

Poly[(acetato- κ^2O,O')aqua(μ_4 -1*H*-benzimidazole-5,6-dicarboxylato- $\kappa^5N^3:O^5,O^5',O^6:O^6'$)praseodymium(III)]

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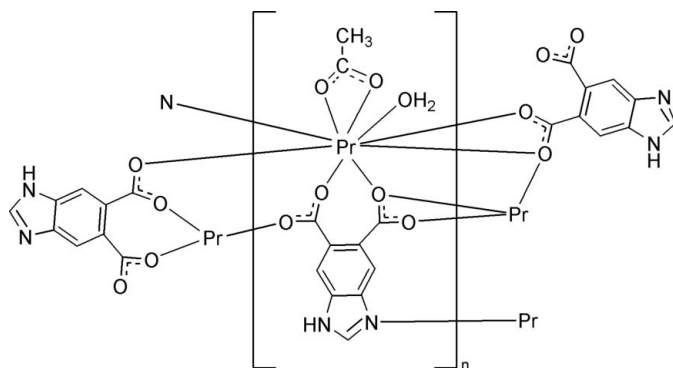
Received 20 August 2010; accepted 15 September 2010

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.005$ Å; disorder in main residue; R factor = 0.028; wR factor = 0.072; data-to-parameter ratio = 11.7.

In the title complex, $[\text{Pr}(\text{C}_9\text{H}_4\text{N}_2\text{O}_4)(\text{C}_2\text{H}_3\text{O}_2)(\text{H}_2\text{O})]_n$, the Pr^{III} ion is coordinated by five O atoms and one N atom from four benzimidazole-5,6-dicarboxylate ligands, two O atoms from an acetate ligand and one water molecule, giving a tricapped trigonal-prismatic geometry. The benzimidazole-5,6-dicarboxylate and acetate ligands connect the Pr^{III} ions, forming a layer in the ac plane; the layers are further linked by $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonding and $\pi-\pi$ stacking interactions between neighboring pyridine rings [the centroid-centroid distance is 3.467 (1) Å], assembling a three-dimensional supramolecular network. The acetate methyl group is disordered over two positions with site-occupancy factors of 0.75 and 0.25.

Related literature

For related structures, see: Gao *et al.* (2008); Lo *et al.* (2007); Wang *et al.* (2009); Wei *et al.* (2008); Yao *et al.* (2008); Zhai (2009).



Experimental

Crystal data

$[\text{Pr}(\text{C}_9\text{H}_4\text{N}_2\text{O}_4)(\text{C}_2\text{H}_3\text{O}_2)(\text{H}_2\text{O})]$	$\gamma = 84.274 (1)^\circ$
$M_r = 422.11$	$V = 645.77 (8) \text{ \AA}^3$
Triclinic, $P\bar{1}$	$Z = 2$
$a = 7.4284 (5) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 9.0109 (7) \text{ \AA}$	$\mu = 3.81 \text{ mm}^{-1}$
$c = 9.7239 (7) \text{ \AA}$	$T = 296 \text{ K}$
$\alpha = 87.075 (1)^\circ$	$0.26 \times 0.22 \times 0.19 \text{ mm}$
$\beta = 86.498 (1)^\circ$	

Data collection

Bruker SMART APEX CCD diffractometer	3963 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2004)	2327 independent reflections
$T_{\text{min}} = 0.386$, $T_{\text{max}} = 0.485$	2184 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.028$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.072$	$\Delta\rho_{\text{max}} = 1.23 \text{ e \AA}^{-3}$
$S = 1.04$	$\Delta\rho_{\text{min}} = -1.45 \text{ e \AA}^{-3}$
2327 reflections	
199 parameters	
22 restraints	

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{O6}^i$	0.85 (2)	1.90 (3)	2.712 (5)	159 (5)
$\text{O1W}-\text{H1W}\cdots\text{O2}^{ii}$	0.83 (2)	2.06 (3)	2.854 (4)	159 (6)
$\text{O1W}-\text{H2W}\cdots\text{O5}^{iii}$	0.84 (2)	1.96 (2)	2.794 (4)	176 (5)

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; 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.

The authors acknowledge the Natural Science Foundation of Guangdong Province (No. 9151063101000037) for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2264).

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supporting information

Acta Cryst. (2010). E66, m1302 [doi:10.1107/S1600536810036986]

Poly[(acetato- κ^2 O,O')aqua(μ_4 -1*H*-benzimidazole-5,6-dicarboxylato- κ^5 N³:O⁵,O^{5'}:O⁵,O⁶:O^{6'})praseodymium(III)]

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S1. Comment

In recent years, studies of coordination polymers built using metals and multifunctional organic ligands, has been a rapidly expanding field. This has been due to their intriguing structural motifs and functional properties, such as molecular adsorption, magnetism, and luminescence. Benzimidazole-5,6-dicarboxylic acid (H₂L) is such a multifunctional ligand with both nitrogen and oxygen donor atoms (Gao *et al.*, 2008; Lo *et al.*, 2007; Wang *et al.*, 2009; Wei *et al.*, 2008; Yao *et al.*, 2008; Zhai *et al.*, 2009). For example, Yao and co-workers have successfully synthesized six novel two-dimensional coordination polymers based on this ligand, namely, [MnL]_n (1), {[Ni₂L₂(H₂O)₄].(H₂O)₃]_n (2), {[Tb(L)(HL)(H₂O)].(H₂O)]_n (3) and {[Ln₂L₂(HL)₂(H₂O)₂]_n (Ln=Ho (4), Er (5), Lu (6)) (Yao *et al.*, 2008). Wei *et al.* also obtained a novel five coordinated Mn(II) polymer ([Mn(HL)]_n) possessing abundant hydrogen bonds and π - π stacking interactions (Wei *et al.*, 2008). Herein, we report the hydrothermal synthesis, structure of the novel coordination polymer.

In the structure of the title compound (Fig. 1), each Pr^{III} centre is nine-coordinated by five oxygen atoms and one N atom from four benzimidazole-5,6-dicarboxylato ligands, two oxygen atoms from an acetate ligand, and one water molecule. The structure can be described as having a bicapped trigonal prismatic geometry with Pr \cdots O distances and O \cdots Pr \cdots O angles ranging from 2.373 (3) Å to 2.645 (3) Å and 69.84 (9) ° to 152.88 (1) °, respectively. The benzimidazole-5,6-dicarboxylate and acetate ligands, act as bridging ligands, linking the Pr^{III} metal centres into a layer parallel to the ac plane (Fig. 2). Those layers are further connected via O—H \cdots O and N—H \cdots O hydrogen bonding interactions (Table 1) to form a three-dimensional supramolecular motif, which is stabilized by π - π stacking interactions between neighboring pyridyl rings (the centroid \cdots centroid distance is 3.467 (1) Å).

S2. Experimental

A mixture of Pr₆O₁₁ (0.170 g; 0.17 mmol), benzimidazole-5,6-dicarboxylic acid (0.206 g; 1 mmol), acetic acid (0.06 g; 1 mmol), water (10 ml) was stirred vigorously for 30 min and then sealed in a teflon-lined stainless-steel autoclave (20 ml, capacity). The autoclave was heated and maintained at 423 K for 3 days, and then cooled to room temperature at 5 K h⁻¹, which produced colorless block-shaped crystals.

S3. Refinement

Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O—H = 0.84 Å and H \cdots H = 1.35 Å, and with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$. The H atom bound to the N1 nitrogen atom was refined with distance restraints of N—H = 0.86 Å, and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{O})$. All other H atoms were placed at calculated positions and treated as riding on the parent atoms, with C—H = 0.93 Å or 0.96 Å, and with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5 U_{\text{eq}}(\text{C})$.

$\beta = 86.498 (1)^\circ$
 $\gamma = 84.274 (1)^\circ$
 $V = 645.77 (8) \text{ \AA}^3$
 $Z = 2$
 $F(000) = 408$
 $D_x = 2.171 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2989 reflections
 $\theta = 2.3\text{--}28.4^\circ$
 $\mu = 3.81 \text{ mm}^{-1}$
 $T = 296 \text{ K}$
 Block, colourless
 $0.26 \times 0.22 \times 0.19 \text{ mm}$

Data collection

Bruker SMART APEX CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2004)
 $T_{\min} = 0.386$, $T_{\max} = 0.485$

3963 measured reflections
 2327 independent reflections
 2184 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$
 $\theta_{\max} = 25.2^\circ$, $\theta_{\min} = 2.3^\circ$
 $h = -8 \rightarrow 8$
 $k = -10 \rightarrow 10$
 $l = -7 \rightarrow 11$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.072$
 $S = 1.04$
 2327 reflections
 199 parameters
 22 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
 $w = 1/[\sigma^2(F_o^2) + (0.0394P)^2 + 1.0511P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.23 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -1.45 \text{ e \AA}^{-3}$
 Extinction correction: SHELXL97 (Sheldrick,
 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.0091 (12)

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 $F^2 > 2\sigma(F^2)$ 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>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Pr1	0.35344 (3)	0.35784 (2)	-0.10574 (2)	0.01137 (13)	
O1	0.1245 (4)	0.2800 (3)	0.0551 (3)	0.0171 (6)	
O1W	0.6206 (5)	0.2207 (4)	0.0136 (4)	0.0286 (8)	
H1W	0.713 (5)	0.260 (5)	0.032 (6)	0.034*	
H2W	0.626 (7)	0.135 (3)	0.051 (6)	0.034*	
O2	-0.1348 (4)	0.4123 (3)	0.1093 (3)	0.0187 (7)	
O3	0.5275 (4)	0.4696 (4)	0.2957 (3)	0.0229 (7)	
O4	0.3620 (4)	0.4864 (3)	0.1165 (3)	0.0169 (6)	

O5	0.3704 (4)	0.0699 (3)	-0.1295 (3)	0.0213 (7)	
O6	0.5234 (4)	0.2005 (3)	-0.2842 (3)	0.0222 (7)	
N1	-0.1290 (5)	0.2444 (4)	0.6358 (4)	0.0197 (8)	
H1	-0.237 (4)	0.219 (6)	0.642 (6)	0.024*	
N2	0.1301 (5)	0.3045 (4)	0.7108 (4)	0.0183 (8)	
C1	0.0176 (5)	0.3514 (4)	0.1395 (4)	0.0124 (8)	
C2	0.0663 (5)	0.3516 (4)	0.2883 (4)	0.0128 (8)	
C3	-0.0669 (6)	0.3032 (5)	0.3815 (5)	0.0179 (9)	
H3	-0.1780	0.2820	0.3522	0.021*	
C4	-0.0292 (5)	0.2876 (5)	0.5200 (5)	0.0158 (9)	
C5	0.1336 (5)	0.3240 (4)	0.5684 (4)	0.0137 (8)	
C6	0.2660 (5)	0.3744 (4)	0.4746 (4)	0.0138 (8)	
H6	0.3747	0.3995	0.5056	0.017*	
C7	0.2352 (5)	0.3872 (4)	0.3345 (4)	0.0121 (8)	
C8	0.3828 (5)	0.4492 (4)	0.2436 (4)	0.0117 (8)	
C9	-0.0292 (6)	0.2583 (5)	0.7442 (5)	0.0191 (9)	
H9	-0.0696	0.2371	0.8348	0.023*	
C10	0.4743 (7)	0.0768 (5)	-0.2356 (6)	0.0304 (9)	
C11	0.5650 (11)	-0.0621 (7)	-0.2989 (8)	0.0304 (9)	0.75
H11A	0.6777	-0.0907	-0.2569	0.046*	0.75
H11B	0.5877	-0.0431	-0.3961	0.046*	0.75
H11C	0.4876	-0.1412	-0.2840	0.046*	0.75
C11'	0.477 (3)	-0.055 (2)	-0.332 (2)	0.0304 (9)	0.25
H11D	0.5368	-0.1430	-0.2891	0.046*	0.25
H11E	0.5413	-0.0309	-0.4178	0.046*	0.25
H11F	0.3551	-0.0717	-0.3491	0.046*	0.25

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.01163 (17)	0.01259 (17)	0.00993 (17)	-0.00185 (9)	0.00044 (10)	-0.00098 (10)
O1	0.0192 (15)	0.0188 (15)	0.0137 (16)	-0.0041 (12)	0.0014 (12)	-0.0035 (12)
O1W	0.0286 (18)	0.0164 (16)	0.042 (2)	-0.0047 (14)	-0.0170 (16)	0.0049 (15)
O2	0.0167 (15)	0.0199 (15)	0.0190 (17)	0.0033 (12)	-0.0052 (13)	-0.0022 (13)
O3	0.0175 (16)	0.0315 (18)	0.0207 (18)	-0.0097 (13)	-0.0023 (13)	0.0039 (14)
O4	0.0200 (15)	0.0180 (15)	0.0131 (16)	-0.0055 (12)	0.0002 (12)	0.0008 (12)
O5	0.0240 (16)	0.0159 (15)	0.0239 (18)	-0.0040 (12)	0.0013 (14)	-0.0006 (13)
O6	0.0206 (16)	0.0198 (16)	0.0252 (18)	-0.0003 (12)	0.0048 (13)	-0.0019 (13)
N1	0.0150 (18)	0.029 (2)	0.016 (2)	-0.0078 (15)	0.0018 (15)	0.0025 (16)
N2	0.0203 (19)	0.0214 (18)	0.0130 (19)	-0.0036 (15)	0.0017 (15)	-0.0006 (15)
C1	0.0136 (19)	0.0106 (18)	0.013 (2)	-0.0035 (15)	0.0002 (16)	0.0017 (16)
C2	0.0128 (19)	0.0126 (19)	0.013 (2)	-0.0012 (15)	-0.0005 (16)	-0.0008 (16)
C3	0.014 (2)	0.022 (2)	0.018 (2)	-0.0019 (17)	-0.0023 (17)	-0.0015 (18)
C4	0.013 (2)	0.019 (2)	0.015 (2)	-0.0007 (16)	0.0010 (17)	-0.0014 (17)
C5	0.015 (2)	0.0135 (19)	0.012 (2)	-0.0001 (15)	0.0013 (16)	-0.0017 (16)
C6	0.0109 (19)	0.0138 (19)	0.017 (2)	-0.0015 (15)	0.0002 (16)	-0.0017 (17)
C7	0.0126 (19)	0.0108 (18)	0.013 (2)	-0.0006 (15)	0.0012 (16)	-0.0015 (16)
C8	0.015 (2)	0.0105 (18)	0.010 (2)	-0.0011 (15)	-0.0008 (16)	-0.0011 (15)

C9	0.022 (2)	0.025 (2)	0.010 (2)	-0.0049 (18)	0.0024 (17)	0.0032 (18)
C10	0.037 (2)	0.0221 (19)	0.031 (2)	0.0040 (18)	0.0026 (19)	-0.0054 (17)
C11	0.037 (2)	0.0221 (19)	0.031 (2)	0.0040 (18)	0.0026 (19)	-0.0054 (17)
C11'	0.037 (2)	0.0221 (19)	0.031 (2)	0.0040 (18)	0.0026 (19)	-0.0054 (17)

Geometric parameters (Å, °)

Pr1—O1	2.373 (3)	N2—C9	1.310 (6)
Pr1—O6	2.498 (3)	N2—C5	1.386 (6)
Pr1—O2 ⁱ	2.501 (3)	N2—Pr1 ^{iv}	2.603 (4)
Pr1—O4	2.511 (3)	C1—C2	1.512 (6)
Pr1—O3 ⁱⁱ	2.528 (3)	C2—C3	1.389 (6)
Pr1—O1W	2.541 (3)	C2—C7	1.429 (6)
Pr1—N2 ⁱⁱⁱ	2.603 (4)	C3—C4	1.389 (6)
Pr1—O5	2.606 (3)	C3—H3	0.9300
Pr1—O4 ⁱⁱ	2.646 (3)	C4—C5	1.399 (6)
Pr1—C8 ⁱⁱ	2.963 (4)	C5—C6	1.394 (6)
O1—C1	1.261 (5)	C6—C7	1.393 (6)
O1W—H1W	0.833 (19)	C6—H6	0.9300
O1W—H2W	0.836 (19)	C7—C8	1.499 (6)
O2—C1	1.253 (5)	C8—Pr1 ⁱⁱ	2.963 (4)
O2—Pr1 ⁱ	2.501 (3)	C9—H9	0.9300
O3—C8	1.250 (5)	C10—C11	1.503 (8)
O3—Pr1 ⁱⁱ	2.528 (3)	C10—C11'	1.55 (2)
O4—C8	1.278 (5)	C11—H11A	0.9600
O4—Pr1 ⁱⁱ	2.646 (3)	C11—H11B	0.9600
O5—C10	1.253 (6)	C11—H11C	0.9600
O6—C10	1.267 (6)	C11'—H11D	0.9600
N1—C9	1.342 (6)	C11'—H11E	0.9600
N1—C4	1.372 (6)	C11'—H11F	0.9600
N1—H1	0.85 (2)		
O1—Pr1—O6	125.76 (10)	C10—O6—Pr1	96.4 (3)
O1—Pr1—O2 ⁱ	79.97 (10)	C9—N1—C4	107.0 (4)
O6—Pr1—O2 ⁱ	135.37 (10)	C9—N1—H1	125 (4)
O1—Pr1—O4	69.81 (9)	C4—N1—H1	128 (4)
O6—Pr1—O4	147.25 (10)	C9—N2—C5	104.1 (4)
O2 ⁱ —Pr1—O4	70.88 (10)	C9—N2—Pr1 ^{iv}	122.6 (3)
O1—Pr1—O3 ⁱⁱ	152.91 (11)	C5—N2—Pr1 ^{iv}	133.1 (3)
O6—Pr1—O3 ⁱⁱ	72.06 (11)	O2—C1—O1	123.2 (4)
O2 ⁱ —Pr1—O3 ⁱⁱ	73.82 (11)	O2—C1—C2	117.7 (4)
O4—Pr1—O3 ⁱⁱ	106.94 (10)	O1—C1—C2	118.8 (3)
O1—Pr1—O1W	96.60 (11)	C3—C2—C7	120.7 (4)
O6—Pr1—O1W	74.37 (12)	C3—C2—C1	113.5 (4)
O2 ⁱ —Pr1—O1W	145.00 (11)	C7—C2—C1	125.7 (4)
O4—Pr1—O1W	75.25 (11)	C2—C3—C4	118.0 (4)
O3 ⁱⁱ —Pr1—O1W	108.74 (11)	C2—C3—H3	121.0
O1—Pr1—N2 ⁱⁱⁱ	84.24 (11)	C4—C3—H3	121.0

O6—Pr1—N2 ⁱⁱⁱ	71.46 (11)	N1—C4—C3	132.5 (4)
O2 ⁱ —Pr1—N2 ⁱⁱⁱ	76.78 (11)	N1—C4—C5	104.9 (4)
O4—Pr1—N2 ⁱⁱⁱ	141.25 (11)	C3—C4—C5	122.5 (4)
O3 ⁱⁱ —Pr1—N2 ⁱⁱⁱ	83.25 (11)	N2—C5—C6	130.8 (4)
O1W—Pr1—N2 ⁱⁱⁱ	137.92 (11)	N2—C5—C4	109.9 (4)
O1—Pr1—O5	75.84 (10)	C6—C5—C4	119.3 (4)
O6—Pr1—O5	50.87 (10)	C7—C6—C5	119.8 (4)
O2 ⁱ —Pr1—O5	141.76 (10)	C7—C6—H6	120.1
O4—Pr1—O5	125.30 (10)	C5—C6—H6	120.1
O3 ⁱⁱ —Pr1—O5	122.16 (11)	C6—C7—C2	119.7 (4)
O1W—Pr1—O5	67.81 (10)	C6—C7—C8	115.3 (3)
N2 ⁱⁱⁱ —Pr1—O5	71.75 (11)	C2—C7—C8	124.8 (4)
O1—Pr1—O4 ⁱⁱ	139.88 (10)	O3—C8—O4	119.5 (4)
O6—Pr1—O4 ⁱⁱ	86.63 (10)	O3—C8—C7	118.6 (4)
O2 ⁱ —Pr1—O4 ⁱⁱ	92.78 (10)	O4—C8—C7	121.9 (3)
O4—Pr1—O4 ⁱⁱ	70.53 (11)	O3—C8—Pr1 ⁱⁱ	57.8 (2)
O3 ⁱⁱ —Pr1—O4 ⁱⁱ	49.85 (9)	O4—C8—Pr1 ⁱⁱ	63.2 (2)
O1W—Pr1—O4 ⁱⁱ	67.41 (10)	C7—C8—Pr1 ⁱⁱ	165.0 (3)
N2 ⁱⁱⁱ —Pr1—O4 ⁱⁱ	132.75 (10)	N2—C9—N1	114.0 (4)
O5—Pr1—O4 ⁱⁱ	124.59 (9)	N2—C9—H9	123.0
O1—Pr1—C8 ⁱⁱ	159.06 (10)	N1—C9—H9	123.0
O6—Pr1—C8 ⁱⁱ	75.06 (10)	O5—C10—O6	121.2 (4)
O2 ⁱ —Pr1—C8 ⁱⁱ	85.58 (10)	O5—C10—C11	121.3 (5)
O4—Pr1—C8 ⁱⁱ	91.20 (10)	O6—C10—C11	117.1 (5)
O3 ⁱⁱ —Pr1—C8 ⁱⁱ	24.71 (10)	O5—C10—C11'	115.5 (10)
O1W—Pr1—C8 ⁱⁱ	86.57 (11)	O6—C10—C11'	119.2 (10)
N2 ⁱⁱⁱ —Pr1—C8 ⁱⁱ	107.21 (11)	C10—C11—H11A	109.5
O5—Pr1—C8 ⁱⁱ	124.02 (10)	C10—C11—H11B	109.5
O4 ⁱⁱ —Pr1—C8 ⁱⁱ	25.55 (10)	H11A—C11—H11B	109.5
C1—O1—Pr1	131.7 (3)	C10—C11—H11C	109.5
Pr1—O1W—H1W	124 (3)	H11A—C11—H11C	109.5
Pr1—O1W—H2W	127 (3)	H11B—C11—H11C	109.5
H1W—O1W—H2W	108 (3)	C10—C11'—H11D	109.5
C1—O2—Pr1 ⁱ	148.2 (3)	C10—C11'—H11E	109.5
C8—O3—Pr1 ⁱⁱ	97.5 (2)	H11D—C11'—H11E	109.5
C8—O4—Pr1	137.6 (3)	C10—C11'—H11F	109.5
C8—O4—Pr1 ⁱⁱ	91.2 (2)	H11D—C11'—H11F	109.5
Pr1—O4—Pr1 ⁱⁱ	109.47 (11)	H11E—C11'—H11F	109.5
C10—O5—Pr1	91.6 (3)		
O6—Pr1—O1—C1	-171.8 (3)	O2—C1—C2—C3	49.4 (5)
O2 ⁱ —Pr1—O1—C1	-32.1 (3)	O1—C1—C2—C3	-124.8 (4)
O4—Pr1—O1—C1	41.1 (3)	O2—C1—C2—C7	-134.6 (4)
O3 ⁱⁱ —Pr1—O1—C1	-46.8 (5)	O1—C1—C2—C7	51.3 (6)
O1W—Pr1—O1—C1	112.7 (4)	C7—C2—C3—C4	-1.4 (6)
N2 ⁱⁱⁱ —Pr1—O1—C1	-109.6 (4)	C1—C2—C3—C4	174.8 (4)
O5—Pr1—O1—C1	177.8 (4)	C9—N1—C4—C3	-176.2 (5)
O4 ⁱⁱ —Pr1—O1—C1	50.3 (4)	C9—N1—C4—C5	1.1 (5)

C8 ⁱⁱ —Pr1—O1—C1	15.0 (5)	C2—C3—C4—N1	179.5 (4)
O1—Pr1—O4—C8	58.8 (4)	C2—C3—C4—C5	2.5 (6)
O6—Pr1—O4—C8	-66.6 (4)	C9—N2—C5—C6	178.5 (4)
O2 ⁱ —Pr1—O4—C8	144.9 (4)	Pr1 ^{iv} —N2—C5—C6	3.1 (7)
O3 ⁱⁱ —Pr1—O4—C8	-149.6 (4)	C9—N2—C5—C4	0.0 (5)
O1W—Pr1—O4—C8	-44.1 (4)	Pr1 ^{iv} —N2—C5—C4	-175.3 (3)
N2 ⁱⁱⁱ —Pr1—O4—C8	109.9 (4)	N1—C4—C5—N2	-0.7 (5)
O5—Pr1—O4—C8	4.3 (4)	C3—C4—C5—N2	177.0 (4)
O4 ⁱⁱ —Pr1—O4—C8	-114.9 (4)	N1—C4—C5—C6	-179.3 (4)
C8 ⁱⁱ —Pr1—O4—C8	-130.2 (3)	C3—C4—C5—C6	-1.7 (6)
O1—Pr1—O4—Pr1 ⁱⁱ	173.75 (13)	N2—C5—C6—C7	-178.6 (4)
O6—Pr1—O4—Pr1 ⁱⁱ	48.4 (2)	C4—C5—C6—C7	-0.3 (6)
O2 ⁱ —Pr1—O4—Pr1 ⁱⁱ	-100.20 (12)	C5—C6—C7—C2	1.3 (6)
O3 ⁱⁱ —Pr1—O4—Pr1 ⁱⁱ	-34.66 (13)	C5—C6—C7—C8	177.3 (4)
O1W—Pr1—O4—Pr1 ⁱⁱ	70.84 (12)	C3—C2—C7—C6	-0.4 (6)
N2 ⁱⁱⁱ —Pr1—O4—Pr1 ⁱⁱ	-135.22 (14)	C1—C2—C7—C6	-176.2 (4)
O5—Pr1—O4—Pr1 ⁱⁱ	119.17 (11)	C3—C2—C7—C8	-176.0 (4)
O4 ⁱⁱ —Pr1—O4—Pr1 ⁱⁱ	0.0	C1—C2—C7—C8	8.2 (6)
C8 ⁱⁱ —Pr1—O4—Pr1 ⁱⁱ	-15.29 (12)	Pr1 ⁱⁱ —O3—C8—O4	14.5 (4)
O1—Pr1—O5—C10	169.4 (3)	Pr1 ⁱⁱ —O3—C8—C7	-163.1 (3)
O6—Pr1—O5—C10	0.2 (3)	Pr1—O4—C8—O3	107.5 (4)
O2 ⁱ —Pr1—O5—C10	117.0 (3)	Pr1 ⁱⁱ —O4—C8—O3	-13.7 (4)
O4—Pr1—O5—C10	-138.6 (3)	Pr1—O4—C8—C7	-75.0 (5)
O3 ⁱⁱ —Pr1—O5—C10	11.5 (3)	Pr1 ⁱⁱ —O4—C8—C7	163.8 (3)
O1W—Pr1—O5—C10	-87.3 (3)	Pr1—O4—C8—Pr1 ⁱⁱ	121.2 (3)
N2 ⁱⁱⁱ —Pr1—O5—C10	80.8 (3)	C6—C7—C8—O3	7.4 (5)
O4 ⁱⁱ —Pr1—O5—C10	-49.0 (3)	C2—C7—C8—O3	-176.9 (4)
C8 ⁱⁱ —Pr1—O5—C10	-18.0 (3)	C6—C7—C8—O4	-170.1 (4)
O1—Pr1—O6—C10	-13.2 (3)	C2—C7—C8—O4	5.6 (6)
O2 ⁱ —Pr1—O6—C10	-128.3 (3)	C6—C7—C8—Pr1 ⁱⁱ	-64.3 (11)
O4—Pr1—O6—C10	96.2 (3)	C2—C7—C8—Pr1 ⁱⁱ	111.4 (10)
O3 ⁱⁱ —Pr1—O6—C10	-170.2 (3)	C5—N2—C9—N1	0.7 (5)
O1W—Pr1—O6—C10	73.6 (3)	Pr1 ^{iv} —N2—C9—N1	176.7 (3)
N2 ⁱⁱⁱ —Pr1—O6—C10	-81.4 (3)	C4—N1—C9—N2	-1.2 (5)
O5—Pr1—O6—C10	-0.2 (3)	Pr1—O5—C10—O6	-0.4 (5)
O4 ⁱⁱ —Pr1—O6—C10	141.1 (3)	Pr1—O5—C10—C11	171.3 (5)
C8 ⁱⁱ —Pr1—O6—C10	164.2 (3)	Pr1—O5—C10—C11'	-157.3 (10)
Pr1 ⁱ —O2—C1—O1	-128.3 (5)	Pr1—O6—C10—O5	0.4 (5)
Pr1 ⁱ —O2—C1—C2	57.8 (7)	Pr1—O6—C10—C11	-171.7 (5)
Pr1—O1—C1—O2	88.8 (5)	Pr1—O6—C10—C11'	156.5 (11)
Pr1—O1—C1—C2	-97.4 (4)		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 ^v —O6 ^v	0.85 (2)	1.90 (3)	2.712 (5)	159 (5)

O1W—H1W...O2 ^{vi}	0.83 (2)	2.06 (3)	2.854 (4)	159 (6)
O1W—H2W...O5 ^{vii}	0.84 (2)	1.96 (2)	2.794 (4)	176 (5)

Symmetry codes: (v) $x-1, y, z+1$; (vi) $x+1, y, z$; (vii) $-x+1, -y, -z$.