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# *catena*-Poly[[diaqua[$\mu_2$-4-(4-carboxyphenoxy)benzoato]($\mu_2$-4,4′-oxydibenzoato)praseodymium(III)] monohydrate]

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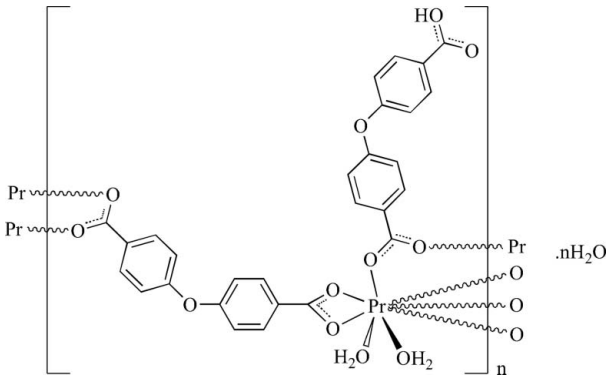
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.025; $wR$ factor = 0.059; data-to-parameter ratio = 13.0.

In the title compound, $\{[Pr(C_{14}H_8O_5)(C_{14}H_9O_5)(H_2O)_2]\cdot H_2O\}_n$, the $Pr^{III}$ cation is eight-coordinated by six carboxyl O atoms from both a monoanionic 4-(4-carboxyphenoxy)benzoate and a dianionic 4,4′-oxydibenzoate ligand (four bridging with two from a bidentate chelate interaction), and two O-atom donors from water molecules. A single water molecule of solvation is also present. The complex units are linked through carboxyl *O*:*O*′ bridges giving a two-dimensional sheet polymer lying parallel to (001). An overall three-dimensional network structure is generated through intermolecular carboxylic acid and water O—H···O hydrogen bonds and weak C—H···O interactions.

## Related literature

For the potential properties of metal-organic complexes involving polycarboxylate ligands, see: Li *et al.* (2011); Wang *et al.* (2004, 2005); Lin *et al.* (2010); Sun *et al.* (2009); Xu *et al.* (2011); Łyszczek & Mazur (2012). For similar structures, see: Thirumurugan & Natarajan (2004); Zhang *et al.* (2005).




## Experimental

### Crystal data

$[Pr(C_{14}H_8O_5)(C_{14}H_9O_5)(H_2O)_2]\cdot H_2O$
$M_r$ = 708.37
Monoclinic, $C2/c$
$a$ = 27.3970 (17) Å
$b$ = 9.5764 (6) Å
$c$ = 21.6754 (14) Å
$\beta$ = 97.433 (1)°
$V$ = 5639.1 (6) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 1.80 mm$^{-1}$
$T$ = 296 K
0.21 × 0.16 × 0.15 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min}$ = 0.704, $T_{max}$ = 0.774
20449 measured reflections
4972 independent reflections
4498 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.059
$S$ = 1.08
4972 reflections
381 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.51 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Pr1—O9$^{i}$ | 2.3983 (18) | Pr1—O11 | 2.4719 (18) |
| Pr1—O5 | 2.4105 (19) | Pr1—O10 | 2.5152 (19) |
| Pr1—O12$^{ii}$ | 2.412 (2) | Pr1—O1 | 2.5163 (19) |
| Pr1—O8$^{iii}$ | 2.4692 (19) | Pr1—O7$^{iii}$ | 2.6534 (19) |

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

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3···O1$^{iv}$ | 0.82 | 2.02 | 2.822 (3) | 166 |
| O10—H10$B$···O2$^{v}$ | 0.85 | 2.09 | 2.880 (3) | 154 |
| O11—H11$A$···O4$^{vi}$ | 0.84 | 1.84 | 2.683 (3) | 176 |
| O11—H11$B$···O8$^{vii}$ | 0.84 | 1.89 | 2.707 (3) | 163 |
| C9—H9···O3$^{vi}$ | 0.93 | 2.48 | 3.337 (4) | 153 |
| C25—H25···O13$^{iii}$ | 0.93 | 2.59 | 3.454 (7) | 155 |

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2278).

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# supporting information

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## *catena*-Poly[[diaqua[$\mu_2$-4-(4-carboxyphenoxy)benzoato]($\mu_2$-4,4′-oxydibenzoato)praseodymium(III)] monohydrate]

**Ping Li, Duo-Meng Su and Chang-Ge Zheng**

### S1. Comment

Metal–organic frameworks (MOFs) with lanthanides have attracted much attention because of their abundant structural chemistry and valuable optical and magnetic properties (Lin *et al.*, 2010). In contrast to coordination polymers with other transition metals, the architecture of lanthanide coordination polymers is hard to control owing to large coordination numbers and flexible coordination geometries of the lanthanide atom. The ligand 4-(4-carboxyphenoxy)benzoic acid ($H_2$oba) can be deprotonated, giving Hoba$^-$ or oba$^{2-}$ species and as *V*-shaped ligands, they can offer more many coordination modes compared to a linear ligand. Owing to the nonlinear flexibility around the etheric oxygen, this ligand can readily generate helical coordination polymers (Łyszczek & Mazur, 2012).

In the title praseodymium(III) complex with 4-(4-carboxyphenoxy)benzoic acid, $\{[Pr(C_{14}H_{11}O_6)(C_{14}H_{10}O_6)(H_2O)_2]\cdot H_2O\}_n$, the $Pr^{III}$ cations have irregular eight-coordinate stereochemistry, the asymmetric unit comprising one $Pr^{III}$ cation, an an Hoba$^-$ ligand, an oba$^{2-}$ ligand, two monodentate water molecules (O10 and O11) and one water molecule of solvation (O13) (Fig. 1). There are two types of coordination modes with the oba$^{2-}$ and Hoba$^-$ ligands: (*a*) two carboxylate groups of the oba$^{2-}$ ligand adopt a bridging bidentate mode (O5, O12$^{ii}$) and a bidentate chelate mode (O7$^{iii}$, O8$^{iii}$), respectively, connecting three $Pr^{III}$ atoms; (*b*) one carboxylate group of the Hoba$^-$ ligand adopts a bridging bidentate (O1, O9$^{i}$) mode, connecting two $Pr^{III}$ atoms. For symmetry codes, see Table 1. The carboxylic acid group (O4, O3) is uncoordinated. The Pr—O bond lengths [range 2.3983 (18)–2.6534 (19) Å] (Table 1) are comparable with those in similar $Pr^{III}$ complexes (Thirumurugan & Natarajan, 2004; Zhang *et al.*, 2005). A two-dimensional coordination polymer is generated, lying parallel to (0 0 1). Adjacent layers are joined into a three-dimensional framework structure (Fig. 2) through intermolecular carboxylic acid and water O—H···O hydrogen bonds and weak C—H···O hydrogen-bonding interactions (Table 2).

### S2. Experimental

A mixture of 4-(4-carboxyphenoxy)benzoic acid (0.026 g, 0.1 mmol), $Pr(NO_3)_3\,6H_2O$ (0.15 mmol, 62.2 mg), and deionized water (8 ml) was sealed in a teflon-lined stainless steel vessel (25 ml) and heated at 433 K for 72 h. The vessel was then cooled slowly to room temperature. Green block-like crystals were obtained by filtration and washed with water. Yield: 50.4 mg (47.5%, based on Pr). Elemental analysis: calcd. for $C_{28}H_{23}O_{13}Pr$, C 47.59%, H 3.25%. Found: C 47.48%, H 3.19%.

### S3. Refinement

C-Bound H atoms were were placed in calculated positions and were treated as riding, with C—H = 0.93 Å, with $U_{iso}$(H) = 1.2$U_{eq}$(C). O-Bound H-atoms were also placed in calculated positions (O—H = 0.82–0.85 Å) and were allowed to ride with $U_{iso}$(H) = 1.2–1.5$U_{eq}$(O).

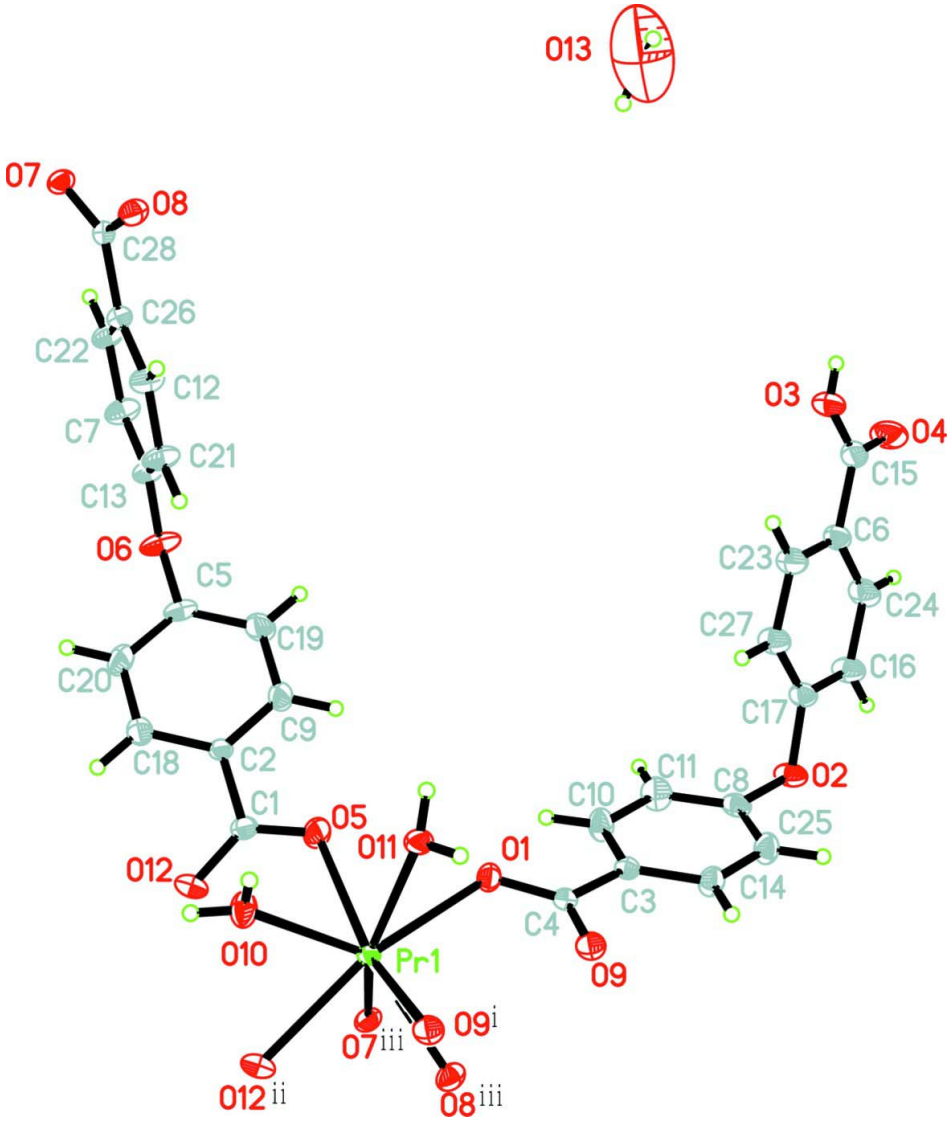


**Figure 1**

The asymmetric unit of the title complex showing 30% probability displacement ellipsoids and the atom-numbering scheme. For symmetry codes: (i) -*x*, -*y* +1, -*z*; (ii) -*x*, -*y*, -*z*; (iii) *x* -1/2, *y* +1/2, *z*.

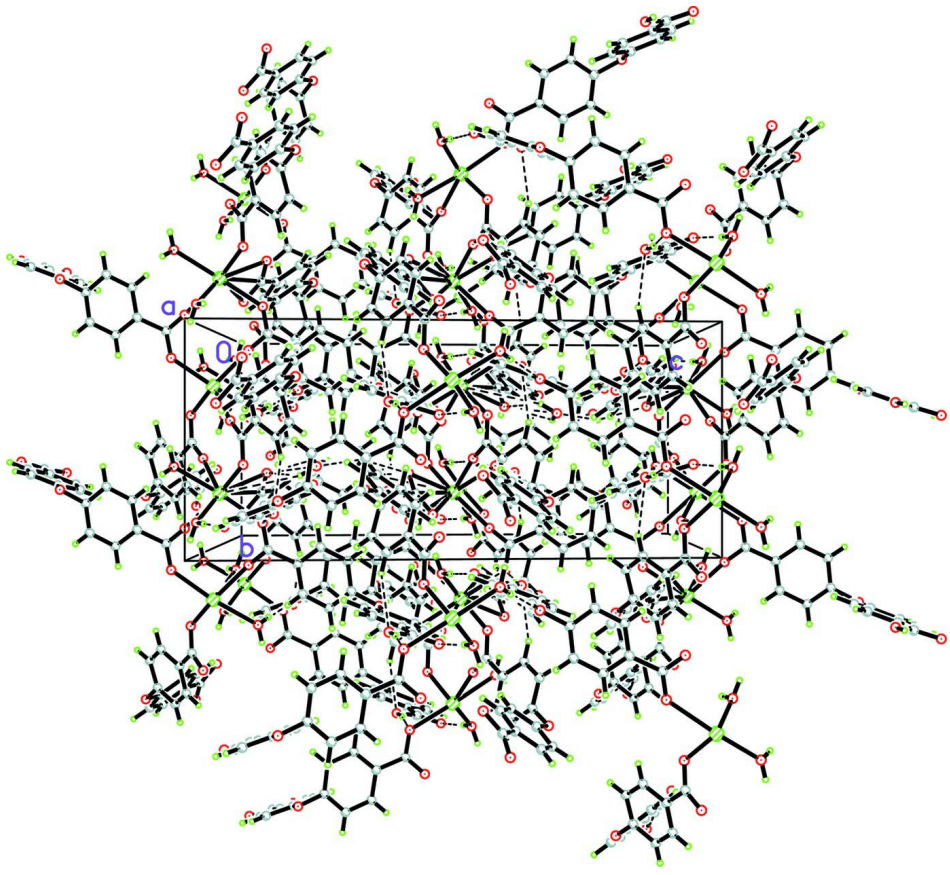


**Figure 2**

A packing diagram for the three-dimensional structure formed through O—H···O and C—H···O hydrogen-bonding interactions. Hydrogen bonds are indicated by dashed lines.

### *catena*-Poly[[diaqua[$\mu_2$-4-(4-carboxyphenoxy)benzoato]($\mu_2$-4,4′-oxydibenzoato)praseodymium(III)] monohydrate]

*Crystal data*

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Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a$ = 27.3970 (17) Å
$b$ = 9.5764 (6) Å
$c$ = 21.6754 (14) Å
$\beta$ = 97.433 (1)°
$V$ = 5639.1 (6) Å$^3$
$Z$ = 8
$F(000)$ = 2832
$D_x$ = 1.669 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9984 reflections
$\theta$ = 2.4–27.6°
$\mu$ = 1.80 mm$^{-1}$
$T$ = 296 K
Block, green
0.21 × 0.16 × 0.15 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min}$ = 0.704, $T_{max}$ = 0.774
20449 measured reflections
4972 independent reflections

4498 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$h = -32 \rightarrow 27$
$k = -11 \rightarrow 11$
$l = -25 \rightarrow 25$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.059$
$S = 1.08$
4972 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
$w = 1/[\sigma^2(F_o^2) + (0.0163P)^2 + 15.8309P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.59$ e Å$^{-3}$
$\Delta\rho_{min} = -0.51$ 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)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Pr1 | 0.014443 (5) | 0.250000 (14) | 0.008512 (7) | 0.02218 (6) |
| C1 | 0.08267 (9) | −0.0154 (3) | 0.06113 (13) | 0.0281 (6) |
| C2 | 0.12798 (9) | −0.0851 (3) | 0.09282 (12) | 0.0257 (6) |
| C3 | 0.05948 (9) | 0.5746 (3) | 0.17173 (12) | 0.0258 (6) |
| C4 | 0.04362 (9) | 0.5108 (3) | 0.10933 (12) | 0.0254 (6) |
| C5 | 0.21188 (10) | −0.2111 (3) | 0.15102 (14) | 0.0341 (7) |
| C6 | 0.26088 (11) | 0.8308 (3) | 0.39077 (15) | 0.0377 (7) |
| C7 | 0.33610 (11) | −0.3437 (3) | 0.18593 (14) | 0.0397 (7) |
| H7 | 0.3323 | −0.3976 | 0.2207 | 0.048* |
| C8 | 0.09428 (10) | 0.6972 (3) | 0.28360 (13) | 0.0327 (6) |
| C9 | 0.15967 (11) | −0.0134 (3) | 0.13644 (16) | 0.0418 (8) |
| H9 | 0.1527 | 0.0785 | 0.1459 | 0.050* |
| C10 | 0.08283 (12) | 0.4950 (3) | 0.22016 (14) | 0.0401 (7) |
| H10 | 0.0867 | 0.3995 | 0.2148 | 0.048* |
| C11 | 0.10043 (13) | 0.5567 (4) | 0.27647 (14) | 0.0447 (8) |
| H11 | 0.1162 | 0.5033 | 0.3089 | 0.054* |
| C12 | 0.34745 (11) | −0.1805 (3) | 0.08407 (14) | 0.0378 (7) |
| H12 | 0.3513 | −0.1246 | 0.0500 | 0.045* |
| C13 | 0.29695 (11) | −0.2675 (3) | 0.15686 (14) | 0.0324 (7) |
| C14 | 0.05244 (12) | 0.7155 (3) | 0.18124 (14) | 0.0365 (7) |
| H14 | 0.0355 | 0.7690 | 0.1496 | 0.044* |
| C15 | 0.31376 (12) | 0.8545 (3) | 0.41214 (17) | 0.0430 (8) |

| | | | | |
|---|---|---|---|---|
| C16 | 0.17743 (11) | 0.8314 (4) | 0.41406 (14) | 0.0432 (8) |
| H16 | 0.1548 | 0.8484 | 0.4417 | 0.052* |
| C17 | 0.16187 (11) | 0.7811 (3) | 0.35461 (14) | 0.0333 (7) |
| C18 | 0.13862 (12) | −0.2214 (3) | 0.07976 (17) | 0.0437 (8) |
| H18 | 0.1172 | −0.2720 | 0.0513 | 0.052* |
| C19 | 0.20161 (12) | −0.0762 (4) | 0.16618 (16) | 0.0459 (8) |
| H19 | 0.2225 | −0.0279 | 0.1960 | 0.055* |
| C20 | 0.18108 (13) | −0.2837 (4) | 0.10883 (18) | 0.0492 (9) |
| H20 | 0.1884 | −0.3754 | 0.0994 | 0.059* |
| C21 | 0.30232 (11) | −0.1854 (4) | 0.10597 (15) | 0.0413 (8) |
| H21 | 0.2759 | −0.1340 | 0.0866 | 0.050* |
| C22 | 0.38089 (11) | −0.3398 (3) | 0.16320 (14) | 0.0357 (7) |
| H22 | 0.4071 | −0.3926 | 0.1823 | 0.043* |
| C23 | 0.24464 (12) | 0.7818 (4) | 0.33152 (15) | 0.0414 (8) |
| H23 | 0.2672 | 0.7660 | 0.3037 | 0.050* |
| C24 | 0.22675 (12) | 0.8557 (4) | 0.43135 (15) | 0.0452 (8) |
| H24 | 0.2374 | 0.8894 | 0.4710 | 0.054* |
| C25 | 0.07024 (12) | 0.7778 (3) | 0.23706 (14) | 0.0396 (7) |
| H25 | 0.0660 | 0.8730 | 0.2430 | 0.048* |
| C26 | 0.38714 (10) | −0.2577 (3) | 0.11215 (14) | 0.0284 (6) |
| C27 | 0.19530 (12) | 0.7562 (3) | 0.31339 (15) | 0.0404 (8) |
| H27 | 0.1847 | 0.7224 | 0.2737 | 0.048* |
| C28 | 0.43485 (10) | −0.2515 (3) | 0.08701 (13) | 0.0273 (6) |
| O1 | 0.05551 (7) | 0.3854 (2) | 0.10037 (9) | 0.0348 (5) |
| O2 | 0.11178 (8) | 0.7623 (2) | 0.34028 (10) | 0.0405 (6) |
| O3 | 0.34277 (8) | 0.8348 (3) | 0.36883 (12) | 0.0494 (6) |
| H3 | 0.3715 | 0.8454 | 0.3840 | 0.074* |
| O4 | 0.32852 (9) | 0.8911 (3) | 0.46497 (12) | 0.0614 (7) |
| O5 | 0.08076 (8) | 0.1151 (2) | 0.06299 (11) | 0.0446 (6) |
| O6 | 0.25350 (8) | −0.2782 (3) | 0.18227 (11) | 0.0452 (6) |
| O7 | 0.46781 (7) | −0.3427 (2) | 0.10035 (9) | 0.0312 (4) |
| O8 | 0.44170 (7) | −0.1528 (2) | 0.04974 (10) | 0.0350 (5) |
| O9 | 0.01975 (7) | 0.5838 (2) | 0.06788 (9) | 0.0328 (4) |
| O10 | 0.04446 (8) | 0.1241 (2) | −0.08121 (10) | 0.0385 (5) |
| H10A | 0.0200 | 0.0888 | −0.1040 | 0.058* |
| H10B | 0.0591 | 0.1815 | −0.1024 | 0.058* |
| O11 | 0.08179 (7) | 0.38020 (19) | −0.03119 (9) | 0.0326 (4) |
| H11B | 0.0752 | 0.4617 | −0.0446 | 0.039* |
| H11A | 0.1106 | 0.3833 | −0.0120 | 0.039* |
| O12 | 0.04866 (7) | −0.0880 (2) | 0.03345 (10) | 0.0393 (5) |
| O13 | 0.5392 (3) | 0.6238 (7) | 0.2092 (3) | 0.251 (4) |
| H13B | 0.5098 | 0.5933 | 0.2009 | 0.377* |
| H13A | 0.5419 | 0.6668 | 0.1755 | 0.377* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pr1 | 0.01793 (9) | 0.02186 (9) | 0.02589 (10) | 0.00108 (5) | −0.00048 (6) | 0.00062 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C1 | 0.0228 (14) | 0.0318 (16) | 0.0294 (15) | 0.0028 (12) | 0.0028 (11) | 0.0000 (12) |
| C2 | 0.0199 (13) | 0.0250 (14) | 0.0317 (15) | 0.0013 (11) | 0.0016 (11) | 0.0019 (11) |
| C3 | 0.0234 (14) | 0.0281 (14) | 0.0245 (14) | −0.0003 (11) | −0.0014 (11) | −0.0007 (11) |
| C4 | 0.0202 (13) | 0.0269 (14) | 0.0289 (14) | −0.0007 (11) | 0.0020 (11) | −0.0017 (11) |
| C5 | 0.0213 (15) | 0.0440 (17) | 0.0377 (17) | 0.0088 (13) | 0.0071 (12) | 0.0143 (14) |
| C6 | 0.0304 (16) | 0.0357 (17) | 0.0446 (18) | −0.0017 (13) | −0.0044 (13) | 0.0023 (14) |
| C7 | 0.0328 (16) | 0.0498 (19) | 0.0375 (17) | 0.0124 (14) | 0.0086 (13) | 0.0182 (15) |
| C8 | 0.0258 (15) | 0.0468 (18) | 0.0249 (15) | −0.0038 (13) | 0.0009 (11) | −0.0083 (13) |
| C9 | 0.0391 (18) | 0.0255 (15) | 0.056 (2) | 0.0058 (13) | −0.0112 (15) | −0.0054 (14) |
| C10 | 0.054 (2) | 0.0275 (16) | 0.0357 (17) | 0.0031 (14) | −0.0073 (14) | 0.0014 (13) |
| C11 | 0.056 (2) | 0.0457 (19) | 0.0278 (16) | 0.0031 (16) | −0.0100 (14) | 0.0035 (14) |
| C12 | 0.0316 (16) | 0.0418 (18) | 0.0407 (17) | 0.0061 (13) | 0.0074 (13) | 0.0163 (14) |
| C13 | 0.0248 (15) | 0.0407 (17) | 0.0322 (16) | 0.0070 (12) | 0.0053 (12) | 0.0079 (13) |
| C14 | 0.0419 (18) | 0.0323 (16) | 0.0322 (16) | 0.0088 (13) | −0.0073 (13) | −0.0025 (13) |
| C15 | 0.0335 (17) | 0.0340 (17) | 0.058 (2) | 0.0008 (14) | −0.0056 (16) | 0.0016 (15) |
| C16 | 0.0330 (17) | 0.064 (2) | 0.0319 (16) | −0.0041 (15) | 0.0032 (13) | −0.0085 (15) |
| C17 | 0.0280 (16) | 0.0407 (17) | 0.0298 (16) | −0.0009 (13) | −0.0012 (12) | −0.0018 (13) |
| C18 | 0.0370 (18) | 0.0334 (17) | 0.057 (2) | 0.0043 (14) | −0.0082 (15) | −0.0103 (15) |
| C19 | 0.0370 (18) | 0.0427 (19) | 0.053 (2) | 0.0028 (15) | −0.0151 (15) | −0.0004 (16) |
| C20 | 0.046 (2) | 0.0336 (17) | 0.065 (2) | 0.0169 (15) | −0.0038 (17) | −0.0079 (16) |
| C21 | 0.0266 (16) | 0.052 (2) | 0.0455 (19) | 0.0139 (14) | 0.0052 (13) | 0.0185 (16) |
| C22 | 0.0276 (15) | 0.0398 (17) | 0.0395 (17) | 0.0119 (13) | 0.0040 (13) | 0.0103 (14) |
| C23 | 0.0320 (18) | 0.052 (2) | 0.0402 (18) | −0.0020 (14) | 0.0054 (14) | −0.0041 (15) |
| C24 | 0.0392 (18) | 0.058 (2) | 0.0354 (17) | −0.0057 (16) | −0.0077 (14) | −0.0089 (15) |
| C25 | 0.048 (2) | 0.0332 (16) | 0.0358 (17) | 0.0049 (14) | −0.0032 (14) | −0.0105 (13) |
| C26 | 0.0241 (15) | 0.0284 (15) | 0.0328 (16) | 0.0021 (11) | 0.0042 (12) | −0.0008 (11) |
| C27 | 0.0337 (18) | 0.057 (2) | 0.0291 (16) | −0.0031 (14) | −0.0003 (13) | −0.0080 (14) |
| C28 | 0.0264 (15) | 0.0236 (14) | 0.0320 (15) | −0.0001 (11) | 0.0036 (12) | −0.0045 (11) |
| O1 | 0.0362 (11) | 0.0281 (11) | 0.0372 (11) | 0.0063 (9) | −0.0059 (9) | −0.0082 (9) |
| O2 | 0.0262 (11) | 0.0669 (16) | 0.0277 (11) | −0.0045 (10) | 0.0008 (9) | −0.0187 (10) |
| O3 | 0.0271 (12) | 0.0528 (15) | 0.0660 (16) | −0.0030 (11) | −0.0029 (11) | −0.0014 (12) |
| O4 | 0.0358 (13) | 0.0807 (19) | 0.0625 (17) | −0.0016 (13) | −0.0140 (12) | −0.0126 (14) |
| O5 | 0.0427 (13) | 0.0291 (12) | 0.0562 (14) | 0.0126 (9) | −0.0158 (11) | −0.0028 (10) |
| O6 | 0.0261 (12) | 0.0661 (15) | 0.0452 (13) | 0.0183 (10) | 0.0115 (10) | 0.0271 (11) |
| O7 | 0.0251 (10) | 0.0284 (10) | 0.0404 (11) | 0.0060 (8) | 0.0058 (8) | 0.0038 (9) |
| O8 | 0.0313 (11) | 0.0269 (10) | 0.0490 (13) | 0.0038 (8) | 0.0139 (9) | 0.0085 (9) |
| O9 | 0.0336 (11) | 0.0345 (11) | 0.0276 (10) | 0.0028 (9) | −0.0064 (8) | 0.0035 (9) |
| O10 | 0.0444 (13) | 0.0315 (11) | 0.0424 (12) | −0.0071 (9) | 0.0161 (10) | −0.0033 (9) |
| O11 | 0.0248 (10) | 0.0259 (10) | 0.0462 (12) | 0.0007 (8) | 0.0009 (9) | 0.0057 (9) |
| O12 | 0.0240 (11) | 0.0488 (13) | 0.0428 (12) | −0.0061 (9) | −0.0045 (9) | −0.0011 (10) |
| O13 | 0.354 (10) | 0.169 (6) | 0.185 (6) | 0.015 (6) | −0.141 (6) | 0.009 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Pr1—O9$^{i}$ | 2.3983 (18) | C12—C26 | 1.389 (4) |
| Pr1—O5 | 2.4105 (19) | C12—H12 | 0.9300 |
| Pr1—O12$^{ii}$ | 2.412 (2) | C13—C21 | 1.378 (4) |
| Pr1—O8$^{iii}$ | 2.4692 (19) | C13—O6 | 1.379 (3) |

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|---|---|---|---|
| Pr1—O11 | 2.4719 (18) | C14—C25 | 1.380 (4) |
| Pr1—O10 | 2.5152 (19) | C14—H14 | 0.9300 |
| Pr1—O1 | 2.5163 (19) | C15—O4 | 1.216 (4) |
| Pr1—O7$^{iii}$ | 2.6534 (19) | C15—O3 | 1.320 (4) |
| C1—O5 | 1.252 (3) | C16—C24 | 1.375 (4) |
| C1—O12 | 1.252 (3) | C16—C17 | 1.390 (4) |
| C1—C2 | 1.496 (4) | C16—H16 | 0.9300 |
| C2—C18 | 1.375 (4) | C17—O2 | 1.379 (4) |
| C2—C9 | 1.381 (4) | C17—C27 | 1.380 (4) |
| C3—C14 | 1.382 (4) | C18—C20 | 1.384 (5) |
| C3—C10 | 1.385 (4) | C18—H18 | 0.9300 |
| C3—C4 | 1.497 (4) | C19—H19 | 0.9300 |
| C4—O9 | 1.254 (3) | C20—H20 | 0.9300 |
| C4—O1 | 1.266 (3) | C21—H21 | 0.9300 |
| C5—C20 | 1.353 (5) | C22—C26 | 1.386 (4) |
| C5—C19 | 1.371 (5) | C22—H22 | 0.9300 |
| C5—O6 | 1.404 (3) | C23—C27 | 1.380 (5) |
| C6—C24 | 1.385 (5) | C23—H23 | 0.9300 |
| C6—C23 | 1.386 (4) | C24—H24 | 0.9300 |
| C6—C15 | 1.480 (4) | C25—H25 | 0.9300 |
| C7—C22 | 1.381 (4) | C26—C28 | 1.481 (4) |
| C7—C13 | 1.381 (4) | C27—H27 | 0.9300 |
| C7—H7 | 0.9300 | C28—O7 | 1.262 (3) |
| C8—C11 | 1.367 (5) | C28—O8 | 1.273 (3) |
| C8—C25 | 1.369 (4) | O3—H3 | 0.8200 |
| C8—O2 | 1.406 (3) | O10—H10A | 0.8499 |
| C9—C19 | 1.381 (4) | O10—H10B | 0.8500 |
| C9—H9 | 0.9300 | O11—H11B | 0.8444 |
| C10—C11 | 1.385 (4) | O11—H11A | 0.8444 |
| C10—H10 | 0.9300 | O13—H13B | 0.8542 |
| C11—H11 | 0.9300 | O13—H13A | 0.8500 |
| C12—C21 | 1.381 (4) | | |

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|---|---|---|---|
| O9$^{i}$—Pr1—O5 | 153.69 (8) | O6—C13—C7 | 116.0 (3) |
| O9$^{i}$—Pr1—O12$^{ii}$ | 88.26 (7) | C25—C14—C3 | 120.8 (3) |
| O5—Pr1—O12$^{ii}$ | 107.34 (7) | C25—C14—H14 | 119.6 |
| O9$^{i}$—Pr1—O8$^{iii}$ | 74.83 (7) | C3—C14—H14 | 119.6 |
| O5—Pr1—O8$^{iii}$ | 128.11 (7) | O4—C15—O3 | 123.6 (3) |
| O12$^{ii}$—Pr1—O8$^{iii}$ | 78.82 (7) | O4—C15—C6 | 122.1 (3) |
| O9$^{i}$—Pr1—O11 | 70.57 (6) | O3—C15—C6 | 114.2 (3) |
| O5—Pr1—O11 | 83.78 (7) | C24—C16—C17 | 118.9 (3) |
| O12$^{ii}$—Pr1—O11 | 136.39 (7) | C24—C16—H16 | 120.5 |
| O8$^{iii}$—Pr1—O11 | 127.57 (6) | C17—C16—H16 | 120.5 |
| O9$^{i}$—Pr1—O10 | 85.53 (7) | O2—C17—C27 | 123.8 (3) |
| O5—Pr1—O10 | 79.66 (7) | O2—C17—C16 | 115.5 (3) |
| O12$^{ii}$—Pr1—O10 | 71.94 (7) | C27—C17—C16 | 120.7 (3) |
| O8$^{iii}$—Pr1—O10 | 145.13 (7) | C2—C18—C20 | 120.2 (3) |
| O11—Pr1—O10 | 68.85 (6) | C2—C18—H18 | 119.9 |

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| O9$^{i}$—Pr1—O1 | 107.40 (6) | C20—C18—H18 | 119.9 |
| O5—Pr1—O1 | 69.94 (7) | C5—C19—C9 | 118.9 (3) |
| O12$^{ii}$—Pr1—O1 | 148.79 (7) | C5—C19—H19 | 120.6 |
| O8$^{iii}$—Pr1—O1 | 79.55 (7) | C9—C19—H19 | 120.6 |
| O11—Pr1—O1 | 74.82 (7) | C5—C20—C18 | 120.0 (3) |
| O10—Pr1—O1 | 134.54 (7) | C5—C20—H20 | 120.0 |
| O9$^{i}$—Pr1—O7$^{iii}$ | 123.84 (6) | C18—C20—H20 | 120.0 |
| O5—Pr1—O7$^{iii}$ | 81.88 (7) | C13—C21—C12 | 119.2 (3) |
| O12$^{ii}$—Pr1—O7$^{iii}$ | 71.13 (7) | C13—C21—H21 | 120.4 |
| O8$^{iii}$—Pr1—O7$^{iii}$ | 50.58 (6) | C12—C21—H21 | 120.4 |
| O11—Pr1—O7$^{iii}$ | 152.06 (6) | C7—C22—C26 | 120.5 (3) |
| O10—Pr1—O7$^{iii}$ | 131.07 (6) | C7—C22—H22 | 119.7 |
| O1—Pr1—O7$^{iii}$ | 77.77 (6) | C26—C22—H22 | 119.7 |
| O5—C1—O12 | 122.6 (3) | C27—C23—C6 | 120.6 (3) |
| O5—C1—C2 | 117.8 (2) | C27—C23—H23 | 119.7 |
| O12—C1—C2 | 119.7 (2) | C6—C23—H23 | 119.7 |
| C18—C2—C9 | 118.8 (3) | C16—C24—C6 | 121.2 (3) |
| C18—C2—C1 | 121.0 (3) | C16—C24—H24 | 119.4 |
| C9—C2—C1 | 120.2 (2) | C6—C24—H24 | 119.4 |
| C14—C3—C10 | 118.9 (3) | C8—C25—C14 | 118.9 (3) |
| C14—C3—C4 | 120.3 (2) | C8—C25—H25 | 120.5 |
| C10—C3—C4 | 120.8 (2) | C14—C25—H25 | 120.5 |
| O9—C4—O1 | 122.7 (2) | C22—C26—C12 | 118.8 (3) |
| O9—C4—C3 | 118.9 (2) | C22—C26—C28 | 121.5 (3) |
| O1—C4—C3 | 118.4 (2) | C12—C26—C28 | 119.7 (3) |
| C20—C5—C19 | 121.1 (3) | C23—C27—C17 | 119.5 (3) |
| C20—C5—O6 | 119.2 (3) | C23—C27—H27 | 120.3 |
| C19—C5—O6 | 119.6 (3) | C17—C27—H27 | 120.3 |
| C24—C6—C23 | 119.0 (3) | O7—C28—O8 | 119.9 (3) |
| C24—C6—C15 | 119.3 (3) | O7—C28—C26 | 121.8 (2) |
| C23—C6—C15 | 121.7 (3) | O8—C28—C26 | 118.2 (2) |
| C22—C7—C13 | 119.8 (3) | O7—C28—Pr1$^{iv}$ | 64.72 (15) |
| C22—C7—H7 | 120.1 | O8—C28—Pr1$^{iv}$ | 56.40 (14) |
| C13—C7—H7 | 120.1 | C26—C28—Pr1$^{iv}$ | 166.2 (2) |
| C11—C8—C25 | 121.7 (3) | C4—O1—Pr1 | 120.84 (17) |
| C11—C8—O2 | 120.2 (3) | C17—O2—C8 | 118.1 (2) |
| C25—C8—O2 | 118.1 (3) | C15—O3—H3 | 109.5 |
| C19—C9—C2 | 121.0 (3) | C1—O5—Pr1 | 123.47 (18) |
| C19—C9—H9 | 119.5 | C13—O6—C5 | 117.6 (2) |
| C2—C9—H9 | 119.5 | C28—O7—Pr1$^{iv}$ | 89.80 (16) |
| C3—C10—C11 | 120.5 (3) | C28—O8—Pr1$^{iv}$ | 98.18 (16) |
| C3—C10—H10 | 119.8 | C4—O9—Pr1$^{i}$ | 170.37 (18) |
| C11—C10—H10 | 119.8 | Pr1—O10—H10A | 109.2 |
| C8—C11—C10 | 119.0 (3) | Pr1—O10—H10B | 109.4 |
| C8—C11—H11 | 120.5 | H10A—O10—H10B | 109.5 |
| C10—C11—H11 | 120.5 | Pr1—O11—H11B | 116.8 |
| C21—C12—C26 | 121.1 (3) | Pr1—O11—H11A | 122.6 |
| C21—C12—H12 | 119.5 | H11B—O11—H11A | 106.3 |

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|---|---|---|---|
| C26—C12—H12 | 119.5 | C1—O12—Pr1$^{ii}$ | 172.3 (2) |
| C21—C13—O6 | 123.3 (3) | H13B—O13—H13A | 99.7 |
| C21—C13—C7 | 120.7 (3) | | |
| | | | |
| O5—C1—C2—C18 | −163.0 (3) | C7—C22—C26—C12 | −0.5 (5) |
| O12—C1—C2—C18 | 16.2 (4) | C7—C22—C26—C28 | 179.8 (3) |
| O5—C1—C2—C9 | 17.7 (4) | C21—C12—C26—C22 | −0.4 (5) |
| O12—C1—C2—C9 | −163.1 (3) | C21—C12—C26—C28 | 179.2 (3) |
| C14—C3—C4—O9 | −6.8 (4) | C6—C23—C27—C17 | 0.7 (5) |
| C10—C3—C4—O9 | 175.4 (3) | O2—C17—C27—C23 | 178.2 (3) |
| C14—C3—C4—O1 | 172.3 (3) | C16—C17—C27—C23 | −0.1 (5) |
| C10—C3—C4—O1 | −5.6 (4) | C22—C26—C28—O7 | 17.2 (4) |
| C18—C2—C9—C19 | 0.6 (5) | C12—C26—C28—O7 | −162.4 (3) |
| C1—C2—C9—C19 | 179.9 (3) | C22—C26—C28—O8 | −164.6 (3) |
| C14—C3—C10—C11 | −2.3 (5) | C12—C26—C28—O8 | 15.7 (4) |
| C4—C3—C10—C11 | 175.5 (3) | C22—C26—C28—Pr1$^{iv}$ | 131.9 (7) |
| C25—C8—C11—C10 | 1.5 (5) | C12—C26—C28—Pr1$^{iv}$ | −47.8 (9) |
| O2—C8—C11—C10 | 180.0 (3) | O9—C4—O1—Pr1 | −16.0 (4) |
| C3—C10—C11—C8 | 0.2 (5) | C3—C4—O1—Pr1 | 165.01 (17) |
| C22—C7—C13—C21 | −1.1 (5) | O9$^{i}$—Pr1—O1—C4 | 21.5 (2) |
| C22—C7—C13—O6 | 179.5 (3) | O5—Pr1—O1—C4 | 173.8 (2) |
| C10—C3—C14—C25 | 2.9 (5) | O12$^{ii}$—Pr1—O1—C4 | −95.6 (2) |
| C4—C3—C14—C25 | −175.0 (3) | O8$^{iii}$—Pr1—O1—C4 | −48.8 (2) |
| C24—C6—C15—O4 | 2.3 (5) | O11—Pr1—O1—C4 | 85.0 (2) |
| C23—C6—C15—O4 | −176.4 (3) | O10—Pr1—O1—C4 | 122.68 (19) |
| C24—C6—C15—O3 | −176.6 (3) | O7$^{iii}$—Pr1—O1—C4 | −100.5 (2) |
| C23—C6—C15—O3 | 4.7 (5) | C28$^{iii}$—Pr1—O1—C4 | −74.6 (2) |
| C24—C16—C17—O2 | −178.6 (3) | C27—C17—O2—C8 | 8.6 (4) |
| C24—C16—C17—C27 | −0.2 (5) | C16—C17—O2—C8 | −173.0 (3) |
| C9—C2—C18—C20 | −1.7 (5) | C11—C8—O2—C17 | 73.5 (4) |
| C1—C2—C18—C20 | 179.0 (3) | C25—C8—O2—C17 | −108.0 (3) |
| C20—C5—C19—C9 | −1.6 (5) | O12—C1—O5—Pr1 | −4.2 (4) |
| O6—C5—C19—C9 | −177.9 (3) | C2—C1—O5—Pr1 | 174.99 (17) |
| C2—C9—C19—C5 | 1.0 (5) | O9$^{i}$—Pr1—O5—C1 | −115.7 (2) |
| C19—C5—C20—C18 | 0.6 (5) | O12$^{ii}$—Pr1—O5—C1 | 8.3 (3) |
| O6—C5—C20—C18 | 176.9 (3) | O8$^{iii}$—Pr1—O5—C1 | 97.6 (2) |
| C2—C18—C20—C5 | 1.1 (6) | O11—Pr1—O5—C1 | −128.5 (2) |
| O6—C13—C21—C12 | 179.5 (3) | O10—Pr1—O5—C1 | −58.9 (2) |
| C7—C13—C21—C12 | 0.2 (5) | O1—Pr1—O5—C1 | 155.5 (3) |
| C26—C12—C21—C13 | 0.6 (5) | O7$^{iii}$—Pr1—O5—C1 | 75.6 (2) |
| C13—C7—C22—C26 | 1.3 (5) | C28$^{iii}$—Pr1—O5—C1 | 82.5 (2) |
| C24—C6—C23—C27 | −0.9 (5) | C21—C13—O6—C5 | 5.7 (5) |
| C15—C6—C23—C27 | 177.9 (3) | C7—C13—O6—C5 | −175.0 (3) |
| C17—C16—C24—C6 | −0.1 (5) | C20—C5—O6—C13 | 92.8 (4) |
| C23—C6—C24—C16 | 0.6 (5) | C19—C5—O6—C13 | −90.9 (4) |
| C15—C6—C24—C16 | −178.2 (3) | O8—C28—O7—Pr1$^{iv}$ | −12.0 (3) |
| C11—C8—C25—C14 | −1.0 (5) | C26—C28—O7—Pr1$^{iv}$ | 166.1 (2) |

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| O2—C8—C25—C14 | −179.5 (3) | O7—C28—O8—Pr1$^{iv}$ | 13.1 (3) |
| C3—C14—C25—C8 | −1.2 (5) | C26—C28—O8—Pr1$^{iv}$ | −165.1 (2) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O3—H3···O1$^{v}$ | 0.82 | 2.02 | 2.822 (3) | 166 |
| O10—H10*B*···O2$^{vi}$ | 0.85 | 2.09 | 2.880 (3) | 154 |
| O11—H11*A*···O4$^{vii}$ | 0.84 | 1.84 | 2.683 (3) | 176 |
| O11—H11*B*···O8$^{viii}$ | 0.84 | 1.89 | 2.707 (3) | 163 |
| C9—H9···O3$^{vii}$ | 0.93 | 2.48 | 3.337 (4) | 153 |
| C25—H25···O13$^{iii}$ | 0.93 | 2.59 | 3.454 (7) | 155 |

Symmetry codes: (iii) *x*−1/2, *y*+1/2, *z*; (v) −*x*+1/2, *y*+1/2, −*z*+1/2; (vi) *x*, −*y*+1, *z*−1/2; (vii) −*x*+1/2, *y*−1/2, −*z*+1/2; (viii) −*x*+1/2, −*y*+1/2, −*z*.