1—HO1A	97.1 (14)	C8—C7—H7A	102.6 (13)
Cd1—O1—HO1B	118.0 (18)	C6—C7—H7A	113.1 (14)
HO1A—O1—HO1B	109 (2)	C8—C7—H7B	102.8 (12)
C8—O3—Cd1 ^{iv}	124.02 (8)	C6—C7—H7B	111.3 (12)

N1—C1—C2	122.56 (13)	H7A—C7—H7B	108.6 (17)
N1—C1—H1	115.2 (11)	O3—C8—O2	125.36 (12)
C2—C1—H1	122.3 (11)	O3—C8—C7	118.03 (12)
C1—C2—C3	118.88 (13)	O2—C8—C7	116.59 (11)

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

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
O1—HO1B...O2 ^v	0.83 (3)	2.01 (3)	2.8361 (16)	174 (2)
O1—HO1A...O2 ⁱⁱ	0.88 (2)	1.94 (2)	2.7546 (17)	155 (2)

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