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Diaquabis[3-(4-methylphenyl)-5-(pyridin-2-yl-κN)-1*H*-1,2,4-triazolato-κN^1]cadmium trihydrate

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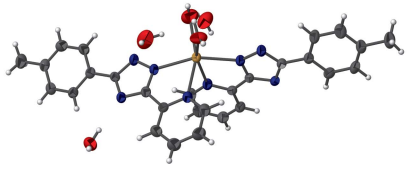
Keywords: crystal structure; triazolyl ligand; Cd^{II} complex; hydrogen bonds.

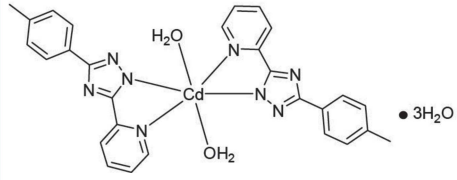
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[Cd(C_{14}H_{11}N_4)_2(H_2O)_2]\cdot 3H_2O$, the Cd^{II} cation is chelated by two 3-(4-methylphenyl)-5-(pyridin-2-yl)-1*H*-1,2,4-triazolate anions and coordinated by two water molecules in a distorted N_4O_2 octahedral geometry. Within the organic ligands, the methylphenyl rings are twisted with respect to the mean planes of chelating rings by 18.31 (16) and 14.89 (15)°. In the crystal, extensive O—H···O and O—H···N hydrogen bonds and weak C—H···O interactions link the molecules into a three-dimensional supramolecular architecture.

3D view



Chemical scheme



Structure description

Metal–azolate coordination polymers have attracted intense attention in recent years due to their interesting structures and potential applications (Yan *et al.*, 2012). Many efforts have focused on symmetrical molecules based on the flexible bridging mode of 1,2,4-triazoles and their derivatives (Chen *et al.*, 2011). It was found that the size and shape of the 3- and 5-substituents may be a crucial factor in determining the final structures of coordination polymers. However, there are few reports using asymmetrical triazolate ligands in the synthesis of metal–azolate coordination polymers (Liu *et al.*, 2017). Here, we report the synthesis and crystal structure of the title complex.

The title mononuclear complex consists of one Cd^{II} cation, two bidentate organic anions, two coordinating water molecules and three crystal water molecules. As shown in Fig. 1, the Cd^{II} cation is chelated by two organic ligands and is coordinated by two water molecules in a distorted octahedral geometry. In the organic ligands, the methylphenyl rings are twisted with respect to the mean planes of chelating rings by 18.31 (16) and 14.89 (15)°.

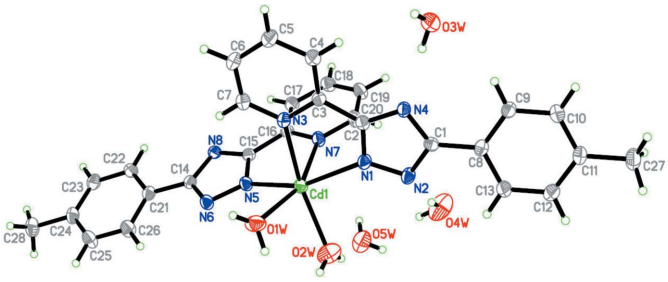


Figure 1
The structures of the molecular entities of the title complex, showing the atom labeling and 30% probability displacement ellipsoids.

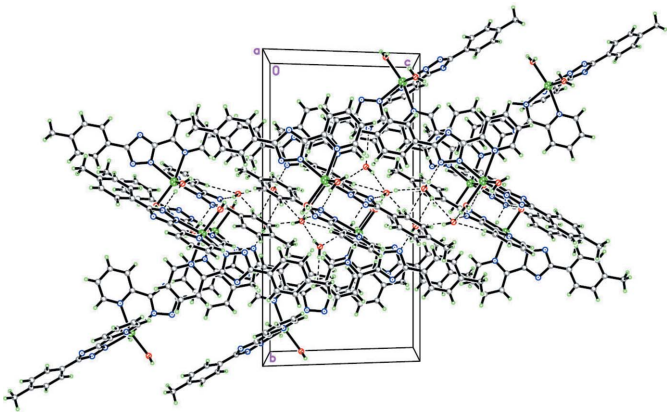


Figure 2
A view of the crystal packing of the title complex. Hydrogen bonds are shown as dashed lines.

In the crystal, extensive O—H···O and O—H···N hydrogen bonds and weak C—H···O interactions link the molecules into a three-dimensional supramolecular architecture (Table 1, Fig. 2).

Synthesis and crystallization

A mixture of cadmium acetate dihydrate (26.7 mg, 0.1 mmol), aqueous ammonia (25%, 0.2 ml), water (4 ml) and 3-(4-methylphenyl)-5-(pyridin-2-yl)-1*H*-1,2,4-triazole (47.2 mg, 0.2 mmol) was sealed in a 20 ml Teflon-lined reactor and placed in an oven at 393 K for 72 h. The resulting mixture was filtered and the resulting colorless blocks were washed with ethanol (yield 75%, based on Cd). Analysis calculated (wt%) for $C_{28}H_{32}CdN_8O_5$: C 49.92, H 4.75, N 16.64; found: C 49.02, H 5.15, N 17.13..

Refinement

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1A···N6^{i}	0.86	2.02	2.869 (4)	170
O1W—H1B···O3W^{ii}	0.83	2.08	2.907 (4)	176
O2W—H2A···N6^{i}	0.85	2.59	3.424 (4)	167
O2W—H2B···O5W	0.83	2.32	3.084 (4)	154
O3W—H3A···N4	0.83	2.09	2.920 (3)	175
O3W—H3B···O5W^{iii}	0.83	2.35	3.168 (4)	168
O4W—H4A···N2	0.82	1.98	2.785 (4)	167
O4W—H4B···O5W	0.94	2.48	3.408 (5)	175
O5W—H5A···N8^{iv}	0.83	2.19	3.006 (4)	165
O5W—H5B···O4W^{v}	0.74	2.13	2.854 (5)	167
C17—H17···O5W^{iv}	0.93	2.58	3.479 (5)	163

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cd(C_{14}H_{11}N_4)_2(H_2O)_2]\cdot 3H_2O$
M_r	673.01
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	10.919 (2), 23.045 (5), 12.154 (2)
β (°)	107.11 (3)
V (Å^3)	2922.8 (11)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.80
Crystal size (mm)	0.30 × 0.27 × 0.25
Data collection	
Diffractometer	Rigaku *MM007*-HF CCD (Saturn 724+)
Absorption correction	Multi-scan (*ABSCOR*; Higashi, 1995)
T_{min}, T_{max}	0.787, 0.819
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20295, 5124, 4037
R_{int}	0.053
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.599
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.080, 1.03
No. of reflections	5124
No. of parameters	381
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.49

Computer programs: *CrystalStructure* (Rigaku/MSC, 2006), *SHELXT* (Sheldrick, 2015*a*) and *SHELXL2014* (Sheldrick, 2015*b*).

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full crystallographic data

IUCrData (2017). **2**, x170968 [https://doi.org/10.1107/S2414314617009683]

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Crystal data

$[Cd(C_{14}H_{11}N_4)_2(H_2O)_2]\cdot 3H_2O$
M_r = 673.01
Monoclinic, $P2_1/n$
a = 10.919 (2) Å
b = 23.045 (5) Å
c = 12.154 (2) Å
β = 107.11 (3)°
V = 2922.8 (11) Å^3
Z = 4
$F(000)$ = 1376
D_x = 1.529 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 24845 reflections
θ = 3.1–25.0°
μ = 0.80 mm^{-1}
T = 293 K
Block, colorless
0.30 × 0.27 × 0.25 mm

Data collection

Rigaku MM007-HF CCD (Saturn 724+) diffractometer
Radiation source: rotating anode
ω scans at fixed χ = 45°
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
T_{min} = 0.787, T_{max} = 0.819
20295 measured reflections
5124 independent reflections
4037 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 25.2°, θ_{min} = 3.1°
h = −12→12
k = −27→26
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.080
S = 1.03
5124 reflections
381 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0319P)^2 + 1.8376P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-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. H atoms attached to carbons were constrained with C—H = 0.96 Å, and U_{iso}(H) = 1.5U_{eq}(C) of the attached C atom for methyl H atoms and C—H = 0.93 Å and 1.2U_{eq}(C) for other H atoms. The water H atoms were located from a Fourier map and restrained with O—H distance of 0.82–0.94 Å with U_{iso}(H) = 1.5U_{eq}(O).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.80813 (2)	0.08471 (2)	0.89399 (2)	0.03269 (9)
C1	0.7173 (3)	0.19928 (13)	0.5853 (3)	0.0300 (7)
C2	0.7754 (3)	0.20571 (13)	0.7663 (3)	0.0309 (7)
C3	0.8164 (3)	0.22497 (13)	0.8865 (3)	0.0304 (7)
C4	0.8298 (3)	0.28247 (15)	0.9193 (3)	0.0428 (9)
H4	0.8093	0.3116	0.8639	0.051*
C5	0.8737 (4)	0.29671 (17)	1.0343 (3)	0.0518 (10)
H5	0.8838	0.3354	1.0571	0.062*
C6	0.9023 (4)	0.25300 (16)	1.1149 (3)	0.0522 (10)
H6	0.9327	0.2614	1.1930	0.063*
C7	0.8848 (4)	0.19643 (15)	1.0768 (3)	0.0434 (9)
H7	0.9032	0.1668	1.1312	0.052*
C8	0.6779 (3)	0.21194 (14)	0.4612 (3)	0.0333 (8)
C9	0.6327 (3)	0.26643 (14)	0.4183 (3)	0.0354 (8)
H9	0.6294	0.2961	0.4692	0.043*
C10	0.5927 (3)	0.27715 (15)	0.3011 (3)	0.0397 (8)
H10	0.5625	0.3139	0.2750	0.048*
C11	0.5966 (3)	0.23440 (15)	0.2213 (3)	0.0375 (8)
C12	0.6422 (4)	0.18072 (15)	0.2648 (3)	0.0470 (10)
H12	0.6466	0.1513	0.2138	0.056*
C13	0.6815 (4)	0.16917 (15)	0.3814 (3)	0.0427 (9)
H13	0.7108	0.1322	0.4070	0.051*
C14	0.7809 (3)	0.00303 (13)	1.2148 (3)	0.0321 (7)
C15	0.6657 (3)	0.04953 (13)	1.0738 (3)	0.0293 (7)
C16	0.5604 (3)	0.07886 (12)	0.9891 (3)	0.0307 (7)
C17	0.4412 (3)	0.08834 (14)	1.0045 (3)	0.0386 (8)
H17	0.4246	0.0761	1.0716	0.046*
C18	0.3472 (3)	0.11615 (15)	0.9192 (3)	0.0419 (9)
H18	0.2666	0.1228	0.9281	0.050*
C19	0.3745 (4)	0.13391 (15)	0.8208 (3)	0.0445 (9)
H19	0.3132	0.1529	0.7623	0.053*
C20	0.4946 (3)	0.12285 (15)	0.8111 (3)	0.0428 (9)
H20	0.5124	0.1344	0.7441	0.051*
C21	0.8285 (3)	−0.02893 (13)	1.3246 (3)	0.0334 (8)
C22	0.7610 (4)	−0.03023 (15)	1.4050 (3)	0.0441 (9)
H22	0.6841	−0.0101	1.3907	0.053*
C23	0.8074 (4)	−0.06140 (16)	1.5070 (3)	0.0461 (9)
H23	0.7605	−0.0618	1.5597	0.055*
C24	0.9211 (4)	−0.09165 (14)	1.5315 (3)	0.0409 (9)
C25	0.9867 (4)	−0.09115 (16)	1.4503 (3)	0.0498 (10)
H25	1.0633	−0.1116	1.4646	0.060*

C26	0.9411 (3)	−0.06092 (16)	1.3479 (3)	0.0450 (9)
H26	0.9864	−0.0620	1.2941	0.054*
C27	0.5511 (4)	0.24619 (18)	0.0937 (3)	0.0556 (11)
H27A	0.5987	0.2226	0.0555	0.083*
H27B	0.5640	0.2864	0.0798	0.083*
H27C	0.4616	0.2370	0.0644	0.083*
C28	0.9733 (4)	−0.12478 (18)	1.6430 (3)	0.0590 (11)
H28A	0.9876	−0.1645	1.6263	0.089*
H28B	0.9127	−0.1232	1.6863	0.089*
H28C	1.0527	−0.1077	1.6872	0.089*
N1	0.7680 (3)	0.14903 (11)	0.7420 (2)	0.0348 (7)
N2	0.7305 (3)	0.14447 (11)	0.6243 (2)	0.0357 (7)
N3	0.8429 (3)	0.18203 (11)	0.9658 (2)	0.0337 (6)
N4	0.7449 (3)	0.23935 (11)	0.6715 (2)	0.0317 (6)
N5	0.7766 (3)	0.03969 (11)	1.0512 (2)	0.0338 (6)
N6	0.8526 (3)	0.00898 (11)	1.1428 (2)	0.0355 (7)
N7	0.5872 (3)	0.09635 (11)	0.8928 (2)	0.0359 (7)
N8	0.6631 (3)	0.02817 (11)	1.1765 (2)	0.0323 (6)
O1W	1.0361 (2)	0.07738 (10)	0.9683 (2)	0.0555 (7)
H1A	1.0613	0.0520	0.9283	0.083*
H1B	1.0889	0.0931	1.0232	0.083*
O2W	0.8212 (3)	0.00599 (12)	0.7820 (3)	0.0758 (9)
H2A	0.8997	−0.0008	0.7901	0.114*
H2B	0.7597	−0.0156	0.7521	0.114*
O3W	0.7291 (3)	0.36566 (11)	0.6538 (2)	0.0561 (7)
H3A	0.7389	0.3299	0.6600	0.084*
H3B	0.7924	0.3841	0.6928	0.084*
O4W	0.5469 (3)	0.06085 (14)	0.5259 (3)	0.0922 (12)
H4A	0.6092	0.0820	0.5514	0.138*
H4B	0.5420	0.0305	0.5755	0.138*
O5W	0.5504 (3)	−0.04741 (14)	0.7179 (3)	0.0719 (9)
H5A	0.4896	−0.0362	0.7410	0.108*
H5B	0.5206	−0.0556	0.6567	0.108*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03730 (16)	0.03264 (14)	0.03062 (15)	0.00326 (11)	0.01385 (11)	0.00511 (10)
C1	0.0311 (18)	0.0261 (17)	0.0333 (19)	−0.0016 (13)	0.0101 (14)	0.0009 (13)
C2	0.0297 (18)	0.0332 (18)	0.0298 (19)	0.0011 (13)	0.0086 (14)	0.0027 (14)
C3	0.0304 (18)	0.0329 (18)	0.0285 (18)	0.0031 (13)	0.0098 (14)	−0.0004 (13)
C4	0.054 (2)	0.035 (2)	0.036 (2)	0.0035 (16)	0.0088 (18)	0.0013 (15)
C5	0.069 (3)	0.044 (2)	0.037 (2)	0.0007 (19)	0.007 (2)	−0.0083 (17)
C6	0.067 (3)	0.055 (2)	0.028 (2)	0.007 (2)	0.0047 (19)	−0.0080 (17)
C7	0.052 (2)	0.044 (2)	0.032 (2)	0.0063 (17)	0.0074 (18)	0.0044 (16)
C8	0.0329 (19)	0.0380 (19)	0.0287 (19)	−0.0053 (14)	0.0085 (15)	−0.0008 (14)
C9	0.042 (2)	0.0351 (19)	0.0295 (19)	−0.0031 (15)	0.0106 (16)	−0.0020 (14)
C10	0.041 (2)	0.041 (2)	0.035 (2)	−0.0007 (15)	0.0076 (17)	0.0062 (15)

C11	0.035 (2)	0.048 (2)	0.0277 (19)	−0.0042 (15)	0.0063 (15)	0.0020 (15)
C12	0.062 (3)	0.043 (2)	0.036 (2)	0.0020 (18)	0.0131 (19)	−0.0062 (16)
C13	0.056 (2)	0.035 (2)	0.033 (2)	0.0041 (16)	0.0078 (18)	0.0018 (15)
C14	0.038 (2)	0.0324 (18)	0.0266 (18)	0.0014 (14)	0.0107 (15)	0.0004 (13)
C15	0.0337 (19)	0.0271 (17)	0.0294 (19)	0.0001 (13)	0.0129 (15)	0.0019 (13)
C16	0.0352 (19)	0.0281 (17)	0.0307 (18)	0.0008 (14)	0.0125 (15)	−0.0010 (13)
C17	0.041 (2)	0.043 (2)	0.036 (2)	0.0051 (16)	0.0176 (16)	0.0035 (15)
C18	0.033 (2)	0.049 (2)	0.045 (2)	0.0059 (16)	0.0139 (17)	0.0048 (17)
C19	0.038 (2)	0.049 (2)	0.044 (2)	0.0088 (16)	0.0074 (18)	0.0103 (17)
C20	0.040 (2)	0.054 (2)	0.036 (2)	0.0049 (17)	0.0137 (17)	0.0145 (16)
C21	0.038 (2)	0.0334 (18)	0.0285 (19)	−0.0032 (14)	0.0092 (15)	0.0004 (14)
C22	0.048 (2)	0.051 (2)	0.034 (2)	0.0160 (17)	0.0143 (18)	0.0040 (16)
C23	0.059 (3)	0.054 (2)	0.028 (2)	0.0041 (19)	0.0177 (18)	0.0037 (16)
C24	0.047 (2)	0.042 (2)	0.030 (2)	−0.0058 (16)	0.0059 (17)	0.0047 (15)
C25	0.036 (2)	0.062 (3)	0.049 (2)	0.0102 (18)	0.0100 (18)	0.0175 (19)
C26	0.043 (2)	0.057 (2)	0.040 (2)	0.0059 (18)	0.0192 (18)	0.0142 (17)
C27	0.060 (3)	0.069 (3)	0.034 (2)	0.003 (2)	0.008 (2)	0.0082 (18)
C28	0.070 (3)	0.069 (3)	0.033 (2)	0.003 (2)	0.007 (2)	0.0153 (19)
N1	0.0478 (18)	0.0317 (15)	0.0266 (16)	−0.0010 (12)	0.0133 (13)	0.0027 (11)
N2	0.0466 (18)	0.0341 (16)	0.0269 (16)	−0.0057 (12)	0.0117 (14)	0.0008 (11)
N3	0.0385 (17)	0.0357 (16)	0.0260 (16)	0.0015 (12)	0.0082 (13)	0.0018 (11)
N4	0.0363 (16)	0.0323 (15)	0.0255 (15)	−0.0003 (12)	0.0073 (12)	0.0017 (11)
N5	0.0360 (17)	0.0376 (16)	0.0287 (16)	0.0058 (12)	0.0111 (13)	0.0071 (11)
N6	0.0377 (17)	0.0403 (16)	0.0298 (16)	0.0068 (12)	0.0120 (13)	0.0090 (12)
N7	0.0345 (17)	0.0430 (16)	0.0302 (16)	0.0055 (12)	0.0096 (13)	0.0069 (12)
N8	0.0376 (17)	0.0338 (15)	0.0280 (15)	0.0057 (12)	0.0139 (13)	0.0028 (11)
O1W	0.0401 (15)	0.0577 (17)	0.0672 (19)	0.0064 (12)	0.0135 (14)	−0.0171 (13)
O2W	0.084 (2)	0.069 (2)	0.081 (2)	−0.0120 (16)	0.0345 (19)	−0.0199 (16)
O3W	0.0701 (19)	0.0436 (15)	0.0519 (17)	0.0050 (13)	0.0137 (15)	0.0053 (12)
O4W	0.112 (3)	0.087 (2)	0.084 (3)	−0.056 (2)	0.038 (2)	−0.0258 (19)
O5W	0.0491 (18)	0.109 (3)	0.058 (2)	−0.0082 (16)	0.0167 (15)	−0.0098 (17)

Geometric parameters (Å, º)

Cd1—N5	2.288 (3)	C16—N7	1.349 (4)
Cd1—O2W	2.298 (3)	C16—C17	1.386 (5)
Cd1—N1	2.308 (3)	C17—C18	1.383 (5)
Cd1—O1W	2.391 (3)	C17—H17	0.9300
Cd1—N3	2.396 (3)	C18—C19	1.377 (5)
Cd1—N7	2.423 (3)	C18—H18	0.9300
C1—N2	1.342 (4)	C19—C20	1.374 (5)
C1—N4	1.362 (4)	C19—H19	0.9300
C1—C8	1.471 (4)	C20—N7	1.338 (4)
C2—N1	1.336 (4)	C20—H20	0.9300
C2—N4	1.347 (4)	C21—C22	1.387 (5)
C2—C3	1.465 (4)	C21—C26	1.390 (5)
C3—N3	1.352 (4)	C22—C23	1.393 (5)
C3—C4	1.379 (4)	C22—H22	0.9300

C4—C5	1.376 (5)	C23—C24	1.378 (5)
C4—H4	0.9300	C23—H23	0.9300
C5—C6	1.375 (5)	C24—C25	1.380 (5)
C5—H5	0.9300	C24—C28	1.513 (5)
C6—C7	1.378 (5)	C25—C26	1.384 (5)
C6—H6	0.9300	C25—H25	0.9300
C7—N3	1.333 (4)	C26—H26	0.9300
C7—H7	0.9300	C27—H27A	0.9600
C8—C13	1.391 (5)	C27—H27B	0.9600
C8—C9	1.393 (4)	C27—H27C	0.9600
C9—C10	1.383 (5)	C28—H28A	0.9600
C9—H9	0.9300	C28—H28B	0.9600
C10—C11	1.392 (5)	C28—H28C	0.9600
C10—H10	0.9300	N1—N2	1.370 (4)
C11—C12	1.379 (5)	N5—N6	1.373 (4)
C11—C27	1.508 (5)	O1W—H1A	0.8557
C12—C13	1.380 (5)	O1W—H1B	0.8263
C12—H12	0.9300	O2W—H2A	0.8470
C13—H13	0.9300	O2W—H2B	0.8287
C14—N6	1.341 (4)	O3W—H3A	0.8318
C14—N8	1.362 (4)	O3W—H3B	0.8307
C14—C21	1.478 (4)	O4W—H4A	0.8201
C15—N5	1.338 (4)	O4W—H4B	0.9352
C15—N8	1.350 (4)	O5W—H5A	0.8342
C15—C16	1.464 (4)	O5W—H5B	0.7430

N5—Cd1—O2W	100.82 (10)	C16—C17—H17	120.3
N5—Cd1—N1	156.95 (10)	C19—C18—C17	119.1 (3)
O2W—Cd1—N1	93.61 (10)	C19—C18—H18	120.5
N5—Cd1—O1W	92.76 (10)	C17—C18—H18	120.5
O2W—Cd1—O1W	85.91 (10)	C20—C19—C18	118.4 (3)
N1—Cd1—O1W	106.22 (10)	C20—C19—H19	120.8
N5—Cd1—N3	99.62 (9)	C18—C19—H19	120.8
O2W—Cd1—N3	157.52 (10)	N7—C20—C19	123.6 (3)
N1—Cd1—N3	70.29 (9)	N7—C20—H20	118.2
O1W—Cd1—N3	83.85 (9)	C19—C20—H20	118.2
N5—Cd1—N7	70.18 (9)	C22—C21—C26	117.8 (3)
O2W—Cd1—N7	108.61 (10)	C22—C21—C14	121.9 (3)
N1—Cd1—N7	88.27 (10)	C26—C21—C14	120.2 (3)
O1W—Cd1—N7	159.08 (9)	C21—C22—C23	120.6 (3)
N3—Cd1—N7	87.11 (9)	C21—C22—H22	119.7
N2—C1—N4	112.9 (3)	C23—C22—H22	119.7
N2—C1—C8	121.2 (3)	C24—C23—C22	121.4 (3)
N4—C1—C8	125.9 (3)	C24—C23—H23	119.3
N1—C2—N4	112.9 (3)	C22—C23—H23	119.3
N1—C2—C3	119.9 (3)	C23—C24—C25	117.8 (3)
N4—C2—C3	127.2 (3)	C23—C24—C28	121.8 (3)
N3—C3—C4	121.0 (3)	C25—C24—C28	120.5 (3)

N3—C3—C2	115.3 (3)	C24—C25—C26	121.5 (3)
C4—C3—C2	123.7 (3)	C24—C25—H25	119.3
C5—C4—C3	119.9 (3)	C26—C25—H25	119.3
C5—C4—H4	120.0	C25—C26—C21	120.9 (3)
C3—C4—H4	120.0	C25—C26—H26	119.6
C6—C5—C4	119.1 (3)	C21—C26—H26	119.6
C6—C5—H5	120.4	C11—C27—H27A	109.5
C4—C5—H5	120.4	C11—C27—H27B	109.5
C5—C6—C7	118.3 (3)	H27A—C27—H27B	109.5
C5—C6—H6	120.9	C11—C27—H27C	109.5
C7—C6—H6	120.9	H27A—C27—H27C	109.5
N3—C7—C6	123.2 (3)	H27B—C27—H27C	109.5
N3—C7—H7	118.4	C24—C28—H28A	109.5
C6—C7—H7	118.4	C24—C28—H28B	109.5
C13—C8—C9	117.2 (3)	H28A—C28—H28B	109.5
C13—C8—C1	121.0 (3)	C24—C28—H28C	109.5
C9—C8—C1	121.8 (3)	H28A—C28—H28C	109.5
C10—C9—C8	121.1 (3)	H28B—C28—H28C	109.5
C10—C9—H9	119.5	C2—N1—N2	106.6 (2)
C8—C9—H9	119.5	C2—N1—Cd1	117.7 (2)
C9—C10—C11	121.7 (3)	N2—N1—Cd1	135.56 (19)
C9—C10—H10	119.1	C1—N2—N1	105.4 (2)
C11—C10—H10	119.1	C7—N3—C3	118.5 (3)
C12—C11—C10	116.7 (3)	C7—N3—Cd1	124.9 (2)
C12—C11—C27	121.9 (3)	C3—N3—Cd1	116.6 (2)
C10—C11—C27	121.4 (3)	C2—N4—C1	102.2 (3)
C11—C12—C13	122.3 (3)	C15—N5—N6	106.8 (2)
C11—C12—H12	118.8	C15—N5—Cd1	117.5 (2)
C13—C12—H12	118.8	N6—N5—Cd1	135.0 (2)
C12—C13—C8	121.0 (3)	C14—N6—N5	104.6 (3)
C12—C13—H13	119.5	C20—N7—C16	118.1 (3)
C8—C13—H13	119.5	C20—N7—Cd1	126.1 (2)
N6—C14—N8	114.1 (3)	C16—N7—Cd1	115.5 (2)
N6—C14—C21	121.5 (3)	C15—N8—C14	101.3 (3)
N8—C14—C21	124.5 (3)	Cd1—O1W—H1A	107.8
N5—C15—N8	113.3 (3)	Cd1—O1W—H1B	132.5
N5—C15—C16	120.3 (3)	H1A—O1W—H1B	119.7
N8—C15—C16	126.4 (3)	Cd1—O2W—H2A	108.2
N7—C16—C17	121.5 (3)	Cd1—O2W—H2B	123.3
N7—C16—C15	115.0 (3)	H2A—O2W—H2B	127.1
C17—C16—C15	123.5 (3)	H3A—O3W—H3B	113.1
C18—C17—C16	119.4 (3)	H4A—O4W—H4B	113.5
C18—C17—H17	120.3	H5A—O5W—H5B	105.0

N1—C2—C3—N3	−0.7 (4)	C23—C24—C25—C26	0.6 (6)
N4—C2—C3—N3	−179.2 (3)	C28—C24—C25—C26	−179.7 (4)
N1—C2—C3—C4	178.3 (3)	C24—C25—C26—C21	1.3 (6)
N4—C2—C3—C4	−0.2 (5)	C22—C21—C26—C25	−2.5 (5)

N3—C3—C4—C5	1.5 (5)	C14—C21—C26—C25	−179.9 (3)
C2—C3—C4—C5	−177.4 (3)	N4—C2—N1—N2	0.0 (4)
C3—C4—C5—C6	−0.6 (6)	C3—C2—N1—N2	−178.7 (3)
C4—C5—C6—C7	−0.5 (6)	N4—C2—N1—Cd1	−177.3 (2)
C5—C6—C7—N3	0.8 (6)	C3—C2—N1—Cd1	4.0 (4)
N2—C1—C8—C13	−14.9 (5)	N4—C1—N2—N1	0.3 (4)
N4—C1—C8—C13	164.5 (3)	C8—C1—N2—N1	179.8 (3)
N2—C1—C8—C9	163.5 (3)	C2—N1—N2—C1	−0.2 (3)
N4—C1—C8—C9	−17.1 (5)	Cd1—N1—N2—C1	176.4 (2)
C13—C8—C9—C10	0.3 (5)	C6—C7—N3—C3	0.1 (5)
C1—C8—C9—C10	−178.2 (3)	C6—C7—N3—Cd1	−179.3 (3)
C8—C9—C10—C11	−0.4 (5)	C4—C3—N3—C7	−1.3 (5)
C9—C10—C11—C12	0.1 (5)	C2—C3—N3—C7	177.8 (3)
C9—C10—C11—C27	179.1 (3)	C4—C3—N3—Cd1	178.2 (2)
C10—C11—C12—C13	0.4 (6)	C2—C3—N3—Cd1	−2.8 (3)
C27—C11—C12—C13	−178.6 (4)	N1—C2—N4—C1	0.2 (4)
C11—C12—C13—C8	−0.6 (6)	C3—C2—N4—C1	178.7 (3)
C9—C8—C13—C12	0.2 (5)	N2—C1—N4—C2	−0.3 (4)
C1—C8—C13—C12	178.7 (3)	C8—C1—N4—C2	−179.8 (3)
N5—C15—C16—N7	−2.6 (4)	N8—C15—N5—N6	1.2 (4)
N8—C15—C16—N7	179.9 (3)	C16—C15—N5—N6	−176.6 (3)
N5—C15—C16—C17	177.2 (3)	N8—C15—N5—Cd1	−171.0 (2)
N8—C15—C16—C17	−0.2 (5)	C16—C15—N5—Cd1	11.3 (4)
N7—C16—C17—C18	0.3 (5)	N8—C14—N6—N5	−0.4 (4)
C15—C16—C17—C18	−179.6 (3)	C21—C14—N6—N5	179.0 (3)
C16—C17—C18—C19	−0.2 (5)	C15—N5—N6—C14	−0.5 (3)
C17—C18—C19—C20	0.4 (5)	Cd1—N5—N6—C14	169.7 (2)
C18—C19—C20—N7	−0.8 (6)	C19—C20—N7—C16	0.9 (5)
N6—C14—C21—C22	173.1 (3)	C19—C20—N7—Cd1	−172.5 (3)
N8—C14—C21—C22	−7.6 (5)	C17—C16—N7—C20	−0.6 (5)
N6—C14—C21—C26	−9.6 (5)	C15—C16—N7—C20	179.2 (3)
N8—C14—C21—C26	169.7 (3)	C17—C16—N7—Cd1	173.5 (2)
C26—C21—C22—C23	1.8 (5)	C15—C16—N7—Cd1	−6.7 (3)
C14—C21—C22—C23	179.1 (3)	N5—C15—N8—C14	−1.3 (3)
C21—C22—C23—C24	0.2 (6)	C16—C15—N8—C14	176.3 (3)
C22—C23—C24—C25	−1.4 (6)	N6—C14—N8—C15	1.0 (4)
C22—C23—C24—C28	179.0 (4)	C21—C14—N8—C15	−178.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*A*···N6^{i}	0.86	2.02	2.869 (4)	170
O1*W*—H1*B*···O3*W*^{ii}	0.83	2.08	2.907 (4)	176
O2*W*—H2*A*···N6^{i}	0.85	2.59	3.424 (4)	167
O2*W*—H2*B*···O5*W*	0.83	2.32	3.084 (4)	154
O3*W*—H3*A*···N4	0.83	2.09	2.920 (3)	175
O3*W*—H3*B*···O5*W*^{iii}	0.83	2.35	3.168 (4)	168
O4*W*—H4*A*···N2	0.82	1.98	2.785 (4)	167

O4*W*—H4*B*···O5*W*	0.94	2.48	3.408 (5)	175
O5*W*—H5*A*···N8^{iv}	0.83	2.19	3.006 (4)	165
O5*W*—H5*B*···O4*W*^{v}	0.74	2.13	2.854 (5)	167
C17—H17···O5*W*^{iv}	0.93	2.58	3.479 (5)	163

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