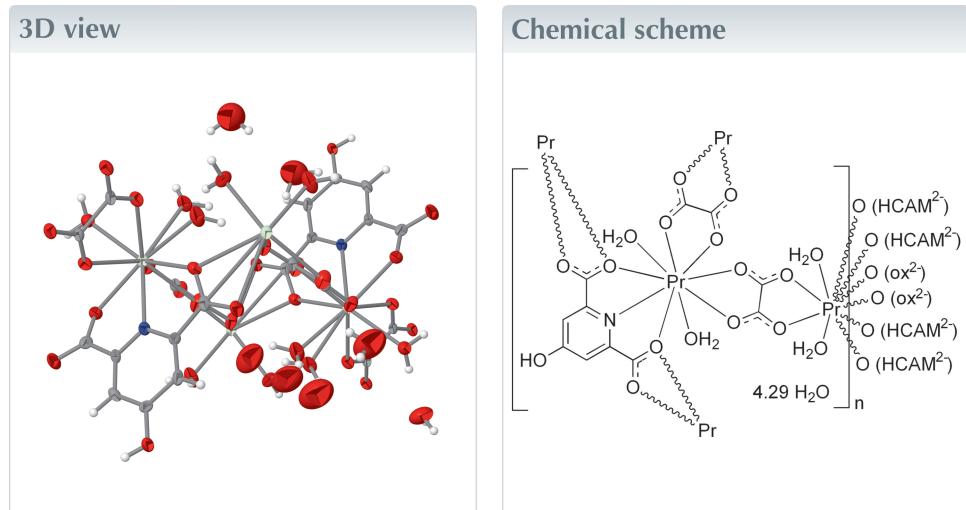


Poly[[tetraaqua(μ_3 -4-hydroxypyridine-2,6-dicarboxylato)di- μ_2 -oxalato-diprasedymium(III)] 4.29-hydrate]

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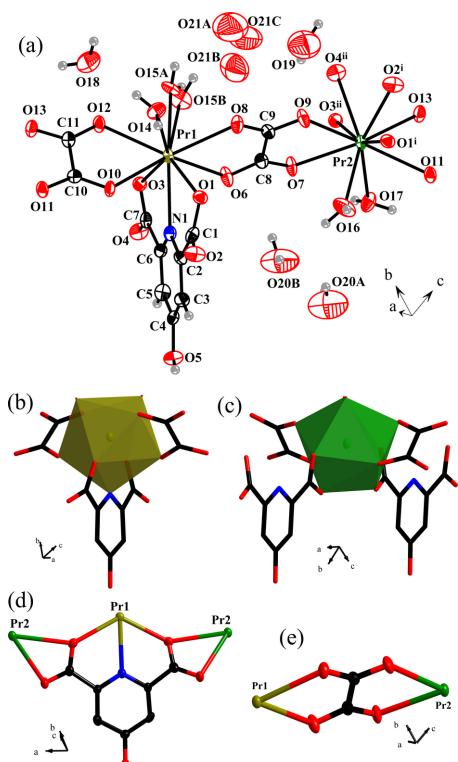
The coordination polymer of crystal formula $[\text{Pr}^{\text{III}}_2(\text{C}_7\text{H}_2\text{NO}_5)(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_4] \cdot 4.29\text{H}_2\text{O}$ or $[\text{Pr}^{\text{III}}_2(\text{HCAM})(\text{ox})_2(\text{H}_2\text{O})_4] \cdot 4.29\text{H}_2\text{O}$ was synthesized from praseodymium(III) nitrate in water using chelidamic acid (H_3CAM) and oxalic acid (H_2ox). There are two Pr^{III} atoms in the asymmetric unit. One metal ion has nine-fold coordination from one pyridyl nitrogen and eight oxygen atoms from one HCAM^{2-} , two ox^{2-} , and two coordinating water molecules leading to the formation of a tricapped trigonal $\{\text{Pr}^{\text{III}}\text{NO}_8\}$ prism. The other metal ion is coordinated by ten oxygen atoms from two HCAM^{2-} , two ox^{2-} , and two coordinating water molecules, forming a bicapped square $\{\text{Pr}^{\text{III}}\text{O}_{10}\}$ unit. The HCAM^{2-} linker has a $\mu_2\text{-}\kappa^2\text{:}\kappa^1$ chelating coordination mode *via* its carboxylates and N-pyridyl donors, linking the $\{\text{Pr}^{\text{III}}\text{NO}_8\}$ and $\{\text{Pr}^{\text{III}}\text{O}_{10}\}$ units into infinite chains. The $\mu_2\text{-}\kappa^1\text{:}\kappa^1\text{:}\kappa^1\text{:}\kappa^1$ bridging carboxylates of the ox^{2-} linkers connect adjacent chains into sheets in the *ac* plane. Adjacent layers further aggregate through intermolecular hydrogen bonding, most of which involves the water molecules of crystallization, and $\pi\text{-}\pi$ interactions to form a tri-periodic supramolecular framework. Some of the co-crystallizing water molecules as well as one of the metal-coordinating water molecules are disordered.



Structure description

A coordination polymer (CP) is a metal coordination compound with repeating coordination entities consisting of metal ions or clusters - the nodes - that are connected through coordinating ligands into an infinite solid-state assembly with different periodicities. Lanthanide-CPs ($\text{Ln}^{\text{III}}\text{-CPs}$) in which the metal nodes are lanthanide ions are of interest as they combine the characteristics of CPs such as an often high chemical and

thermal stability and a capability to be tailor-made to include functional groups with the lanthanide's unique properties based on their various coordination geometries and characteristic optical and magnetic properties (Li *et al.*, 2015; Bünzli, 2014). These merits can provide Ln^{III} -CPs with fascinating structures and functions. Their well-known applications include catalysis (Zhang *et al.*, 2021), luminescent sensing (Wang *et al.*, 2023) and gas adsorption (Roy *et al.*, 2014), to name just a few. All Ln^{III} ions have a high oxophilicity, so organic polycarboxylates are commonly employed as organic linkers in Ln^{III} -CPs (Bünzli, 2014). The high coordination numbers and flexible coordination geometries of Ln^{III} , as well as a lack of directionality of Ln —O bonds do, however, make it difficult to predict the exact nature of the resultant polymeric framework, which is also greatly affected by the choice of solvent used during synthesis, which is often incorporated into the coordination polymer structure (Bünzli, 2014; Patra & Pal, 2025). Owing to their often labile nature, the solvent molecules tend to exhibit disorder, even though they can consolidate the framework structure by promoting intermolecular hydrogen-bonding interactions. The introduction of hydrogen-bond-promoting groups such as hydroxyl on an organic linker is therefore expected to support the framework structure of CPs by transfixing the solvent molecules. Chelidamic acid (H_3CAM) containing an —OH group on a pyridyl ring was selected to be the organic linker to bind with

**Figure 1**

A depiction of (a) an extended asymmetric unit of title compound drawn using 50% probability ellipsoids, (b) $TPRS\{-Pr^{III}NO_8\}$ building unit of Pr1, (c) $SAPRS\{-Pr^{III}O_{10}\}$ building unit of Pr2, (d) coordination mode adopted by $HCAM^{2-}$, and (e) coordination mode adopted by ox^{2-} . [Symmetry codes: (i) $-x, -y + 1, -z + 1$; (ii) $-x + 1, -y + 1, -z + 1$].

Table 1
Selected bond lengths (Å).

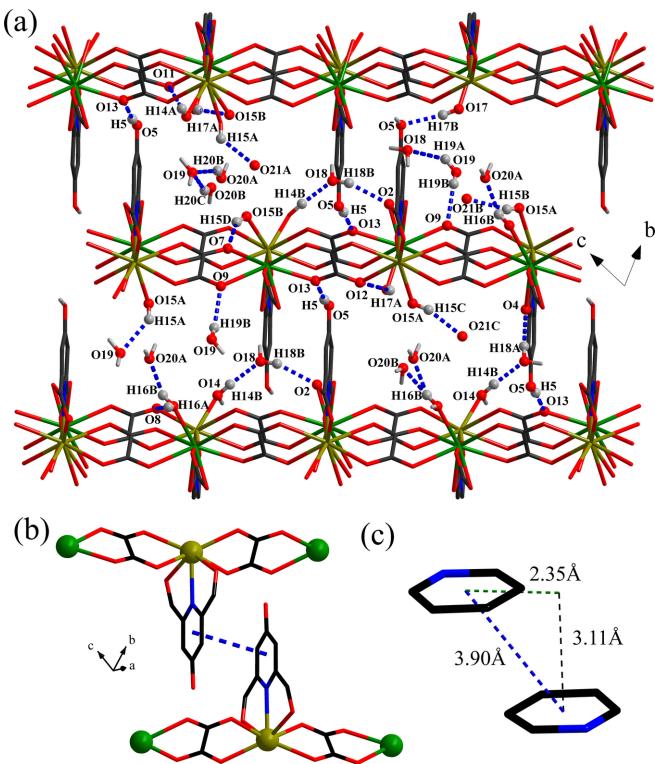
Pr1—O1	2.517 (3)	Pr2—O1 ⁱ	2.746 (3)
Pr1—O3	2.526 (3)	Pr2—O2 ⁱ	2.580 (3)
Pr1—O6	2.503 (3)	Pr2—O3 ⁱⁱ	2.772 (3)
Pr1—O8	2.535 (3)	Pr2—O4 ⁱⁱ	2.608 (3)
Pr1—O10	2.532 (3)	Pr2—O7	2.478 (3)
Pr1—O12	2.520 (3)	Pr2—O9	2.538 (3)
Pr1—O14	2.510 (3)	Pr2—O11 ⁱⁱⁱ	2.519 (3)
Pr1—O15A	2.523 (16)	Pr2—O13 ⁱⁱⁱ	2.550 (3)
Pr1—O15B	2.501 (16)	Pr2—O16	2.496 (4)
Pr1—N1	2.555 (4)	Pr2—O17	2.487 (3)

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

praseodymium(III) (Pr^{III}) in this work. Oxalic acid (H_2Ox) was also used as another small organic linker to help prevent the coordination of labile solvent molecules to the coordination sphere of Pr^{III} and to provide the possibility of obtaining a new Pr^{III} -CP structure with high dimensionality.

The asymmetric unit of the title compound, *i.e.* $[Pr^{III}_2(H-CAM)(ox)_2(H_2O)_4] \cdot 4.29H_2O$, is made up of two Pr^{III} ions (Pr1 and Pr2), one complete $HCAM^{2-}$ dianion, two ox^{2-} dianions, four metal-coordinating water molecules (two at each Pr^{III} ion), and approximately four and a third co-crystallizing water molecules (Fig. 1a). One of the coordinating water molecules is disordered over two sites (O15A and O15B). Two of the four crystallizing water molecule are not disordered (O18 and O19), whilst O20 is hydrogen bonded to its own symmetry equivalent by inversion, inducing site disorder splitting to O20A and O20B, each of which exhibit 50% occupancy. The other co-crystallizing water molecules are extensively disordered and were refined over three partially occupied sites (O21A, O21B and O21C), which share a total site occupancy of 1.294 water molecules. The correlated disorder prevents their hydrogen atoms to be resolved.

The Pr1 and Pr2 ions show two different coordination environments. Pr1 has a nine-fold coordination environment defined by one pyridyl nitrogen atom of $HCAM^{2-}$ and eight oxygen atoms from one $HCAM^{2-}$, two ox^{2-} , and two coordinating water molecules, leading to the formation of a tricapped trigonal-prismatic building unit, *i.e.* $TPRS\{-Pr^{III}NO_8\}$ (Fig. 1b). Pr2 is tenfold coordinated to oxygen atoms from two $HCAM^{2-}$, two ox^{2-} , and two coordinating water molecules, forming a bicapped square antiprism, *i.e.* $SAPRS\{-Pr^{III}O_{10}\}$ (Fig. 1c). The Pr—O bond lengths are in the range of 2.478 (3)–2.550 (3) Å (Table 1), which agrees well with those for other reported Pr^{III} frameworks containing $HCAM^{2-}$ and ox^{2-} (Chen *et al.*, 2008; Zou *et al.*, 2009, 2010, 2011; Zhao *et al.*, 2009). The $HCAM^{2-}$ linker has a $\mu_2\kappa^2:\kappa^1$ chelating coordination mode *via* both carboxylate groups and the N-pyridyl donor, thus creating infinite chains made up from alternating and edge-sharing $TPRS\{-Pr^{III}NO_8\}$ and $SAPRS\{-Pr^{III}O_{10}\}$ units that extend along [100]. The chains are connected to adjacent chains through bridging carboxylates of the ox^{2-} linkers that adopt the common $\mu_2\kappa^1\kappa^1:\kappa^1\kappa^1$ mode of coordination (Fig. 1e) along the *c*-axis, resulting in sheets in the *ac* plane. Neighboring sheets are connected to one another through both hydrogen-bonding interactions involving the

**Figure 2**

Views of (a) hydrogen-bonding interactions in the crystal structure of title compound (only hydrogen atoms involving the hydrogen bonding interactions are shown), (b) interlayer π - π interaction, and (c) displaced π - π stacking geometry.

coordinating and crystallizing water molecules (Table 2, Fig. 2a) and intermolecular π - π interactions between the pyridyl rings of the HCAM^{2-} ligands that protrude from the parallel sheets (Fig. 2b), leading to formation of a tri-periodic supramolecular network. The π - π interactions are slightly offset from each other (Banerjee *et al.*, 2019; Yao *et al.*, 2018) and have a centroid-to-centroid distance of *ca* 3.90 Å, an offset distance of *ca* 2.35 Å, and are exactly parallel (Fig. 2c). The interplanar stacking distance is 3.11 Å. The supramolecular architecture established by these stabilizing interactions has an interlayer distance between parallel sheets of *ca* 9.33 Å. Disregarding the co-crystallized not metal-coordinating water molecules, the total potential solvent area volume within the interlayer space is estimated to be *ca* 20% of the unit-cell volume, based on a calculation performed by PLATON software (Spek, 2020).

Synthesis and crystallization

All chemicals used in this work were obtained commercially and used without purification: Pr_6O_{11} (TJTM, 99.99%), chelidamic acid (H_3CAM ; $\text{C}_7\text{H}_5\text{NO}_5$, Macklin, 98%), oxalic acid ($\text{H}_2\text{Ox}\cdot 2\text{H}_2\text{O}$; $\text{C}_2\text{H}_2\text{O}_4\cdot 2\text{H}_2\text{O}$, Fluka Chemika, ≥99%), nitric acid (HNO_3 , RCI Labscan, 65%). $\text{Pr}^{\text{III}}(\text{NO}_3)_3\cdot 6\text{H}_2\text{O}$ was prepared by dissolving Pr_6O_{11} in small amount of concentrated solution of nitric acid followed by slow crystallization.

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

$D\cdots H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H5···O13 ^{iv}	0.82	1.81	2.626 (4)	170
O14—H14A···O11 ^v	0.82 (2)	1.92 (2)	2.735 (4)	173 (5)
O14—H14B···O18	0.83 (2)	1.93 (2)	2.755 (5)	175 (5)
O15A—H15A···O19 ^{vi}	0.83 (2)	2.16 (4)	2.81 (3)	135 (3)
O15A—H15A···O21A	0.83 (2)	2.26 (2)	2.89 (2)	134 (4)
O15A—H15B···O21B	0.84 (2)	2.02 (9)	2.71 (3)	138 (11)
O15B—H15C···O21C	0.84 (2)	2.15 (6)	2.93 (3)	155 (10)
O15B—H15D···O7 ^{vii}	0.86 (2)	1.96 (4)	2.75 (2)	152 (5)
O16—H16A···O8 ⁱ	0.86 (2)	1.85 (2)	2.705 (4)	179 (5)
O16—H16B···O20A ^{viii}	0.83 (2)	2.17 (4)	2.96 (3)	159 (6)
O16—H16B···O20B	0.83 (2)	2.12 (3)	2.94 (2)	172 (5)
O17—H17A···O12 ^{ix}	0.83 (2)	2.33 (4)	2.922 (4)	129 (4)
O17—H17A···O15A ⁱⁱ	0.83 (2)	2.13 (3)	2.892 (19)	153 (5)
O17—H17A···O15B ⁱⁱ	0.83 (2)	2.15 (3)	2.865 (18)	144 (4)
O17—H17B···O5 ^{vii}	0.83 (2)	2.09 (2)	2.914 (4)	171 (5)
O18—H18A···O4 ^{viii}	0.85 (2)	2.10 (2)	2.951 (6)	177 (6)
O18—H18B···O2 ^v	0.85 (2)	2.21 (3)	3.011 (6)	156 (7)
O19—H19A···O18 ^{vi}	0.83 (2)	2.56 (7)	3.161 (8)	130 (7)
O19—H19B···O9	0.83 (2)	2.15 (2)	2.904 (7)	151 (5)
O20A—H20A···O20B	0.87	2.17	2.901 (14)	141
O20A—H20B···O19 ^{ix}	0.85	2.13	2.87 (3)	146
O20B—H20C···O19 ⁱ	0.85	2.13	2.87 (2)	145

Symmetry codes: (i) $-x, -y + 1, -z + 1$; (ii) $-x + 1, -y + 1, -z + 1$; (iv) $x, y - 1, z$; (v) $-x, -y + 2, -z$; (vi) $-x, -y + 2, -z + 1$; (vii) $-x + 1, -y, -z + 1$; (viii) $x - 1, y + 1, z$; (ix) $x + 1, y - 1, z$.

To synthesize the title compound, a mixture of $\text{Pr}^{\text{III}}(\text{NO}_3)_3\cdot 6\text{H}_2\text{O}$ (43.5 mg, 0.100 mmol), H_3CAM (20.5 mg, 0.100 mmol) and oxalic acid (12.6 mg, 0.100 mmol) was prepared in 10.0 ml of deionized water. The mixture was then transferred to a Teflon lined autoclave and heated at 130°C for 5 d under autogenous pressure. After cooling down to room temperature, brown block-shaped crystals (34% yield based on Pr^{III}) were obtained, collected and washed with deionized water. The crystals were characterized using FT-IR spectroscopy (PerkinElmer/Frontier FT-IR instrument; ATR mode; cm^{-1}): 3675–2814(*br*), 1647(*m*), 1562(*s*), 1443(*m*), 1396(*m*), 1354(*m*), 1305(*m*), 1251(*w*), 1121(*w*), 1027(*m*), 750(*m*), 486(*m*).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

The oxygen atom of a coordinating water molecule (O15) shows site disorder splitting to two sites of O15A and O15B with site occupancies of 0.45 (4) and 0.55 (4), respectively. A SIMU command with an effective standard deviation of 0.01 Å² was used to restrain O15A and O15B to have similar U_{ij}^{eff} components. An oxygen atom of a crystallizing water molecule (O20) is hydrogen bonded to its symmetry-equivalent counterpart which across a nearby inversion center (0.5 0 0.5), inducing disorder and splitting into two sites (O20A and O20B). As O20A and O20B are too close to be compatible with each other, one of them was moved across the inversion center. A SIMU ($s = 0.01, st = 0.01, d_{\text{max}} = 3$) together with a ISOR ($s = 0.01, st = 0.02$) command were applied to O20A and O20B to restrain their U_{ij}^{eff} components to approximate isotropic behavior. The region where O21A, O21B and O21C of water molecules of crystallization were

placed originally contained several large electron densities, with O21B being in hydrogen-bonding distance to its own counterpart by inversion. The large number of permutations prevented an exact disorder modeling or placement of hydrogen atoms. However, the total number of site occupancies in this region was estimated to be about one and a third (1.294). A SIMU ($s = 0.01$, $st = 0.02$, $d_{\max} = 2$) command was applied to O21A, O21B and O21C to restrain to have similar U^{ij} components.

The carbon-bound hydrogen atoms were positioned geometrically and refined isotropically using a riding model (AFIX 43). The C–H bond lengths in the pyridyl ring of HCAM²⁻ were constrained to 0.93 Å [$U_{iso}(\text{H}) = 1.2U_{iso}(\text{C})$]. A hydrogen atom of an –OH group of HCAM²⁻ was positioned geometrically and refined isotropically with allowing a rotation with a tetrahedral C–O–H angle (AFIX 147) to best fit the experimental electron density. The O–H bond length of this –OH group was set to be 0.82 Å [$U_{iso}(\text{H}) = 1.5U_{iso}(\text{O})$]. The hydrogen atoms of water molecules (both coordinating and crystallizing water) were refined isotropically, and the O–H bond lengths and H···H distances were restrained to 0.84 (2) Å and 1.36 (2) Å, respectively, [$U_{iso}(\text{H}) = 1.5U_{iso}(\text{O})$]. There were some hydrogen atoms of water molecules that were additionally restrained based on hydrogen-bonding considerations, *i.e.* H19B···O9 and H20A···O20B distances were restrained to 2.15 (2) Å, and the H15A···O21A distance was restrained to 2.25 (2) Å. The hydrogen atoms of O20A and O20B were initially refined in the same manner while a damping factor was applied. In the final refinement cycles, the damping factor was removed and the hydrogen atoms were constrained to ride on their carrying oxygen atoms (AFIX 3).

Acknowledgements

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Table 3
Experimental details.

Crystal data	[Pr ₂ (C ₇ H ₃ NO ₅)(C ₂ O ₄) ₂ (H ₂ O) ₄]·4.29H ₂ O
Chemical formula	
M_r	785.78
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	298
a, b, c (Å)	9.9236 (3), 10.3042 (4), 12.9748 (5)
α, β, γ (°)	66.684 (4), 80.942 (3), 66.660 (3)
V (Å ³)	1118.69 (8)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	4.41
Crystal size (mm)	0.2 × 0.2 × 0.1
Data collection	
Diffractometer	SuperNova, Single source at offset/far, HyPix3000
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2021)
T_{\min}, T_{\max}	0.768, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18710, 4715, 3799
R_{int}	0.088
(sin θ/λ) _{max} (Å ⁻¹)	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.085, 1.05
No. of reflections	4715
No. of parameters	399
No. of restraints	71
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å ⁻³)	1.47, -1.78

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT2018/2* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

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full crystallographic data

IUCrData (2025). **10**, x250456 [https://doi.org/10.1107/S2414314625004560]

Poly[[tetraaqua(μ_3 -4-hydroxypyridine-2,6-dicarboxylato)di- μ_2 -oxalato-dipraseodymium(III)] 4.29-hydrate]

Aaqib Khurshid, Apinpus Rujiwatra and Thammanoon Chuasaard

Poly[[tetraaqua(μ_3 -4-hydroxypyridine-2,6-dicarboxylato)di- μ_2 -oxalato-dipraseodymium(III)] 4.29-hydrate]

Crystal data



$M_r = 785.78$

Triclinic, $P\bar{1}$

$a = 9.9236 (3)$ Å

$b = 10.3042 (4)$ Å

$c = 12.9748 (5)$ Å

$\alpha = 66.684 (4)^\circ$

$\beta = 80.942 (3)^\circ$

$\gamma = 66.660 (3)^\circ$

$V = 1118.69 (8)$ Å³

$Z = 2$

$F(000) = 757$

$D_x = 2.333$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 11399 reflections

$\theta = 2.3\text{--}27.2^\circ$

$\mu = 4.41$ mm⁻¹

$T = 298$ K

Block, clear brownish colourless

0.2 × 0.2 × 0.1 mm

Data collection

SuperNova, Single source at offset/far,
HyPix3000
diffractometer

Radiation source: micro-focus sealed X-ray
tube, SuperNova (Mo) X-ray Source

Detector resolution: 10.0000 pixels mm⁻¹
 ω scans

Absorption correction: multi-scan
(CrysAlisPro; Rigaku OD, 2021)

$T_{\min} = 0.768$, $T_{\max} = 1.000$

18710 measured reflections

4715 independent reflections

3799 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.088$

$\theta_{\max} = 28.3^\circ$, $\theta_{\min} = 2.2^\circ$

$h = -12 \rightarrow 12$

$k = -12 \rightarrow 12$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.085$

$S = 1.05$

4715 reflections

399 parameters

71 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

$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.47$ e Å⁻³

$\Delta\rho_{\min} = -1.78$ 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.

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	0.23196 (2)	0.77685 (3)	0.25657 (2)	0.01644 (9)	
Pr2	0.23512 (2)	0.29264 (3)	0.76177 (2)	0.01623 (9)	
O1	0.0556 (3)	0.6667 (3)	0.2380 (3)	0.0213 (7)	
O2	-0.0132 (3)	0.5827 (4)	0.1307 (3)	0.0307 (8)	
O3	0.5023 (3)	0.6898 (3)	0.2099 (3)	0.0216 (7)	
O4	0.7077 (3)	0.5102 (4)	0.1918 (3)	0.0289 (8)	
O5	0.4995 (3)	0.2189 (4)	0.0567 (3)	0.0259 (8)	
H5	0.433892	0.212745	0.029681	0.039*	
O6	0.3619 (3)	0.5268 (4)	0.4061 (3)	0.0304 (8)	
O7	0.3719 (3)	0.3733 (4)	0.5863 (3)	0.0252 (8)	
O8	0.0950 (3)	0.7142 (3)	0.4408 (3)	0.0256 (8)	
O9	0.0969 (3)	0.5504 (4)	0.6168 (3)	0.0275 (8)	
O10	0.1736 (3)	0.8820 (3)	0.0496 (2)	0.0213 (7)	
O11	0.1805 (3)	1.0576 (3)	-0.1203 (2)	0.0216 (7)	
O12	0.2910 (3)	1.0092 (3)	0.1385 (3)	0.0242 (7)	
O13	0.3127 (3)	1.1706 (3)	-0.0329 (2)	0.0234 (7)	
O14	-0.0079 (4)	0.9973 (4)	0.2305 (3)	0.0302 (8)	
H14A	-0.066 (5)	0.983 (6)	0.201 (4)	0.045*	
H14B	-0.016 (5)	1.088 (3)	0.200 (4)	0.045*	
O15A	0.298 (3)	0.894 (3)	0.3700 (17)	0.028 (4)	0.45 (4)
H15A	0.234 (5)	0.956 (5)	0.395 (3)	0.043*	0.45 (4)
H15B	0.369 (8)	0.842 (8)	0.415 (8)	0.043*	0.45 (4)
O15B	0.342 (2)	0.828 (3)	0.3904 (16)	0.042 (4)	0.55 (4)
H15C	0.293 (5)	0.859 (12)	0.440 (6)	0.064*	0.55 (4)
H15D	0.427 (5)	0.767 (8)	0.420 (6)	0.064*	0.55 (4)
O16	0.1824 (4)	0.2134 (5)	0.6187 (3)	0.0400 (10)	
H16A	0.094 (3)	0.236 (6)	0.601 (4)	0.060*	
H16B	0.233 (5)	0.209 (7)	0.562 (3)	0.060*	
O17	0.4416 (3)	0.0634 (4)	0.7485 (3)	0.0304 (9)	
H17A	0.522 (3)	0.073 (5)	0.736 (4)	0.046*	
H17B	0.454 (5)	-0.020 (3)	0.800 (3)	0.046*	
O18	-0.0349 (5)	1.2962 (5)	0.1190 (4)	0.0638 (13)	
H18A	-0.109 (5)	1.355 (6)	0.143 (5)	0.096*	
H18B	-0.017 (7)	1.350 (6)	0.053 (3)	0.096*	
O19	-0.1396 (7)	0.7992 (7)	0.6626 (6)	0.106 (2)	
H19A	-0.150 (8)	0.811 (12)	0.724 (5)	0.159*	
H19B	-0.055 (4)	0.743 (7)	0.655 (8)	0.159*	
O20A	0.599 (3)	-0.1133 (16)	0.544 (2)	0.126 (6)	0.5
H20A	0.516875	-0.037798	0.542562	0.189*	0.5

H20B	0.661995	-0.098201	0.570062	0.189*	0.5
O20B	0.389 (3)	0.1898 (16)	0.4318 (19)	0.112 (5)	0.5
H20C	0.299245	0.227002	0.411383	0.168*	0.5
H20D	0.402974	0.255335	0.447541	0.168*	0.5
O21A	0.1227 (19)	0.9358 (19)	0.5629 (13)	0.131 (6)	0.488 (17)
O21C	0.214 (3)	0.838 (3)	0.608 (2)	0.108 (6)	0.253 (13)
O21B	0.3984 (11)	0.7322 (11)	0.5831 (8)	0.097 (5)	0.553 (15)
N1	0.3350 (4)	0.5635 (4)	0.1792 (3)	0.0188 (8)	
C1	0.0848 (5)	0.5939 (5)	0.1735 (4)	0.0228 (11)	
C2	0.2449 (4)	0.5154 (5)	0.1506 (4)	0.0171 (10)	
C3	0.2935 (5)	0.4015 (5)	0.1089 (4)	0.0218 (10)	
H3	0.226867	0.373002	0.088373	0.026*	
C4	0.4425 (5)	0.3294 (5)	0.0978 (4)	0.0194 (10)	
C5	0.5398 (5)	0.3766 (5)	0.1287 (4)	0.0237 (11)	
H5A	0.640885	0.328970	0.123911	0.028*	
C6	0.4805 (4)	0.4958 (5)	0.1664 (4)	0.0181 (10)	
C7	0.5711 (5)	0.5680 (5)	0.1928 (4)	0.0193 (10)	
C9	0.1529 (5)	0.5941 (5)	0.5226 (4)	0.0193 (10)	
C8	0.3103 (5)	0.4884 (5)	0.5036 (4)	0.0202 (10)	
C11	0.2745 (5)	1.0625 (5)	0.0363 (4)	0.0195 (10)	
C10	0.2019 (5)	0.9932 (5)	-0.0159 (4)	0.0177 (10)	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.01715 (16)	0.01723 (16)	0.01250 (17)	-0.00734 (12)	0.00045 (11)	-0.00222 (12)
Pr2	0.01536 (16)	0.01812 (15)	0.01234 (16)	-0.00743 (12)	0.00053 (11)	-0.00168 (12)
O1	0.0189 (16)	0.0243 (18)	0.0231 (19)	-0.0089 (14)	0.0049 (13)	-0.0122 (15)
O2	0.0163 (17)	0.043 (2)	0.045 (2)	-0.0117 (16)	0.0039 (15)	-0.0283 (18)
O3	0.0233 (18)	0.0244 (18)	0.0215 (19)	-0.0128 (15)	0.0024 (14)	-0.0097 (15)
O4	0.0166 (18)	0.032 (2)	0.042 (2)	-0.0098 (15)	0.0002 (15)	-0.0170 (18)
O5	0.0178 (17)	0.0267 (18)	0.038 (2)	-0.0046 (15)	-0.0057 (15)	-0.0177 (16)
O6	0.0258 (19)	0.034 (2)	0.0159 (19)	-0.0058 (16)	0.0034 (14)	-0.0006 (16)
O7	0.0206 (17)	0.0287 (19)	0.0137 (18)	-0.0078 (15)	-0.0005 (13)	0.0034 (15)
O8	0.0241 (18)	0.0224 (18)	0.0198 (19)	-0.0068 (15)	0.0003 (14)	0.0008 (15)
O9	0.0251 (18)	0.033 (2)	0.0153 (19)	-0.0090 (15)	0.0067 (14)	-0.0035 (15)
O10	0.0301 (18)	0.0207 (17)	0.0138 (18)	-0.0158 (15)	-0.0012 (13)	-0.0001 (14)
O11	0.0257 (18)	0.0258 (18)	0.0132 (18)	-0.0136 (15)	-0.0039 (13)	-0.0016 (14)
O12	0.0335 (19)	0.0266 (18)	0.0133 (19)	-0.0168 (15)	-0.0052 (14)	-0.0004 (15)
O13	0.0284 (18)	0.0259 (18)	0.0181 (19)	-0.0177 (15)	-0.0024 (14)	-0.0017 (15)
O14	0.027 (2)	0.0250 (19)	0.040 (2)	-0.0093 (16)	-0.0066 (16)	-0.0112 (18)
O15A	0.029 (9)	0.042 (9)	0.023 (7)	-0.012 (7)	0.004 (5)	-0.023 (7)
O15B	0.028 (7)	0.060 (11)	0.046 (7)	-0.016 (7)	0.000 (5)	-0.027 (8)
O16	0.026 (2)	0.069 (3)	0.039 (3)	-0.019 (2)	0.0060 (18)	-0.034 (2)
O17	0.0188 (18)	0.0220 (19)	0.041 (2)	-0.0083 (15)	0.0046 (16)	-0.0036 (16)
O18	0.075 (4)	0.036 (3)	0.070 (4)	-0.012 (2)	0.003 (3)	-0.019 (2)
O19	0.098 (4)	0.087 (4)	0.116 (5)	-0.008 (4)	0.010 (4)	-0.049 (4)
O20A	0.125 (7)	0.110 (13)	0.150 (10)	-0.017 (11)	-0.032 (7)	-0.069 (11)

O20B	0.124 (7)	0.097 (12)	0.131 (10)	-0.017 (10)	-0.027 (7)	-0.071 (11)
O21A	0.160 (12)	0.094 (10)	0.119 (10)	-0.013 (8)	-0.012 (8)	-0.048 (8)
O21C	0.145 (11)	0.082 (9)	0.089 (9)	-0.011 (8)	-0.020 (8)	-0.047 (8)
O21B	0.115 (8)	0.081 (7)	0.063 (7)	-0.006 (6)	-0.017 (5)	-0.019 (5)
N1	0.015 (2)	0.021 (2)	0.019 (2)	-0.0091 (17)	0.0012 (16)	-0.0049 (17)
C1	0.019 (3)	0.018 (2)	0.029 (3)	-0.009 (2)	0.001 (2)	-0.004 (2)
C2	0.014 (2)	0.023 (2)	0.014 (2)	-0.0065 (19)	-0.0006 (18)	-0.007 (2)
C3	0.023 (3)	0.028 (3)	0.022 (3)	-0.014 (2)	-0.001 (2)	-0.011 (2)
C4	0.024 (3)	0.014 (2)	0.017 (3)	-0.007 (2)	-0.0011 (19)	-0.002 (2)
C5	0.015 (2)	0.026 (3)	0.027 (3)	-0.005 (2)	-0.005 (2)	-0.007 (2)
C6	0.018 (2)	0.017 (2)	0.018 (3)	-0.0061 (19)	-0.0011 (19)	-0.005 (2)
C7	0.018 (3)	0.023 (3)	0.016 (3)	-0.011 (2)	-0.0003 (19)	-0.002 (2)
C9	0.016 (2)	0.023 (3)	0.017 (3)	-0.006 (2)	0.0000 (19)	-0.007 (2)
C8	0.016 (2)	0.024 (3)	0.020 (3)	-0.008 (2)	0.001 (2)	-0.007 (2)
C11	0.015 (2)	0.023 (3)	0.019 (3)	-0.008 (2)	-0.0031 (19)	-0.004 (2)
C10	0.015 (2)	0.020 (2)	0.019 (3)	-0.0051 (19)	-0.0039 (18)	-0.007 (2)

Geometric parameters (\AA , ^\circ)

Pr1—O1	2.517 (3)	O11—C10	1.260 (5)
Pr1—O3	2.526 (3)	O12—C11	1.227 (5)
Pr1—O6	2.503 (3)	O13—C11	1.275 (5)
Pr1—O8	2.535 (3)	O14—H14A	0.821 (19)
Pr1—O10	2.532 (3)	O14—H14B	0.832 (19)
Pr1—O12	2.520 (3)	O15A—H15A	0.830 (19)
Pr1—O14	2.510 (3)	O15A—H15B	0.84 (2)
Pr1—O15A	2.523 (16)	O15B—H15C	0.84 (2)
Pr1—O15B	2.501 (16)	O15B—H15D	0.86 (2)
Pr1—N1	2.555 (4)	O16—H16A	0.856 (19)
Pr2—O1 ⁱ	2.746 (3)	O16—H16B	0.826 (19)
Pr2—O2 ⁱ	2.580 (3)	O17—H17A	0.826 (18)
Pr2—O3 ⁱⁱ	2.772 (3)	O17—H17B	0.832 (19)
Pr2—O4 ⁱⁱ	2.608 (3)	O18—H18A	0.85 (2)
Pr2—O7	2.478 (3)	O18—H18B	0.85 (2)
Pr2—O9	2.538 (3)	O19—H19A	0.83 (2)
Pr2—O11 ⁱⁱⁱ	2.519 (3)	O19—H19B	0.831 (19)
Pr2—O13 ⁱⁱⁱ	2.550 (3)	O20A—H20A	0.8688
Pr2—O16	2.496 (4)	O20A—H20B	0.8471
Pr2—O17	2.487 (3)	O20B—H20C	0.8540
Pr2—C1 ⁱ	3.025 (4)	O20B—H20D	0.8435
Pr2—C7 ⁱⁱ	3.054 (4)	N1—C2	1.336 (5)
O1—C1	1.263 (5)	N1—C6	1.348 (5)
O2—C1	1.256 (5)	C1—C2	1.513 (6)
O3—C7	1.259 (5)	C2—C3	1.370 (6)
O4—C7	1.247 (5)	C3—H3	0.9300
O5—H5	0.8200	C3—C4	1.381 (6)
O5—C4	1.333 (5)	C4—C5	1.407 (6)
O6—C8	1.256 (5)	C5—H5A	0.9300

O7—C8	1.248 (5)	C5—C6	1.381 (6)
O8—C9	1.256 (5)	C6—C7	1.519 (6)
O9—C9	1.247 (5)	C9—C8	1.559 (7)
O10—C10	1.235 (5)	C11—C10	1.559 (6)
O1—Pr1—O3	125.52 (9)	O16—Pr2—O9	79.58 (12)
O1—Pr1—O8	71.98 (10)	O16—Pr2—O11 ⁱⁱⁱ	77.00 (11)
O1—Pr1—O10	73.53 (9)	O16—Pr2—O13 ⁱⁱⁱ	137.51 (12)
O1—Pr1—O12	134.40 (10)	O16—Pr2—C1 ⁱ	92.58 (12)
O1—Pr1—O15A	144.9 (4)	O16—Pr2—C7 ⁱⁱ	142.54 (11)
O1—Pr1—N1	63.08 (10)	O17—Pr2—O1 ⁱ	123.96 (10)
O3—Pr1—O8	131.86 (10)	O17—Pr2—O2 ⁱ	150.18 (10)
O3—Pr1—O10	89.35 (9)	O17—Pr2—O3 ⁱⁱ	70.95 (10)
O3—Pr1—N1	62.46 (10)	O17—Pr2—O4 ⁱⁱ	119.01 (10)
O6—Pr1—O1	88.21 (10)	O17—Pr2—O9	133.08 (10)
O6—Pr1—O3	71.33 (10)	O17—Pr2—O11 ⁱⁱⁱ	70.13 (10)
O6—Pr1—O8	64.40 (10)	O17—Pr2—O13 ⁱⁱⁱ	82.94 (11)
O6—Pr1—O10	138.63 (11)	O17—Pr2—O16	69.13 (12)
O6—Pr1—O12	135.43 (9)	O17—Pr2—C1 ⁱ	142.91 (10)
O6—Pr1—O14	138.35 (11)	O17—Pr2—C7 ⁱⁱ	95.28 (11)
O6—Pr1—O15A	85.8 (7)	C1 ⁱ —Pr2—C7 ⁱⁱ	116.61 (12)
O6—Pr1—N1	68.80 (11)	Pr1—O1—Pr2 ⁱ	144.80 (13)
O8—Pr1—N1	114.36 (10)	C1—O1—Pr1	120.3 (3)
O10—Pr1—O8	137.05 (9)	C1—O1—Pr2 ⁱ	90.1 (2)
O10—Pr1—N1	69.83 (10)	C1—O2—Pr2 ⁱ	98.1 (3)
O12—Pr1—O3	72.10 (10)	Pr1—O3—Pr2 ⁱⁱ	143.18 (13)
O12—Pr1—O8	131.56 (10)	C7—O3—Pr1	123.1 (3)
O12—Pr1—O10	64.34 (9)	C7—O3—Pr2 ⁱⁱ	90.4 (2)
O12—Pr1—O15A	66.4 (5)	C7—O4—Pr2 ⁱⁱ	98.6 (3)
O12—Pr1—N1	114.05 (10)	C4—O5—H5	109.5
O14—Pr1—O1	78.28 (10)	C8—O6—Pr1	121.4 (3)
O14—Pr1—O3	146.68 (10)	C8—O7—Pr2	121.3 (3)
O14—Pr1—O8	73.95 (10)	C9—O8—Pr1	120.6 (3)
O14—Pr1—O10	74.65 (11)	C9—O9—Pr2	119.4 (3)
O14—Pr1—O12	74.62 (10)	C10—O10—Pr1	120.7 (3)
O14—Pr1—O15A	83.6 (6)	C10—O11—Pr2 ^{iv}	123.2 (3)
O14—Pr1—N1	133.09 (11)	C11—O12—Pr1	120.1 (3)
O15A—Pr1—O3	84.8 (5)	C11—O13—Pr2 ^{iv}	121.0 (3)
O15A—Pr1—O8	74.3 (4)	Pr1—O14—H14A	108 (4)
O15A—Pr1—O10	129.7 (6)	Pr1—O14—H14B	124 (3)
O15A—Pr1—N1	143.2 (6)	H14A—O14—H14B	110 (5)
O15B—Pr1—O1	144.6 (4)	Pr1—O15A—H15A	122 (3)
O15B—Pr1—O3	76.7 (5)	Pr1—O15A—H15B	121 (3)
O15B—Pr1—O6	72.4 (7)	H15A—O15A—H15B	109 (3)
O15B—Pr1—O8	72.9 (4)	Pr1—O15B—H15C	123 (3)
O15B—Pr1—O10	139.4 (5)	Pr1—O15B—H15D	121 (3)
O15B—Pr1—O12	75.1 (6)	H15C—O15B—H15D	105 (3)
O15B—Pr1—O14	96.5 (6)	Pr2—O16—H16A	121 (3)

O15B—Pr1—N1	130.4 (6)	Pr2—O16—H16B	124 (3)
O1 ⁱ —Pr2—O3 ⁱⁱ	164.06 (9)	H16A—O16—H16B	107 (6)
O1 ⁱ —Pr2—C1 ⁱ	24.67 (10)	Pr2—O17—H17A	114 (4)
O1 ⁱ —Pr2—C7 ⁱⁱ	140.12 (11)	Pr2—O17—H17B	119 (3)
O2 ⁱ —Pr2—O1 ⁱ	48.86 (9)	H17A—O17—H17B	107 (3)
O2 ⁱ —Pr2—O3 ⁱⁱ	115.62 (9)	H18A—O18—H18B	106 (3)
O2 ⁱ —Pr2—O4 ⁱⁱ	72.16 (9)	H19A—O19—H19B	112 (4)
O2 ⁱ —Pr2—C1 ⁱ	24.28 (11)	H20A—O20A—H20B	105.4
O2 ⁱ —Pr2—C7 ⁱⁱ	93.86 (11)	H20C—O20B—H20D	107.1
O3 ⁱⁱ —Pr2—C1 ⁱ	139.57 (11)	C2—N1—Pr1	120.4 (3)
O3 ⁱⁱ —Pr2—C7 ⁱⁱ	24.35 (10)	C2—N1—C6	118.0 (4)
O4 ⁱⁱ —Pr2—O1 ⁱ	116.38 (9)	C6—N1—Pr1	121.6 (3)
O4 ⁱⁱ —Pr2—O3 ⁱⁱ	48.16 (9)	O1—C1—Pr2 ⁱ	65.2 (2)
O4 ⁱⁱ —Pr2—C1 ⁱ	93.52 (11)	O1—C1—C2	117.6 (4)
O4 ⁱⁱ —Pr2—C7 ⁱⁱ	23.81 (11)	O2—C1—Pr2 ⁱ	57.6 (2)
O7—Pr2—O1 ⁱ	122.36 (9)	O2—C1—O1	122.4 (4)
O7—Pr2—O2 ⁱ	137.91 (11)	O2—C1—C2	120.0 (4)
O7—Pr2—O3 ⁱⁱ	64.97 (9)	C2—C1—Pr2 ⁱ	172.1 (3)
O7—Pr2—O4 ⁱⁱ	84.16 (10)	N1—C2—C1	113.6 (4)
O7—Pr2—O9	64.76 (10)	N1—C2—C3	123.1 (4)
O7—Pr2—O11 ⁱⁱⁱ	136.21 (10)	C3—C2—C1	123.2 (4)
O7—Pr2—O13 ⁱⁱⁱ	131.51 (9)	C2—C3—H3	120.4
O7—Pr2—O16	69.72 (11)	C2—C3—C4	119.2 (4)
O7—Pr2—O17	71.87 (10)	C4—C3—H3	120.4
O7—Pr2—C1 ⁱ	133.16 (11)	O5—C4—C3	123.3 (4)
O7—Pr2—C7 ⁱⁱ	73.09 (11)	O5—C4—C5	117.9 (4)
O9—Pr2—O1 ⁱ	70.34 (9)	C3—C4—C5	118.8 (4)
O9—Pr2—O2 ⁱ	75.37 (10)	C4—C5—H5A	121.1
O9—Pr2—O3 ⁱⁱ	104.33 (9)	C6—C5—C4	117.9 (4)
O9—Pr2—O4 ⁱⁱ	74.22 (10)	C6—C5—H5A	121.1
O9—Pr2—O13 ⁱⁱⁱ	140.30 (10)	N1—C6—C5	123.0 (4)
O9—Pr2—C1 ⁱ	69.61 (11)	N1—C6—C7	113.3 (4)
O9—Pr2—C7 ⁱⁱ	88.79 (11)	C5—C6—C7	123.7 (4)
O11 ⁱⁱⁱ —Pr2—O1 ⁱ	66.23 (9)	O3—C7—Pr2 ⁱⁱ	65.2 (2)
O11 ⁱⁱⁱ —Pr2—O2 ⁱ	82.52 (10)	O3—C7—C6	117.1 (4)
O11 ⁱⁱⁱ —Pr2—O3 ⁱⁱ	119.82 (9)	O4—C7—Pr2 ⁱⁱ	57.6 (2)
O11 ⁱⁱⁱ —Pr2—O4 ⁱⁱ	133.81 (10)	O4—C7—O3	122.8 (4)
O11 ⁱⁱⁱ —Pr2—O9	135.73 (9)	O4—C7—C6	120.0 (4)
O11 ⁱⁱⁱ —Pr2—O13 ⁱⁱⁱ	63.37 (9)	C6—C7—Pr2 ⁱⁱ	177.2 (3)
O11 ⁱⁱⁱ —Pr2—C1 ⁱ	74.49 (10)	O8—C9—C8	116.4 (4)
O11 ⁱⁱⁱ —Pr2—C7 ⁱⁱ	131.07 (11)	O9—C9—O8	126.7 (4)
O13 ⁱⁱⁱ —Pr2—O1 ⁱ	106.12 (9)	O9—C9—C8	116.9 (4)
O13 ⁱⁱⁱ —Pr2—O2 ⁱ	74.10 (10)	O6—C8—C9	116.7 (4)
O13 ⁱⁱⁱ —Pr2—O3 ⁱⁱ	67.88 (9)	O7—C8—O6	126.5 (4)
O13 ⁱⁱⁱ —Pr2—O4 ⁱⁱ	72.69 (10)	O7—C8—C9	116.8 (4)
O13 ⁱⁱⁱ —Pr2—C1 ⁱ	91.14 (12)	O12—C11—O13	125.7 (4)
O13 ⁱⁱⁱ —Pr2—C7 ⁱⁱ	68.71 (10)	O12—C11—C10	118.3 (4)
O16—Pr2—O1 ⁱ	68.24 (10)	O13—C11—C10	115.9 (4)

O16—Pr2—O2 ⁱ	116.84 (10)	O10—C10—O11	128.1 (4)
O16—Pr2—O3 ⁱⁱ	126.51 (10)	O10—C10—C11	116.3 (4)
O16—Pr2—O4 ⁱⁱ	149.02 (12)	O11—C10—C11	115.6 (4)
Pr1—O1—C1—Pr2 ⁱ	−161.4 (3)	Pr2 ^{iv} —O11—C10—C11	−3.7 (5)
Pr1—O1—C1—O2	−154.6 (3)	Pr2 ^{iv} —O13—C11—O12	−170.6 (4)
Pr1—O1—C1—C2	26.9 (5)	Pr2 ^{iv} —O13—C11—C10	9.8 (5)
Pr1—O3—C7—Pr2 ⁱⁱ	−163.8 (3)	O1—C1—C2—N1	−15.8 (6)
Pr1—O3—C7—O4	−165.4 (3)	O1—C1—C2—C3	161.7 (4)
Pr1—O3—C7—C6	17.9 (5)	O2—C1—C2—N1	165.7 (4)
Pr1—O6—C8—O7	−173.3 (3)	O2—C1—C2—C3	−16.9 (6)
Pr1—O6—C8—C9	7.5 (5)	O5—C4—C5—C6	177.0 (4)
Pr1—O8—C9—O9	−179.6 (3)	O8—C9—C8—O6	−4.7 (6)
Pr1—O8—C9—C8	−0.3 (5)	O8—C9—C8—O7	176.0 (4)
Pr1—O10—C10—O11	179.5 (3)	O9—C9—C8—O6	174.6 (4)
Pr1—O10—C10—C11	0.1 (5)	O9—C9—C8—O7	−4.6 (6)
Pr1—O12—C11—O13	−173.4 (3)	O12—C11—C10—O10	−4.2 (7)
Pr1—O12—C11—C10	6.1 (6)	O12—C11—C10—O11	176.3 (4)
Pr1—N1—C2—C1	−2.4 (5)	O13—C11—C10—O10	175.3 (4)
Pr1—N1—C2—C3	−179.9 (3)	O13—C11—C10—O11	−4.1 (6)
Pr1—N1—C6—C5	177.6 (3)	N1—C2—C3—C4	1.5 (7)
Pr1—N1—C6—C7	−4.8 (5)	N1—C6—C7—O3	−8.1 (6)
Pr2 ⁱ —O1—C1—O2	6.8 (4)	N1—C6—C7—O4	175.1 (4)
Pr2 ⁱ —O1—C1—C2	−171.7 (3)	C1—C2—C3—C4	−175.7 (4)
Pr2 ⁱ —O2—C1—O1	−7.3 (5)	C2—N1—C6—C5	−2.1 (6)
Pr2 ⁱ —O2—C1—C2	171.2 (3)	C2—N1—C6—C7	175.5 (4)
Pr2 ⁱⁱ —O3—C7—O4	−1.6 (4)	C2—C3—C4—O5	−179.1 (4)
Pr2 ⁱⁱ —O3—C7—C6	−178.3 (3)	C2—C3—C4—C5	−0.6 (6)
Pr2 ⁱⁱ —O4—C7—O3	1.7 (5)	C3—C4—C5—C6	−1.5 (6)
Pr2 ⁱⁱ —O4—C7—C6	178.3 (3)	C4—C5—C6—N1	3.0 (7)
Pr2—O7—C8—O6	−168.6 (3)	C4—C5—C6—C7	−174.4 (4)
Pr2—O7—C8—C9	10.6 (5)	C5—C6—C7—O3	169.5 (4)
Pr2—O9—C9—O8	175.9 (3)	C5—C6—C7—O4	−7.3 (7)
Pr2—O9—C9—C8	−3.3 (5)	C6—N1—C2—C1	177.3 (4)
Pr2 ^{iv} —O11—C10—O10	176.9 (3)	C6—N1—C2—C3	−0.2 (6)

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

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

$D\cdots H$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
O5—H5 \cdots O13 ^v	0.82	1.81	2.626 (4)	170
O14—H14A \cdots O11 ^{vi}	0.82 (2)	1.92 (2)	2.735 (4)	173 (5)
O14—H14B \cdots O18	0.83 (2)	1.93 (2)	2.755 (5)	175 (5)
O15A—H15A \cdots O19 ^{vii}	0.83 (2)	2.16 (4)	2.81 (3)	135 (3)
O15A—H15A \cdots O21A	0.83 (2)	2.26 (2)	2.89 (2)	134 (4)
O15A—H15B \cdots O21B	0.84 (2)	2.02 (9)	2.71 (3)	138 (11)
O15B—H15C \cdots O21C	0.84 (2)	2.15 (6)	2.93 (3)	155 (10)

O15 <i>B</i> —H15 <i>D</i> ···O7 ⁱⁱ	0.86 (2)	1.96 (4)	2.75 (2)	152 (5)
O16—H16 <i>A</i> ···O8 ⁱ	0.86 (2)	1.85 (2)	2.705 (4)	179 (5)
O16—H16 <i>B</i> ···O20 <i>A</i> ^{viii}	0.83 (2)	2.17 (4)	2.96 (3)	159 (6)
O16—H16 <i>B</i> ···O20 <i>B</i>	0.83 (2)	2.12 (3)	2.94 (2)	172 (5)
O17—H17 <i>A</i> ···O12 ⁱⁱ	0.83 (2)	2.33 (4)	2.922 (4)	129 (4)
O17—H17 <i>A</i> ···O15 <i>A</i> ⁱⁱ	0.83 (2)	2.13 (3)	2.892 (19)	153 (5)
O17—H17 <i>A</i> ···O15 <i>B</i> ⁱⁱ	0.83 (2)	2.15 (3)	2.865 (18)	144 (4)
O17—H17 <i>B</i> ···O5 ^{viii}	0.83 (2)	2.09 (2)	2.914 (4)	171 (5)
O18—H18 <i>A</i> ···O4 ^{ix}	0.85 (2)	2.10 (2)	2.951 (6)	177 (6)
O18—H18 <i>B</i> ···O2 ^{vi}	0.85 (2)	2.21 (3)	3.011 (6)	156 (7)
O19—H19 <i>A</i> ···O18 ^{vii}	0.83 (2)	2.56 (7)	3.161 (8)	130 (7)
O19—H19 <i>B</i> ···O9	0.83 (2)	2.15 (2)	2.904 (7)	151 (5)
O20 <i>A</i> —H20 <i>A</i> ···O20 <i>B</i>	0.87	2.17	2.901 (14)	141
O20 <i>A</i> —H20 <i>B</i> ···O19 ^x	0.85	2.13	2.87 (3)	146
O20 <i>B</i> —H20 <i>C</i> ···O19 ⁱ	0.85	2.13	2.87 (2)	145

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+1$; (v) $x, y-1, z$; (vi) $-x, -y+2, -z$; (vii) $-x, -y+2, -z+1$; (viii) $-x+1, -y, -z+1$; (ix) $x-1, y+1, z$; (x) $x+1, y-1, z$.