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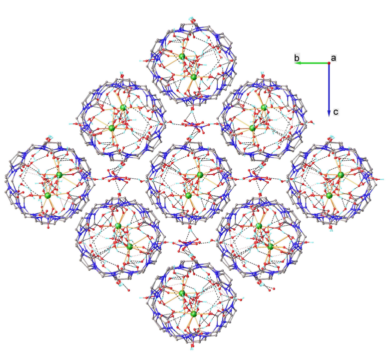



# The crystal structure of a mononuclear Pr$^{III}$ complex with cucurbit[6]uril

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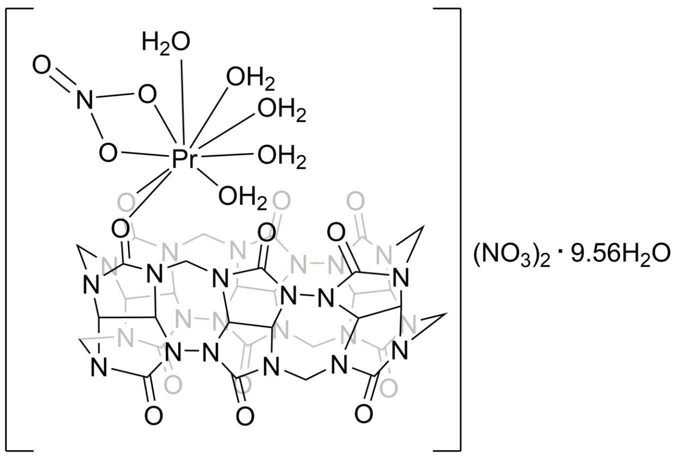
A new mononuclear complex, pentaaqua(cucurbit[6]uril-$\kappa^2O,O'$)(nitrato-$\kappa^2O,O'$)praseodymium(III) dinitrate 9.56-hydrate, $[Pr(NO_3)(CB6)(H_2O)_5]$-$(NO_3)_2\cdot9.56H_2O$ (**1**), was obtained as outcome of the hydrothermal reaction between the macrocyclic ligand cucurbit[6]uril (**CB6**, $C_{36}H_{36}N_{24}O_{12}$) with a tenfold excess of $Pr(NO_3)_3\cdot6H_2O$. Complex **1** crystallizes in the $P2_1/n$ space group with two crystallographically independent but chemically identical $[Pr(CB6)(NO_3)(H_2O)_5]^{2+}$ complex cations, four nitrate counter-anions and 19.12 interstitial water molecules per asymmetric unit. The nonacoordinated Pr$^{III}$ in **1** are located in the $PrO_9$ coordination environment formed by two carbonyl O atoms from bidentate cucurbit[6]uril units, two oxygen atoms from the bidentate nitrate anion and five water molecules. Considering the differences in Pr—O bond distances and O—Pr—O angles in the coordination spheres, the coordination polyhedrons of the two Pr$^{III}$ atoms can be described as distorted spherical capped square antiprismatic and muffin polyhedral.

## 1. Chemical context

Cucurbit[$n$]urils (CB[$n$]s) are 3D cyclic organic molecules possessing a rigid hydrophobic macrocyclic cavity, which is available for the uptake of various guest molecules *via* non-covalent interactions (Lin *et al.*, 2020). Recently, the main interest in cucurbit[$n$]uril chemistry was due to their possible applications in selective catalysis (Nandi *et al.*, 2017), molecular recognition (Barrow *et al.*, 2015) and drug delivery (Das *et al.*, 2019). The presence of several carbonyl oxygen atoms on both sides of the macrocyclic ring makes cucurbit[$n$]urils attractive ligand platforms for the design of discrete and polymeric coordination compounds, which can provide accessible channels due to the peculiarities of the arrangement of the cucurbit[$n$]urils in the crystal structure (Ni *et al.*, 2013). The design of lanthanide(III) complexes with cucurbit[$n$]urils is particularly interesting because of the possible applications in molecular magnetism (Ren *et al.*, 2013) and luminescence (Matsumoto *et al.*, 2022). Depending on the size of the macrocyclic cavity and the lanthanide(III) ionic radii, cucurbit[$n$]urils usually provide two to six oxygen atoms in the coordination sphere of the lanthanide ions (Zhang *et al.*, 2019, 2020; Liang *et al.*, 2013*b*; Zheng & Liu, 2017). In the majority of cases, the interaction between cucurbit[$n$]urils and lanthanide(III) salts leads to the formation of discrete mononuclear assemblies with one coordinated cucurbit[$n$]uril (Ren *et al.*, 2013; Ni *et al.*, 2015); however, examples of polynuclear complexes and coordination polymers have also been reported (Zhang *et al.*, 2019; Zhang *et al.*, 2020; Liang *et al.*, 2013*a*,*b*). Several lanthanide-containing complexes with cucurbit[6]urils have been reported previously (Ren *et al.*, 2013; Zheng & Liu, 2017; Shan *et al.*, 2016; Yang *et al.*, 2016; Xiao *et al.*, 2016). In the absence of additional bridging organic ligands or anionic complexes, the interaction between $Ln^{III}$ salts and cucurbit[6]uril leads to the formation of mononuclear complexes (Ren *et al.*, 2013; Yang *et al.*, 2016; Kovalenko *et al.*, 2021; Samsonenko *et al.*, 2002).



Since cucurbit[6]uril is poorly soluble in water, lanthanide complex formation is usually observed in the presence of strong mineral acids (da Silva *et al.*, 2014) or a substantial excess of the lanthanide salt reaching 25-fold excess (Ren *et al.*, 2013). The observed structure of lanthanide(III)–cucurbit[6]uril complexes depends upon a number of factors, which include an excess of the lanthanide salt in the reaction mixture, the counter-anion, reaction temperature and crystallization conditions.

In this work we report synthesis and crystal structure of a new mononuclear $Pr^{III}$ complex with cucurbit[6]uril, $[Pr(\mathbf{CB6})(NO_3)(H_2O)_5](NO_3)_2{\cdot}9.56\ H_2O$ (**1**), which was synthesized in the presence of a lowered tenfold $Pr^{III}$ excess and is not isomorphous to previously reported $Ln^{III}$ complexes with cucurbit[6]uril.

## 2. Structural commentary

The title complex **1** was prepared and isolated as colorless crystals according to a modified procedure for the analoguous $Dy^{III}$ complex with cucurbit[6]uril, using $Pr(NO_3)_3{\cdot}6H_2O$ for **1** (Ren *et al.*, 2013). The previously reported synthetic strategy employed a 25-fold excess of the $Ln^{III}$ salt in order to promote the solubility of cucurbit[6]uril. In this work we introduced ultrasonication before placing the reaction mixture in hydrothermal conditions, which allowed the excess of the $Ln^{III}$ salt needed for the cucurbit[6]uril to be dissolved to be decreased.

The obtained complex $[Pr(\mathbf{CB6})(NO_3)(H_2O)_5](NO_3)_2{\cdot}9.56\ H_2O$ (**1**) crystallizes in the $P2_1/n$ space group, while previously reported complexes obtained as outcomes of interactions between $Ln(NO_3)_3$ and cucurbit[6]uril crystallized in the orthorhombic $Pna2_1$ space group ($Ln$ = Gd, Dy, Ho and Yb) or in the monoclinic $P2_1/n$ space group in the case of $Ln^{III}$ (Samsonenko *et al.*, 2002; Ren *et al.*, 2013). The different space group in the case of **1** may be caused by a variation of the synthetic conditions or the different lanthanide(III) radii.

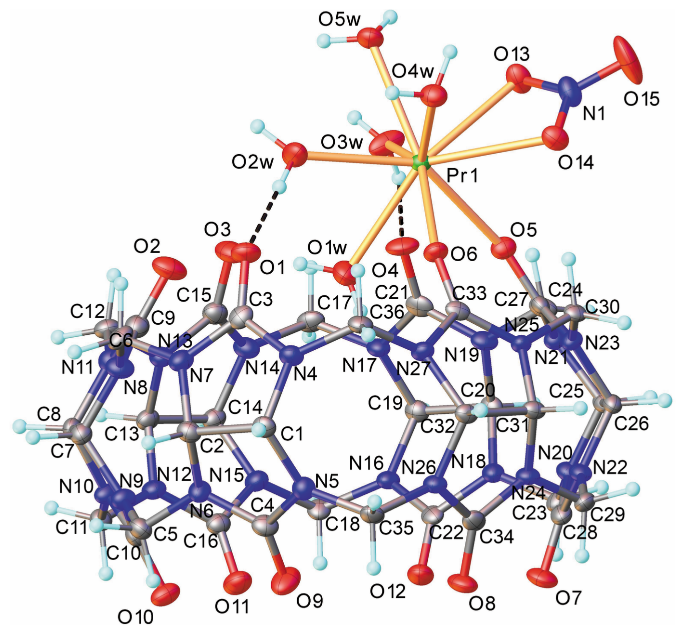


**Figure 1**
The molecular structure of the $[Pr(CB6)(NO_3)(H_2O)_5]^{2+}$ cation (molecule *A*) with selected atom-labeling scheme and displacement ellipsoids drawn at the 50% level.

The unit cell of complex **1** contains eight $Pr^{III}$–cucurbituril cationic $[Pr(\mathbf{CB6})(NO_3)(H_2O)_5]^{2+}$ complex molecules (Fig. 1) per unit cell, non-coordinated water molecules and two nitrate anions per complex cation for charge balance. There are two crystallographically independent complex cations in the asymmetric unit of **1**, however, the differences in the coordination environments of the $Pr^{III}$ ions are minor. The $Pr^{III}$ ions in the complex **1** are nonacoordinated. Two coordination positions of the $Pr^{III}$ ions are occupied by two carbonyl oxygen atoms from the coordinated **CB6** ligands, two positions contain oxygen atoms from the bidentate nitrate anions and the remaining five positions are occupied by oxygen atoms from the coordinated water molecules. The macrocyclic cucurbit[6]uril coordinates in bidentate mode, which is typical for $Ln^{III}$–cucurbit[*n*]uril complexes without additional ligands. The carbonyl oxygen atoms on the opposite side of the macrocycle remain uncoordinated.

The $Pr-O_{carbonyl}$ bond distances in complex **1** are typical for cucurbit[6]uril complexes with $Ln^{III}$ ions (Samsonenko *et al.*, 2002; Ren *et al.*, 2013; da Silva *et al.*, 2014; Lin *et al.*, 2019). The observed bond distances between the $Pr^{III}$ ions and the nitrate oxygen atoms are typical for bidentately coordinated nitrate anions to $Pr^{III}$ ions (Pavlishchuk *et al.*, 2019). However, minor differences in the geometrical parameters of the coordination spheres of Pr1*A* and Pr1*B* are observed (Table 1, (Fig. 2). According to the calculations performed with *Shape 2.1* software (Casanova *et al.*, 2005, Table 2), the nona-

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Pr1*A*—O1*WA* | 2.544 (2) | Pr1*B*—O1*WB* | 2.553 (3) |
| Pr1*A*—O2*WA* | 2.449 (3) | Pr1*B*—O2*WB* | 2.438 (2) |
| Pr1*A*—O3*WA* | 2.442 (2) | Pr1*B*—O3*WB* | 2.448 (2) |
| Pr1*B*—O4*WB* | 2.527 (3) | Pr1*B*—O4*WB* | 2.527 (3) |
| Pr1*A*—O5*A* | 2.493 (2) | Pr1*B*—O5*B* | 2.519 (2) |
| Pr1*A*—O5*WA* | 2.483 (2) | Pr1*B*—O5*WB* | 2.476 (2) |
| Pr1*A*—O6*A* | 2.466 (2) | Pr1*B*—O6*B* | 2.460 (2) |
| Pr1*A*—O13*A* | 2.571 (2) | Pr1*B*—O13*B* | 2.651 (3) |
| Pr1*A*—O14*A* | 2.613 (2) | Pr1*B*—O14*B* | 2.572 (2) |
| | | | |
| O2*WA*—Pr1*A*—O1*WA* | 68.01 (9) | O2*WB*—Pr1*B*—O13*B* | 68.61 (8) |
| O2*WA*—Pr1*A*—O4*WA* | 77.25 (8) | O2*WB*—Pr1*B*—O3*WB* | 84.55 (8) |
| O2*WA*—Pr1*A*—O5*WA* | 67.92 (8) | O2*WB*—Pr1*B*—O6*B* | 96.37 (8) |
| O2*WA*—Pr1*A*—O6*A* | 84.64 (8) | O2*WB*—Pr1*B*—O1*WB* | 67.77 (9) |
| O3*WA*—Pr1*A*—O1*WA* | 73.57 (9) | O2*WB*—Pr1*B*—O5*WB* | 71.46 (8) |
| O3*WA*—Pr1*A*—O2*WA* | 93.13 (9) | O3*WB*—Pr1*B*—O5*WB* | 71.21 (8) |
| O3*WA*—Pr1*A*—O5*WA* | 70.71 (8) | O3*WB*—Pr1*B*—O5*B* | 78.97 (8) |
| O3*WA*—Pr1*A*—O5*A* | 77.35 (8) | O3*WB*—Pr1*B*—O4*WB* | 76.07 (9) |
| O3*WA*—Pr1*A*—O13*A* | 73.92 (8) | O3*WB*—Pr1*B*—O1*WB* | 71.69 (9) |
| O4*WA*—Pr1*A*—O13*A* | 88.91 (8) | O3*WB*—Pr1*B*—O1*WB* | 71.69 (9) |
| O4*WA*—Pr1*A*—O14*A* | 65.33 (8) | O4*WB*—Pr1*B*—O14*B* | 65.36 (8) |
| O5*WA*—Pr1*A*—O4*WA* | 71.24 (8) | O5*B*—Pr1*B*—O4*WB* | 70.75 (8) |
| O5*WA*—Pr1*A*—O13*A* | 70.72 (8) | O5*B*—Pr1*B*—O1*WB* | 71.12 (9) |
| O5*A*—Pr1*A*—O1*WA* | 72.17 (8) | O5*WB*—Pr1*B*—O4*WB* | 69.88 (8) |
| O5*A*—Pr1*A*—O13*A* | 76.26 (8) | O5*WB*—Pr1*B*—O14*B* | 82.62 (8) |
| O5*A*—Pr1*A*—O14*A* | 71.00 (8) | O5*WB*—Pr1*B*—O13*B* | 71.53 (8) |
| O6*A*—Pr1*A*—O1*WA* | 74.26 (8) | O6*B*—Pr1*B*—O1*WB* | 75.85 (9) |
| O6*A*—Pr1*A*—O4*WA* | 70.85 (8) | O6*B*—Pr1*B*—O5*B* | 77.22 (8) |
| O6*A*—Pr1*A*—O5*A* | 82.86 (8) | O6*B*—Pr1*B*—O14*B* | 71.49 (8) |
| O6*A*—Pr1*A*—O14*A* | 78.55 (7) | O6*B*—Pr1*B*—O13*B* | 71.15 (8) |
| O13*A*—Pr1*A*—O14*A* | 49.19 (7) | O14*B*—Pr1*B*—O13*B* | 48.49 (8) |

coordinated $Pr^{III}$ ions in complex **1** exhibit different geometries of the coordination environment: the Pr1*A* ions are located in a spherical capped square-antiprismatic environment (CSAPR-9, $C_{4v}$), while the geometry of the Pr1*B* ions is best described as a muffin polyhedron (MFF-9, $C_s$).

## 3. Supramolecular features

The cationic fragments $[Pr(CB6)(NO_3)(H_2O)_5]^{2+}$ in complex **1** are linked to each other through an extended system of hydrogen bonds (Table 3, Figs. 3 and 4). The carbonyl oxygen atoms, which are located on opposite side of macrocycle with respect to the coordinated $Pr^{III}$ ions are involved in the formation of an extended system of hydrogen-bonded water molecules, which provide the supramolecular organization of **1**. The carbonyl oxygen atoms O11*A*, O9*B* and O10*B* from the uncoordinated sides of the **CB6** ligands form hydrogen bonds with water molecules in the coordination sphere of the $Pr^{III}$ ions from adjacent complex cations (O11*A*–H4*WB*···O4*WB*, O11*A*—H5*WA*···O5*WB*, O9*B*—H5*WD*···O5*WA* and O10*B*—H4*WC*···O4*WA*). In addition, there are intramolecular hydrogen bonds that are formed between the carbonyl oxygen atoms located on the coordinated side of the **CB6** ligands with the water molecules coordinated to the $Pr^{III}$ ions from the same $[Pr(\mathbf{CB6})(NO_3)(H_2O)_5]^{2+}$ fragment (O1*A*—H2*WC*···O2*WA*, O4*A*—H3*WC*···O3*WA*, O1*B*—H2*WB*···O2*WB* and O4*B*—H3*WB*···O3*WB*). Other non-coordinated carbonyl oxygen atoms from **CB6** are involved in

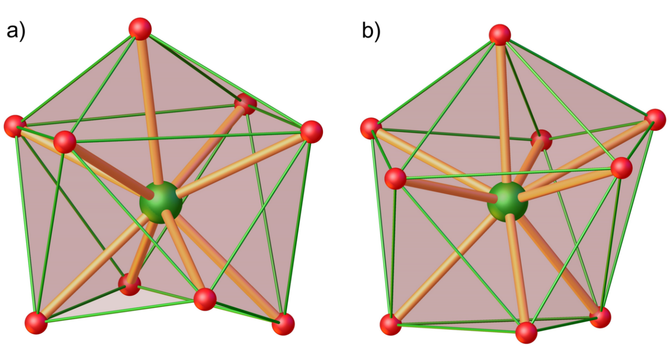



**Figure 2**
Coordination environments of the (*a*) Pr1*A* and (*b*) Pr1*B* ions in complex **1**.

**Table 2**
Continuous shape calculations for nonacoordinated $Pr^{III}$ ions in complex **1** performed with *Shape 2.1* software (Casanova *et al.*, 2005).

Nonacoordinated ions: EP-9 – enneagon (*D9h*); OPY-9 – octagonal pyramid (*C8v*); HBPY-9 – heptagonal bipyramid (*D7h*); JTC-9 – Johnson triangular cupola J3 (*C3v*); JCCU-9 – capped cube J8 (*C4v*); CCU-9 – spherical-relaxed capped cube (*C4v*); JCSAPR-9 – capped square antiprism J10 (*C4v*); CSAPR-9 – spherical capped square antiprism (*C4v*); JTCTPR-9 – tricapped trigonal prism J51 (*D3h*); TCTPR-9 – spherical tricapped trigonal prism (*C3h*); JTDIC-9 – tridiminished icosahedron J63 (*C3v*); HH-9 – hula hoop (*C2v*); MFF-9 – muffin (*Cs*).

| | Pr1*A* | Pr1*B* |
|---|---|---|
| EP-9 | 36.646 | 33.312 |
| OPY-9 | 21.958 | 21.971 |
| HBPY-9 | 18.179 | 15.434 |
| JTC-9 | 16.494 | 14.581 |
| JCCU-9 | 9.826 | 8.982 |
| CCU-9 | 8.542 | 7.654 |
| JCSAPR-9 | 2.258 | 3.376 |
| CSAPR-9 | **1.150** | 2.289 |
| JTCTPR-9 | 2.890 | 3.350 |
| TCTPR-9 | 1.506 | 2.654 |
| JTDIC-9 | 13.110 | 13.482 |
| HH-9 | 10.200 | 8.067 |
| MFF-9 | 1.198 | **1.787** |

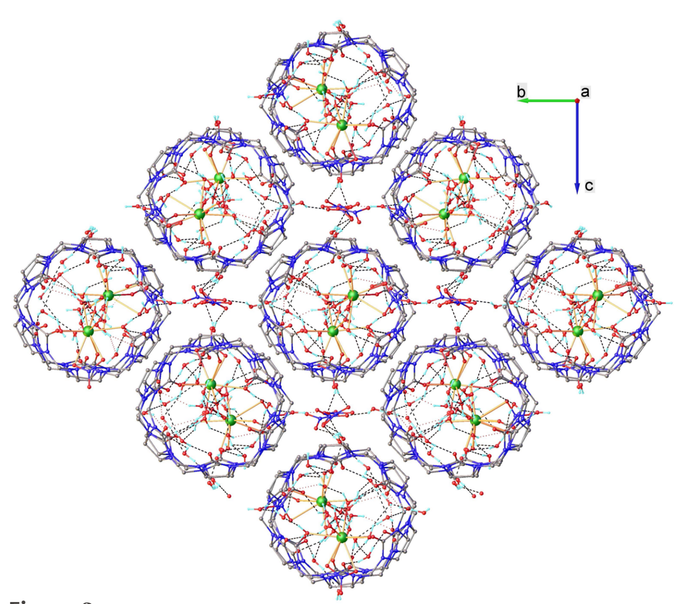



**Figure 3**
Fragment of the crystal structure viewed along the *a* axis.

**Table 3**
Hydrogen-bond geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*WB*—H1*WA*···O3*B* | 0.90 | 2.50 | 3.378 (4) | 169 |
| O2*WB*—H2*WA*···O11*W*$^{i}$ | 0.87 | 1.85 | 2.674 (3) | 157 |
| O2*WB*—H2*WB*···O1*B* | 0.87 | 2.07 | 2.865 (3) | 150 |
| O2*WB*—H2*WB*···O2*B* | 0.87 | 2.46 | 2.894 (4) | 111 |
| O3*WB*—H3*WA*···O2*W*$^{i}$ | 0.87 | 1.88 | 2.709 (4) | 158 |
| O3*WB*—H3*WB*···O4*B* | 0.87 | 1.89 | 2.710 (3) | 156 |
| O4*WB*—H4*WA*···O1*W*$^{i}$ | 0.87 | 2.01 | 2.729 (4) | 139 |
| O4*WB*—H4*WB*···O10*A*$^{ii}$ | 0.87 | 2.48 | 3.211 (3) | 142 |
| O4*WB*—H4*WB*···O11*A*$^{ii}$ | 0.87 | 2.60 | 3.206 (3) | 127 |
| O5*WB*—H5*WA*···O11*A*$^{ii}$ | 0.87 | 2.08 | 2.798 (4) | 140 |
| O5*WB*—H5*WA*···O12*A*$^{ii}$ | 0.87 | 2.44 | 3.018 (3) | 124 |
| O5*WB*—H5*WB*···O4*W*$^{i}$ | 0.87 | 1.86 | 2.712 (4) | 167 |
| O1*WA*—H1*WC*···O2*A* | 0.86 | 2.41 | 3.251 (4) | 167 |
| O1*WA*—H1*WD*···O7*W*$^{c}$ | 0.85 | 1.99 | 2.749 (17) | 148 |
| O1*WA*—H1*WD*···O8*W*$^{a}$ | 0.85 | 2.25 | 2.751 (9) | 118 |
| O2*WA*—H2*WC*···O1*A* | 0.87 | 1.80 | 2.667 (3) | 179 |
| O2*WA*—H2*WD*···O19*W*$^{iii}$ | 0.87 | 1.95 | 2.723 (4) | 147 |
| O3*WA*—H3*WC*···O4*A* | 0.87 | 1.87 | 2.723 (3) | 166 |
| O3*WA*—H3*WD*···O16*W* | 0.87 | 1.93 | 2.733 (4) | 153 |
| O4*WA*—H4*WC*···O10*B*$^{iv}$ | 0.87 | 2.05 | 2.905 (3) | 167 |
| O4*WA*—H4*WD*···O14*W*$^{iii}$ | 0.85 | 1.93 | 2.743 (4) | 159 |
| O5*WA*—H5*WC*···O19*W*$^{iii}$ | 0.87 | 1.93 | 2.766 (5) | 159 |
| O5*WA*—H5*WD*···O9*B*$^{iv}$ | 0.87 | 1.97 | 2.676 (3) | 137 |
| O15*W*—H15*A*···O3*A* | 0.87 | 1.97 | 2.837 (4) | 174 |
| O15*W*—H15*B*···O16*B* | 0.87 | 2.19 | 3.019 (5) | 159 |
| O15*W*—H15*B*···O18*B* | 0.87 | 2.39 | 3.128 (5) | 143 |
| O15*W*—H15*B*···N2*B* | 0.87 | 2.53 | 3.394 (5) | 173 |
| O1*W*—H1*WE*···O21*B* | 0.87 | 1.92 | 2.768 (4) | 165 |
| O1*W*—H1*WF*···O16*A* | 0.87 | 1.89 | 2.750 (4) | 170 |
| O17*W*$^{b}$—H17*E*$^{b}$···O2*A*$^{v}$ | 0.87 | 2.07 | 2.913 (6) | 163 |
| O17*W*$^{b}$—H17*F*$^{b}$···O3*A*$^{v}$ | 0.87 | 2.46 | 3.045 (9) | 126 |
| O3*W*—H3*WE*···O4*W* | 0.87 | 1.86 | 2.734 (4) | 177 |
| O3*W*—H3*WF*···O8*A*$^{vi}$ | 0.87 | 1.98 | 2.764 (3) | 150 |
| O2*W*—H2*WE*···O9*A*$^{vi}$ | 0.87 | 2.41 | 3.047 (3) | 131 |
| O2*W*—H2*WE*···O3*W* | 0.87 | 2.06 | 2.850 (4) | 151 |
| O2*W*—H2*WF*···O10*A*$^{vi}$ | 0.87 | 1.96 | 2.822 (3) | 173 |
| O21*W*$^{a}$—H21*A*$^{a}$···O10*B* | 0.88 | 2.41 | 3.181 (9) | 145 |
| O21*W*$^{a}$—H21*B*$^{a}$···O11*B* | 0.90 | 2.36 | 3.213 (9) | 157 |
| O21*W*$^{a}$—H21*B*$^{a}$···O12*B* | 0.90 | 2.60 | 3.127 (10) | 118 |
| O19*W*—H19*C*···O7*B*$^{i}$ | 0.87 | 2.29 | 2.856 (4) | 123 |
| O19*W*—H19*C*···O8*B*$^{i}$ | 0.87 | 2.28 | 2.939 (4) | 132 |
| O19*W*—H19*D*···O17*W*$^{b}$ | 0.87 | 2.16 | 2.813 (7) | 132 |
| O19*W*—H19*D*···O18*W*$^{a}$ | 0.87 | 1.70 | 2.54 (2) | 160 |
| O14*W*—H14*C*···O11*B*$^{i}$ | 0.87 | 2.42 | 2.870 (4) | 112 |
| O14*W*—H14*C*···O12*B*$^{i}$ | 0.87 | 2.21 | 3.024 (4) | 156 |
| O14*W*—H14*D*···O24*W* | 0.85 | 2.25 | 2.913 (5) | 135 |
| O6*W*—H6*WA*···O9*A* | 0.86 (2) | 2.29 (2) | 3.101 (5) | 159 (4) |
| O6*W*—H6*WB*···O10*A* | 0.87 (2) | 2.31 (2) | 3.117 (5) | 155 (4) |
| O16*W*—H16*A*···O8*B*$^{iv}$ | 0.87 | 2.17 | 3.014 (4) | 163 |
| O16*W*—H16*B*···O15*W* | 0.87 | 1.93 | 2.723 (4) | 152 |
| O7*W*$^{c}$—H7*WA*$^{c}$···O6*W* | 0.89 | 1.79 | 2.673 (17) | 170 |
| O4*W*—H4*WE*···O12*W* | 0.87 | 1.89 | 2.744 (4) | 166 |
| O4*W*—H4*WF*···O7*A*$^{vi}$ | 0.87 | 1.91 | 2.777 (3) | 177 |
| O8*W*$^{a}$—H8*WA*$^{a}$···O6*W* | 0.87 | 1.93 | 2.737 (9) | 153 |
| O8*W*$^{a}$—H8*WB*$^{a}$···N21*A* | 0.87 | 2.66 | 3.316 (9) | 133 |
| O18*W*$^{a}$—H18*E*$^{a}$···O2*A*$^{v}$ | 0.87 | 2.08 | 2.94 (2) | 171 |
| O18*W*$^{a}$—H18*F*$^{a}$···O25*W* | 0.87 | 2.35 | 2.79 (4) | 111 |
| O9*W*$^{b}$—H9*WA*$^{b}$···N19*A* | 0.83 | 2.69 | 3.411 (10) | 146 |
| O9*W*$^{b}$—H9*WB*$^{b}$···O6*W* | 0.86 | 1.94 | 2.805 (10) | 177 |
| O5*W*—H5*WE*···O14*W* | 0.90 | 1.58 | 2.440 (11) | 158 |
| O5*W*—H5*WF*···O20*B*$^{i}$ | 0.87 | 1.99 | 2.786 (12) | 151 |
| O10*W*—H10*A*···O4*B*$^{i}$ | 0.87 | 2.21 | 2.981 (3) | 148 |
| O10*W*—H10*B*···O3*W* | 0.87 | 1.83 | 2.697 (4) | 175 |
| O20*W*$^{b}$—H20*C*$^{b}$···O12*B* | 0.87 | 2.00 | 2.86 (2) | 167 |
| O20*W*$^{b}$—H20*D*$^{b}$···O5*WA*$^{vii}$ | 0.87 | 2.38 | 3.00 (2) | 128 |
| O20*W*$^{b}$—H20*D*$^{b}$···O19*W*$^{i}$ | 0.87 | 2.37 | 3.20 (4) | 160 |
| O11*W*—H11*E*···O13*W* | 0.87 | 1.91 | 2.749 (4) | 161 |
| O11*W*—H11*F*···O12*A*$^{vi}$ | 0.87 | 1.90 | 2.755 (4) | 168 |
| O22*W*$^{a}$—H22*A*$^{a}$···O21*W*$^{a}$ | 0.87 | 1.80 | 2.670 (11) | 179 |
| O22*W*$^{a}$—H22*B*$^{a}$···O1*WB* | 0.87 | 1.93 | 2.763 (8) | 161 |
| O12*W*—H12*E*···O3*B*$^{i}$ | 0.87 | 2.05 | 2.913 (4) | 169 |
| O12*W*—H12*F*···O2*B*$^{i}$ | 0.87 | 2.15 | 2.918 (4) | 147 |
| O25*W*—H25*C*···O21*A* | 0.87 | 2.02 | 2.872 (5) | 166 |
| O25*W*—H25*D*···O18*B*$^{viii}$ | 0.87 | 2.09 | 2.953 (6) | 170 |
| O13*W*—H13*C*···O17*B* | 0.87 | 2.03 | 2.884 (5) | 165 |
| O13*W*—H13*D*···O21*A*$^{ix}$ | 0.87 | 1.96 | 2.800 (4) | 163 |
| O24*W*—H24*E*···O25*W* | 0.87 | 1.93 | 2.790 (5) | 171 |
| O24*W*—H24*F*···O12*B*$^{i}$ | 0.87 | 2.17 | 2.839 (4) | 133 |

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

the formation of hydrogen bonds with non-coordinated water molecules located between adjacent $[Pr(\mathbf{CB6})(NO_3)(H_2O)_5]^{2+}$ fragments (in complex cations with Pr1*A* ions: O2*A*—H17*E*···O17*W*, O3*A*—H17*W*···O17*W*, O3*A*—H15*A*···O15*W*, O7*A*—H4*F*···O4*W*, O8*A*—H3*WF*···O3*W*, O10*A*—H2*WE*···O2*W* and O12*A*—H11*F*···O11*W*; in complex cations with Pr1*B* ions: O2*B*—H12*F*···O12*W*, O3*B*—H12*E*···O12*W*, O7*B*—H19*C*···O19*W*, O8*B*—H16*A*···O16*W*, O11*B*—H14*C*···O14*W* and O12*B*—H24*F*···O24*W*). Water molecules coordinated to $Pr^{III}$ ions in **1** are also involved in the formation of hydrogen bonds with non-coordinated water molecules (water molecules coordinated to Pr1*A*: O1*WA*—H1*WA*···O9*W*, O2*WA*—H2*WD*···O19*W*, O3*WA*—H3*WD*···O16*W*, O4*WA*—H4*WD*···O14*W*, O5*WA*—H5*WC*···O19*W*; water molecules coordinated to Pr1*B*: O2*WB*—H2*WA*···O11*W*, O3*WB*—H3*W*···O2*W*, O4*WB*—H4*WA*···O1*W*, O5*WB*—H5*WB*···O4*W*).

In summary, we have synthesized a new $Pr^{III}$ complex with the macrocyclic cucurbit[6]uril ligand, which crystallizes in space group $P2_1/n$, while previously reported complexes with other lanthanide ions $Ln^{III}$ = La, Gd, Dy, Ho and Yb crystallized in $P2_1/n$ or $Pna2_1$. The crystal structure of **1** contains $[Pr(CB6)(NO_3)(H_2O)_5]^{2+}$ complex cations, two non-coordin-

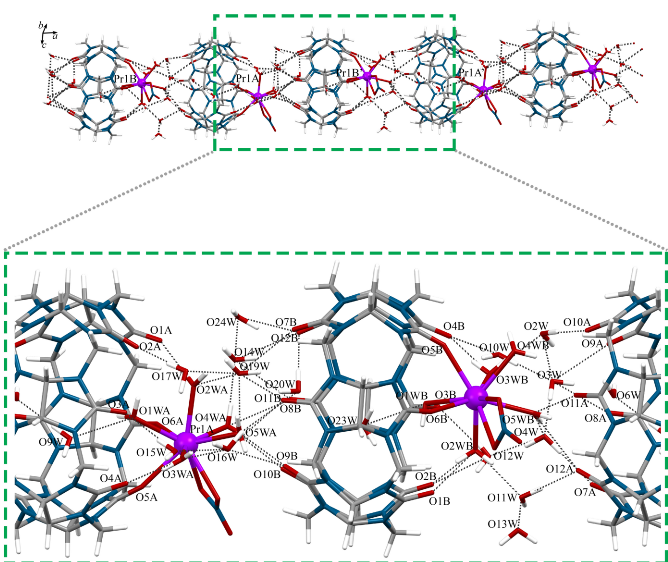



**Figure 4**
System of hydrogen bonds connecting the $[Pr(CB6)(NO_3)(H_2O)_5]^{2+}$ units in complex **1**.

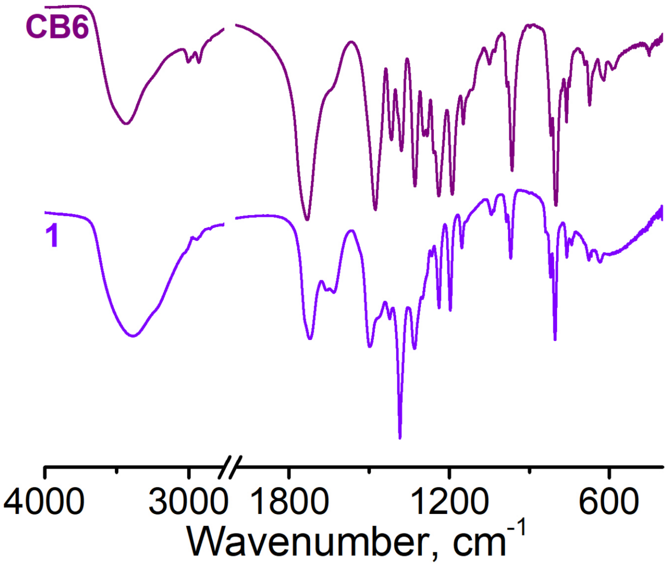



**Figure 5**
IR spectra of **CB6** and complex **1** recorded in a KBr pellet.

ated nitrates per cation and non-coordinated water molecules. Subtle differences in the bond distances and angles in the $Pr^{III}$ coordination spheres leads to the observation of two crystallographically different types of $Pr^{III}$ ions. The composition of the coordination sphere of two types of nonacoordinated $Pr^{III}$ ions in **1** is the same, however the symmetry of the coordination environment of Pr1*A* and Pr1*B* ions is different.

## 4. Synthesis and crystallization

Cucurbit[6]uril was obtained by a modified procedure (Zbruyev *et al.*, 2023). Cucurbit[6]uril ($C_{36}H_{36}N_{24}O_{12}\cdot10H_2O$, **CB6**, 11.8 mg, 0.01 mmol) and $Pr(NO_3)_3\cdot6H_2O$ (42 mg, 0.1 mmol) were placed in a closed vial containing 3 mL of water and ultrasonicated for the enhancement of macrocycle solubility. The obtained suspension was heated for 1 h at 358 K in a sand bath, which was accompanied by dissolution of macrocyclic ligand. Afterwards the observed clear solution had been heated at 363 K for 2 h. Slow cooling in the sand bath led to the formation of colorless crystals of **1** in one day. IR spectra of **CB6** and complex **1** are shown in Fig. 5.

## 5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. H atoms were placed in calculated positions and refined as riding.


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**Table 4**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[Pr(NO_3)(C_{36}H_{36}N_{24}O_{12})(H_2O)_5]$-$(NO_3)_2\cdot9.56H_2O$ |
| $M_r$ | 1586.05 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 180 |
| $a, b, c$ (Å) | 24.1937 (3), 17.01202 (19), 28.6422 (3) |
| $\beta$ (°) | 90.5965 (11) |
| $V$ (Å$^3$) | 11788.0 (2) |
| $Z$ | 8 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.95 |
| Crystal size (mm) | 0.25 × 0.10 × 0.05 |
| | |
| Data collection | |
| Diffractometer | Rigaku Oxford Diffraction Xcalibur, Eos |
| Absorption correction | Multi-scan (*CrysAlis PRO*; Rigaku OD, 2022) |
| $T_{min}, T_{max}$ | 0.892, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 75330, 20820, 17014 |
| $R_{int}$ | 0.043 |
| $(\sin \theta/\lambda)_{max}$ (Å$^{-1}$) | 0.595 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.037, 0.087, 1.04 |
| No. of reflections | 20820 |
| No. of parameters | 1843 |
| No. of restraints | 84 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}, \Delta\rho_{min}$ (e Å$^{-3}$) | 1.26, −0.64 |

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

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# supporting information

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## The crystal structure of a mononuclear Pr$^{III}$ complex with cucurbit[6]uril

**George V. Fedorenko, Oleksandr I. Zbruyev, Anna V. Pavlishchuk, Lyudmila P. Oleksenko, Sergiu G. Shova, Valentyn A. Chebanov and Vitaly V. Pavlishchuk**

### Computing details

### Pentaaqua(cucurbit[6]uril-κ$^2$*O,O′*)(nitrato-κ$^2$*O,O′*)praseodymium(III) dinitrate 9.56-hydrate

*Crystal data*

$[Pr(NO_3)(C_{36}H_{36}N_{24}O_{12})(H_2O)_5](NO_3)_2·9.56H_2O$
$M_r$ = 1586.05
Monoclinic, $P2_1/n$
$a$ = 24.1937 (3) Å
$b$ = 17.01202 (19) Å
$c$ = 28.6422 (3) Å
$β$ = 90.5965 (11)°
$V$ = 11788.0 (2) Å$^3$
$Z$ = 8
$F(000)$ = 6508
$D_x$ = 1.787 Mg m$^{-3}$
Mo $Kα$ radiation, $λ$ = 0.71073 Å
Cell parameters from 28067 reflections
$θ$ = 1.7–29.2°
$μ$ = 0.95 mm$^{-1}$
$T$ = 180 K
Prism, clear light colourless
0.25 × 0.10 × 0.05 mm

*Data collection*

Rigaku Oxford Diffraction Xcalibur, Eos diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1593 pixels mm$^{-1}$
$ω$ scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2022)
$T_{min}$ = 0.892, $T_{max}$ = 1.000
75330 measured reflections
20820 independent reflections
17014 reflections with $I > 2σ(I)$
$R_{int}$ = 0.043
$θ_{max}$ = 25.0°, $θ_{min}$ = 1.7°
$h$ = −28→28
$k$ = −20→20
$l$ = −34→34

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2σ(F^2)]$ = 0.037
$wR(F^2)$ = 0.087
$S$ = 1.04
20820 reflections
1843 parameters
84 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[σ^2(F_o^2) + (0.0337P)^2 + 14.5091P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(Δ/σ)_{max}$ = 0.003
$Δρ_{max}$ = 1.26 e Å$^{-3}$
$Δρ_{min}$ = −0.64 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Pr1B | 0.56080 (2) | 0.81394 (2) | 0.59862 (2) | 0.01479 (5) | |
| O1WB | 0.47590 (11) | 0.73681 (17) | 0.62441 (10) | 0.0377 (7) | |
| H1WA | 0.486182 | 0.690310 | 0.636326 | 0.057* | |
| H1WB | 0.470192 | 0.751057 | 0.653367 | 0.057* | |
| O1B | 0.48772 (10) | 0.91183 (14) | 0.71903 (10) | 0.0270 (6) | |
| O2WB | 0.55961 (10) | 0.79322 (14) | 0.68282 (9) | 0.0227 (6) | |
| H2WA | 0.586751 | 0.819146 | 0.695909 | 0.034* | |
| H2WB | 0.529881 | 0.814445 | 0.694371 | 0.034* | |
| O2B | 0.48542 (11) | 0.72565 (15) | 0.75053 (12) | 0.0422 (8) | |
| O3WB | 0.58270 (10) | 0.67361 (13) | 0.59506 (9) | 0.0255 (6) | |
| H3WA | 0.609936 | 0.666078 | 0.575809 | 0.038* | |
| H3WB | 0.554996 | 0.648289 | 0.582458 | 0.038* | |
| O3B | 0.49472 (10) | 0.55689 (16) | 0.67188 (9) | 0.0328 (7) | |
| O4WB | 0.62515 (10) | 0.80282 (15) | 0.53001 (9) | 0.0282 (6) | |
| H4WA | 0.616218 | 0.761685 | 0.513332 | 0.042* | |
| H4WB | 0.658602 | 0.792674 | 0.540175 | 0.042* | |
| O4B | 0.51371 (10) | 0.55885 (13) | 0.56426 (9) | 0.0220 (6) | |
| O5WB | 0.65703 (9) | 0.79418 (14) | 0.62651 (9) | 0.0239 (6) | |
| H5WA | 0.684114 | 0.827830 | 0.625512 | 0.036* | |
| H5WB | 0.667755 | 0.759336 | 0.646922 | 0.036* | |
| O5B | 0.50626 (9) | 0.77305 (13) | 0.52729 (8) | 0.0178 (5) | |
| O6B | 0.48547 (9) | 0.91097 (14) | 0.59600 (9) | 0.0220 (6) | |
| O7B | 0.25571 (10) | 0.75673 (15) | 0.50609 (10) | 0.0313 (7) | |
| O8B | 0.23920 (10) | 0.93703 (15) | 0.57119 (9) | 0.0247 (6) | |
| O9B | 0.24207 (10) | 0.88557 (14) | 0.68395 (9) | 0.0265 (6) | |
| O10B | 0.23623 (10) | 0.69061 (14) | 0.73399 (10) | 0.0267 (6) | |
| O11B | 0.24724 (10) | 0.52504 (16) | 0.66726 (9) | 0.0299 (6) | |
| O12B | 0.26210 (10) | 0.56796 (15) | 0.55534 (10) | 0.0321 (7) | |
| O13B | 0.59277 (11) | 0.94176 (14) | 0.64444 (9) | 0.0287 (6) | |
| O14B | 0.60014 (10) | 0.94555 (14) | 0.56987 (9) | 0.0237 (6) | |
| O15B | 0.63579 (10) | 1.03954 (14) | 0.61214 (9) | 0.0272 (6) | |
| N1B | 0.60973 (12) | 0.97756 (17) | 0.60905 (11) | 0.0189 (7) | |
| N4B | 0.41097 (11) | 0.98499 (16) | 0.69788 (10) | 0.0163 (6) | |
| N5B | 0.31183 (11) | 0.97714 (16) | 0.68493 (10) | 0.0157 (6) | |
| N6B | 0.30779 (11) | 0.88978 (16) | 0.74275 (10) | 0.0171 (6) | |
| N7B | 0.40668 (11) | 0.90972 (16) | 0.76095 (11) | 0.0200 (7) | |
| N8B | 0.40462 (11) | 0.77192 (16) | 0.78199 (11) | 0.0189 (7) | |
| N9B | 0.30465 (11) | 0.75783 (15) | 0.77427 (10) | 0.0178 (7) | |
| N10B | 0.31271 (11) | 0.62898 (15) | 0.76599 (10) | 0.0162 (6) | |

| | | | | |
|---|---|---|---|---|
| N11B | 0.41256 (11) | 0.64389 (15) | 0.76862 (10) | 0.0175 (6) |
| N12B | 0.32050 (11) | 0.51116 (16) | 0.71870 (10) | 0.0176 (6) |
| N13B | 0.42078 (11) | 0.52820 (16) | 0.71929 (10) | 0.0186 (7) |
| N14B | 0.42782 (12) | 0.46547 (17) | 0.65184 (10) | 0.0194 (7) |
| N15B | 0.32735 (12) | 0.45865 (17) | 0.64833 (10) | 0.0196 (7) |
| N16B | 0.33628 (12) | 0.48466 (17) | 0.56576 (10) | 0.0201 (7) |
| N17B | 0.43743 (12) | 0.47786 (16) | 0.56773 (10) | 0.0179 (6) |
| N18B | 0.33767 (12) | 0.56903 (16) | 0.50693 (11) | 0.0199 (7) |
| N19B | 0.43849 (11) | 0.57223 (16) | 0.51452 (10) | 0.0165 (6) |
| N20B | 0.33547 (12) | 0.70226 (16) | 0.47753 (11) | 0.0196 (7) |
| N21B | 0.43552 (11) | 0.70763 (15) | 0.48855 (10) | 0.0144 (6) |
| N22B | 0.33276 (11) | 0.83151 (16) | 0.48861 (10) | 0.0170 (6) |
| N23B | 0.43332 (11) | 0.83771 (15) | 0.49156 (10) | 0.0145 (6) |
| N24B | 0.32163 (11) | 0.95249 (16) | 0.53227 (10) | 0.0190 (7) |
| N25B | 0.42278 (11) | 0.95266 (16) | 0.54014 (10) | 0.0167 (6) |
| N26B | 0.31293 (11) | 1.00684 (16) | 0.60210 (10) | 0.0164 (6) |
| N27B | 0.41203 (11) | 0.99137 (15) | 0.61323 (10) | 0.0158 (6) |
| C1B | 0.35630 (13) | 1.00089 (19) | 0.71601 (12) | 0.0140 (7) |
| H1B | 0.352366 | 1.056931 | 0.725973 | 0.017* |
| C2B | 0.35189 (13) | 0.94338 (18) | 0.75820 (12) | 0.0149 (7) |
| H2B | 0.341992 | 0.971511 | 0.787609 | 0.018* |
| C3B | 0.43990 (14) | 0.93228 (19) | 0.72489 (13) | 0.0186 (8) |
| C4B | 0.28340 (14) | 0.91371 (19) | 0.70194 (12) | 0.0158 (8) |
| C5B | 0.27999 (14) | 0.83490 (19) | 0.77356 (13) | 0.0188 (8) |
| H5BA | 0.280534 | 0.856499 | 0.805659 | 0.023* |
| H5BB | 0.240865 | 0.830080 | 0.763508 | 0.023* |
| C6B | 0.42404 (15) | 0.84978 (19) | 0.79379 (14) | 0.0226 (8) |
| H6BA | 0.464928 | 0.849079 | 0.795425 | 0.027* |
| H6BB | 0.410342 | 0.863812 | 0.825156 | 0.027* |
| C7B | 0.35437 (14) | 0.73954 (18) | 0.80104 (13) | 0.0168 (8) |
| H7B | 0.350236 | 0.752971 | 0.834817 | 0.020* |
| C8B | 0.36084 (13) | 0.64994 (19) | 0.79352 (12) | 0.0156 (7) |
| H8B | 0.362203 | 0.620768 | 0.823821 | 0.019* |
| C9B | 0.43919 (15) | 0.7150 (2) | 0.76524 (14) | 0.0227 (8) |
| C10B | 0.27990 (14) | 0.69254 (19) | 0.75570 (12) | 0.0175 (8) |
| C11B | 0.29540 (14) | 0.54941 (19) | 0.75811 (12) | 0.0175 (8) |
| H11A | 0.254788 | 0.548881 | 0.753514 | 0.021* |
| H11B | 0.303860 | 0.518325 | 0.786516 | 0.021* |
| C12B | 0.43993 (14) | 0.57008 (19) | 0.76091 (12) | 0.0171 (8) |
| H12A | 0.434301 | 0.536036 | 0.788491 | 0.021* |
| H12B | 0.480117 | 0.579755 | 0.758213 | 0.021* |
| C13B | 0.37447 (14) | 0.47439 (19) | 0.71995 (12) | 0.0166 (8) |
| H13B | 0.377848 | 0.435552 | 0.746033 | 0.020* |
| C14B | 0.37760 (14) | 0.43374 (19) | 0.67130 (12) | 0.0160 (7) |
| H14B | 0.379409 | 0.375225 | 0.674280 | 0.019* |
| C15B | 0.45185 (14) | 0.5212 (2) | 0.67998 (13) | 0.0199 (8) |
| C16B | 0.29387 (14) | 0.50168 (19) | 0.67675 (13) | 0.0190 (8) |
| C17B | 0.45297 (14) | 0.4360 (2) | 0.60984 (12) | 0.0178 (8) |

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|---|---|---|---|---|
| H17A | 0.442744 | 0.379980 | 0.606026 | 0.021* |
| H17B | 0.493642 | 0.438575 | 0.613659 | 0.021* |
| C18B | 0.31179 (15) | 0.4360 (2) | 0.60153 (13) | 0.0218 (8) |
| H18A | 0.271048 | 0.438609 | 0.598368 | 0.026* |
| H18B | 0.323017 | 0.380692 | 0.596402 | 0.026* |
| C19B | 0.38675 (14) | 0.46397 (19) | 0.54149 (12) | 0.0168 (8) |
| H19B | 0.385156 | 0.409391 | 0.528591 | 0.020* |
| C20B | 0.38917 (14) | 0.52679 (19) | 0.50213 (12) | 0.0171 (8) |
| H20B | 0.392401 | 0.502091 | 0.470596 | 0.021* |
| C21B | 0.46726 (14) | 0.53940 (19) | 0.55065 (12) | 0.0159 (7) |
| C22B | 0.30784 (15) | 0.5433 (2) | 0.54383 (13) | 0.0214 (8) |
| C23B | 0.31583 (15) | 0.6223 (2) | 0.47205 (13) | 0.0221 (8) |
| H23A | 0.274979 | 0.622172 | 0.473686 | 0.026* |
| H23B | 0.326201 | 0.603010 | 0.440736 | 0.026* |
| C24B | 0.46224 (14) | 0.63159 (18) | 0.48440 (12) | 0.0163 (7) |
| H24A | 0.459304 | 0.613640 | 0.451587 | 0.020* |
| H24B | 0.501984 | 0.637397 | 0.492208 | 0.020* |
| C25B | 0.38771 (13) | 0.72842 (19) | 0.45926 (12) | 0.0156 (7) |
| H25B | 0.392731 | 0.711757 | 0.426097 | 0.019* |
| C26B | 0.38432 (13) | 0.81872 (19) | 0.46399 (12) | 0.0156 (7) |
| H26B | 0.384405 | 0.845439 | 0.432896 | 0.019* |
| C27B | 0.46232 (14) | 0.77303 (19) | 0.50474 (12) | 0.0153 (7) |
| C28B | 0.30308 (15) | 0.7629 (2) | 0.49235 (13) | 0.0212 (8) |
| C29B | 0.30666 (14) | 0.9083 (2) | 0.49094 (12) | 0.0193 (8) |
| H29A | 0.317092 | 0.938994 | 0.463023 | 0.023* |
| H29B | 0.266041 | 0.901314 | 0.490064 | 0.023* |
| C30B | 0.45060 (14) | 0.91719 (19) | 0.50051 (12) | 0.0154 (7) |
| H30A | 0.443177 | 0.949365 | 0.472334 | 0.018* |
| H30B | 0.490978 | 0.917773 | 0.506459 | 0.018* |
| C31B | 0.37221 (14) | 0.99832 (19) | 0.53747 (12) | 0.0177 (8) |
| H31B | 0.374513 | 1.041237 | 0.513708 | 0.021* |
| C32B | 0.36752 (14) | 1.0314 (2) | 0.58800 (12) | 0.0170 (8) |
| H32B | 0.371819 | 1.089811 | 0.588916 | 0.020* |
| C33B | 0.44358 (14) | 0.94841 (19) | 0.58436 (12) | 0.0164 (8) |
| C34B | 0.28648 (14) | 0.96181 (19) | 0.56926 (12) | 0.0163 (8) |
| C35B | 0.29035 (14) | 1.0259 (2) | 0.64696 (12) | 0.0184 (8) |
| H35A | 0.249667 | 1.019953 | 0.645373 | 0.022* |
| H35B | 0.298532 | 1.081663 | 0.654069 | 0.022* |
| C36B | 0.43400 (14) | 1.0215 (2) | 0.65738 (12) | 0.0187 (8) |
| H36A | 0.474563 | 1.013763 | 0.658018 | 0.022* |
| H36B | 0.426873 | 1.078735 | 0.658897 | 0.022* |
| Pr1A | 0.57442 (2) | 0.76863 (2) | 0.18574 (2) | 0.01388 (5) |
| O1A | 0.52959 (10) | 0.90673 (14) | 0.06042 (9) | 0.0244 (6) |
| O1WA | 0.48655 (11) | 0.74271 (16) | 0.13871 (10) | 0.0338 (7) |
| H1WC | 0.493989 | 0.736521 | 0.109566 | 0.051* |
| H1WD | 0.462049 | 0.777421 | 0.144625 | 0.051* |
| O2A | 0.49150 (11) | 0.72148 (15) | 0.02604 (10) | 0.0319 (7) |
| O2WA | 0.58725 (11) | 0.79270 (15) | 0.10227 (9) | 0.0295 (6) |

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|---|---|---|---|---|
| H2WC | 0.568280 | 0.830052 | 0.088916 | 0.044* |
| H2WD | 0.607064 | 0.773022 | 0.079956 | 0.044* |
| O3WA | 0.56863 (10) | 0.62637 (14) | 0.17536 (10) | 0.0307 (7) |
| H3WC | 0.538318 | 0.604139 | 0.184774 | 0.046* |
| H3WD | 0.584088 | 0.591259 | 0.157684 | 0.046* |
| O3A | 0.47393 (10) | 0.53124 (15) | 0.08121 (10) | 0.0298 (6) |
| O4A | 0.47559 (10) | 0.54094 (14) | 0.19161 (10) | 0.0258 (6) |
| O4WA | 0.64300 (10) | 0.88067 (13) | 0.18532 (9) | 0.0232 (6) |
| H4WC | 0.674158 | 0.864967 | 0.197585 | 0.035* |
| H4WD | 0.648367 | 0.895498 | 0.157396 | 0.035* |
| O5WA | 0.66466 (9) | 0.71843 (14) | 0.15799 (9) | 0.0224 (6) |
| H5WC | 0.660848 | 0.700271 | 0.129599 | 0.034* |
| H5WD | 0.674338 | 0.677470 | 0.174529 | 0.034* |
| O5A | 0.50058 (10) | 0.73070 (13) | 0.24148 (9) | 0.0201 (5) |
| O6A | 0.52373 (9) | 0.89438 (13) | 0.18430 (8) | 0.0197 (5) |
| O7A | 0.25431 (10) | 0.80013 (15) | 0.25809 (10) | 0.0275 (6) |
| O8A | 0.27946 (10) | 0.98195 (15) | 0.19179 (9) | 0.0270 (6) |
| O9A | 0.28105 (11) | 0.95178 (16) | 0.07980 (10) | 0.0340 (7) |
| O10A | 0.24609 (10) | 0.77112 (14) | 0.01672 (9) | 0.0246 (6) |
| O11A | 0.22893 (10) | 0.60894 (15) | 0.07673 (9) | 0.0284 (6) |
| O12A | 0.23249 (10) | 0.62070 (15) | 0.19417 (9) | 0.0262 (6) |
| O13A | 0.62804 (11) | 0.70786 (14) | 0.25481 (9) | 0.0253 (6) |
| O14A | 0.59886 (10) | 0.82552 (13) | 0.26813 (9) | 0.0217 (6) |
| O15A | 0.64832 (15) | 0.76442 (17) | 0.32079 (11) | 0.0532 (10) |
| N1A | 0.62551 (13) | 0.76602 (17) | 0.28276 (11) | 0.0250 (7) |
| N4A | 0.46216 (12) | 0.99487 (16) | 0.08181 (10) | 0.0192 (7) |
| N5A | 0.36272 (11) | 1.02021 (17) | 0.08671 (10) | 0.0199 (7) |
| N6A | 0.35073 (11) | 0.93992 (16) | 0.02598 (10) | 0.0183 (6) |
| N7A | 0.45086 (12) | 0.92786 (17) | 0.01601 (11) | 0.0204 (7) |
| N8A | 0.42725 (12) | 0.79814 (16) | −0.01314 (11) | 0.0220 (7) |
| N9A | 0.32820 (12) | 0.81825 (16) | −0.01343 (10) | 0.0186 (7) |
| N10A | 0.31330 (11) | 0.68980 (16) | −0.01359 (10) | 0.0183 (7) |
| N11A | 0.41303 (12) | 0.66954 (16) | −0.00882 (11) | 0.0202 (7) |
| N12A | 0.29677 (11) | 0.56631 (16) | 0.02689 (10) | 0.0184 (7) |
| N13A | 0.39697 (12) | 0.54957 (16) | 0.03391 (10) | 0.0186 (7) |
| N14A | 0.39014 (12) | 0.47167 (17) | 0.09562 (11) | 0.0210 (7) |
| N15A | 0.29310 (12) | 0.51386 (17) | 0.09766 (10) | 0.0199 (7) |
| N16A | 0.29088 (11) | 0.51562 (16) | 0.18255 (10) | 0.0183 (7) |
| N17A | 0.38934 (11) | 0.48661 (16) | 0.17968 (10) | 0.0183 (7) |
| N18A | 0.30528 (11) | 0.59156 (17) | 0.24436 (10) | 0.0187 (7) |
| N19A | 0.40343 (11) | 0.56116 (16) | 0.24222 (11) | 0.0192 (7) |
| N20A | 0.32296 (12) | 0.71531 (17) | 0.28327 (11) | 0.0200 (7) |
| N21A | 0.42169 (11) | 0.68743 (16) | 0.27817 (10) | 0.0174 (6) |
| N22A | 0.34140 (11) | 0.84330 (16) | 0.28023 (10) | 0.0176 (6) |
| N23A | 0.43991 (11) | 0.81477 (16) | 0.27806 (10) | 0.0157 (6) |
| N24A | 0.35820 (11) | 0.96256 (16) | 0.23646 (10) | 0.0173 (6) |
| N25A | 0.45675 (11) | 0.93532 (16) | 0.23537 (10) | 0.0154 (6) |
| N26A | 0.36452 (11) | 1.03135 (16) | 0.17075 (10) | 0.0175 (6) |

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|---|---|---|---|---|
| N27A | 0.46227 (11) | 0.99413 (16) | 0.16680 (10) | 0.0171 (6) |
| C1A | 0.41290 (14) | 1.0302 (2) | 0.06082 (12) | 0.0177 (8) |
| H1A | 0.419203 | 1.086604 | 0.052585 | 0.021* |
| C2A | 0.40301 (14) | 0.97888 (19) | 0.01633 (13) | 0.0181 (8) |
| H2A | 0.400656 | 1.011773 | −0.012555 | 0.022* |
| C3A | 0.48476 (15) | 0.93862 (19) | 0.05407 (13) | 0.0188 (8) |
| C4A | 0.32705 (14) | 0.9686 (2) | 0.06553 (13) | 0.0204 (8) |
| C5A | 0.31757 (14) | 0.9012 (2) | −0.00957 (13) | 0.0202 (8) |
| H5AA | 0.278013 | 0.909101 | −0.002417 | 0.024* |
| H5AB | 0.324788 | 0.926356 | −0.040077 | 0.024* |
| C6A | 0.46087 (15) | 0.8674 (2) | −0.01824 (13) | 0.0217 (8) |
| H6AA | 0.454236 | 0.889699 | −0.049731 | 0.026* |
| H6AB | 0.500251 | 0.851832 | −0.016240 | 0.026* |
| C7A | 0.37517 (14) | 0.7875 (2) | −0.03791 (13) | 0.0188 (8) |
| H7A | 0.376834 | 0.807493 | −0.070695 | 0.023* |
| C8A | 0.36599 (14) | 0.6974 (2) | −0.03618 (12) | 0.0183 (8) |
| H8A | 0.365282 | 0.673857 | −0.068160 | 0.022* |
| C9A | 0.44835 (15) | 0.7287 (2) | 0.00399 (13) | 0.0220 (8) |
| C10A | 0.29131 (15) | 0.7612 (2) | −0.00146 (12) | 0.0187 (8) |
| C11A | 0.28239 (14) | 0.6171 (2) | −0.01180 (12) | 0.0191 (8) |
| H11C | 0.242538 | 0.629795 | −0.010044 | 0.023* |
| H11D | 0.288281 | 0.587938 | −0.041254 | 0.023* |
| C12A | 0.42587 (14) | 0.5869 (2) | −0.00377 (13) | 0.0204 (8) |
| H12C | 0.416412 | 0.559591 | −0.033300 | 0.024* |
| H12D | 0.466140 | 0.581065 | 0.001627 | 0.024* |
| C13A | 0.34317 (14) | 0.5129 (2) | 0.02782 (13) | 0.0184 (8) |
| H13A | 0.342463 | 0.476458 | 0.000443 | 0.022* |
| C14A | 0.33550 (14) | 0.4682 (2) | 0.07441 (12) | 0.0183 (8) |
| H14A | 0.323378 | 0.412675 | 0.069001 | 0.022* |
| C15A | 0.42500 (15) | 0.5194 (2) | 0.07168 (13) | 0.0208 (8) |
| C16A | 0.26900 (14) | 0.5679 (2) | 0.06818 (13) | 0.0185 (8) |
| C17A | 0.40390 (15) | 0.4378 (2) | 0.14026 (13) | 0.0213 (8) |
| H17C | 0.444165 | 0.427509 | 0.141487 | 0.026* |
| H17D | 0.384728 | 0.386668 | 0.143117 | 0.026* |
| C18A | 0.26556 (14) | 0.4876 (2) | 0.13986 (12) | 0.0191 (8) |
| H18C | 0.226660 | 0.505640 | 0.138729 | 0.023* |
| H18D | 0.265280 | 0.429457 | 0.140346 | 0.023* |
| C19A | 0.33812 (14) | 0.4794 (2) | 0.20486 (12) | 0.0190 (8) |
| H19A | 0.330427 | 0.423601 | 0.213605 | 0.023* |
| C20A | 0.34769 (14) | 0.53184 (19) | 0.24878 (12) | 0.0170 (8) |
| H20A | 0.344245 | 0.501228 | 0.278418 | 0.020* |
| C21A | 0.42744 (15) | 0.53089 (19) | 0.20315 (13) | 0.0196 (8) |
| C22A | 0.27237 (14) | 0.5804 (2) | 0.20566 (12) | 0.0178 (8) |
| C23A | 0.29043 (14) | 0.6442 (2) | 0.28221 (13) | 0.0218 (8) |
| H23C | 0.250884 | 0.658348 | 0.278920 | 0.026* |
| H23D | 0.295274 | 0.616259 | 0.312286 | 0.026* |
| C24A | 0.43424 (14) | 0.60403 (19) | 0.27711 (13) | 0.0203 (8) |
| H24C | 0.474206 | 0.597253 | 0.271219 | 0.024* |

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| H24D | 0.426414 | 0.581224 | 0.308146 | 0.024* | |
| C25A | 0.37665 (13) | 0.7209 (2) | 0.30513 (12) | 0.0165 (7) | |
| H25A | 0.376373 | 0.699985 | 0.337761 | 0.020* | |
| C26A | 0.38905 (13) | 0.81014 (19) | 0.30419 (12) | 0.0165 (7) | |
| H26A | 0.393595 | 0.832126 | 0.336384 | 0.020* | |
| C27A | 0.45769 (14) | 0.74376 (19) | 0.26374 (12) | 0.0157 (7) | |
| C28A | 0.30109 (14) | 0.7879 (2) | 0.27206 (12) | 0.0203 (8) | |
| C29A | 0.33119 (14) | 0.9268 (2) | 0.27605 (12) | 0.0191 (8) | |
| H29C | 0.344162 | 0.953206 | 0.304968 | 0.023* | |
| H29D | 0.290859 | 0.935683 | 0.273178 | 0.023* | |
| C30A | 0.47198 (13) | 0.88587 (19) | 0.27464 (12) | 0.0161 (7) | |
| H30C | 0.511512 | 0.871647 | 0.272038 | 0.019* | |
| H30D | 0.467635 | 0.916426 | 0.303790 | 0.019* | |
| C31A | 0.41402 (13) | 0.99428 (19) | 0.23820 (12) | 0.0166 (8) | |
| H31A | 0.419762 | 1.030211 | 0.265448 | 0.020* | |
| C32A | 0.41934 (13) | 1.03807 (19) | 0.19099 (12) | 0.0158 (7) | |
| H32A | 0.430147 | 1.094279 | 0.195670 | 0.019* | |
| C33A | 0.48415 (13) | 0.93666 (18) | 0.19464 (12) | 0.0155 (7) | |
| C34A | 0.32906 (15) | 0.9904 (2) | 0.19885 (13) | 0.0192 (8) | |
| C35A | 0.34790 (14) | 1.0668 (2) | 0.12692 (12) | 0.0193 (8) | |
| H35C | 0.365426 | 1.119228 | 0.124362 | 0.023* | |
| H35D | 0.307345 | 1.074600 | 0.126828 | 0.023* | |
| C36A | 0.48871 (14) | 1.0214 (2) | 0.12462 (12) | 0.0183 (8) | |
| H36C | 0.527564 | 1.003145 | 0.124874 | 0.022* | |
| H36D | 0.489178 | 1.079590 | 0.124805 | 0.022* | |
| O16B | 0.54381 (15) | 0.2575 (2) | 0.11872 (14) | 0.0720 (12) | |
| O17B | 0.46355 (16) | 0.20587 (19) | 0.13009 (16) | 0.0713 (12) | |
| O18B | 0.47281 (16) | 0.3073 (2) | 0.08550 (15) | 0.0740 (12) | |
| N2B | 0.49486 (17) | 0.2564 (2) | 0.11405 (16) | 0.0478 (10) | |
| O19B | 0.21410 (11) | 0.16709 (15) | 0.62334 (10) | 0.0316 (7) | |
| O20B | 0.23535 (13) | 0.28860 (16) | 0.61011 (11) | 0.0423 (8) | |
| O21B | 0.29113 (11) | 0.19422 (16) | 0.58943 (10) | 0.0322 (7) | |
| N3B | 0.24697 (13) | 0.21708 (19) | 0.60798 (11) | 0.0249 (7) | |
| O19A | 0.70260 (12) | 0.19623 (17) | 0.61611 (11) | 0.0423 (8) | |
| O20A | 0.73974 (13) | 0.31081 (16) | 0.61681 (11) | 0.0423 (8) | |
| O21A | 0.79150 (12) | 0.20722 (18) | 0.61441 (12) | 0.0455 (8) | |
| N3A | 0.74391 (14) | 0.23856 (18) | 0.61561 (11) | 0.0257 (7) | |
| O16A | 0.45706 (13) | 0.1619 (2) | 0.57899 (13) | 0.0570 (10) | |
| O17A | 0.51151 (16) | 0.2472 (2) | 0.61215 (14) | 0.0655 (10) | |
| O18A | 0.53037 (12) | 0.12449 (19) | 0.61361 (10) | 0.0424 (8) | |
| N2A | 0.49932 (14) | 0.1785 (2) | 0.60257 (13) | 0.0364 (9) | |
| O15W | 0.55919 (11) | 0.43362 (16) | 0.11751 (10) | 0.0359 (7) | |
| H15A | 0.531808 | 0.463070 | 0.108221 | 0.054* | |
| H15B | 0.545841 | 0.386081 | 0.117051 | 0.054* | |
| O1W | 0.38077 (11) | 0.27422 (14) | 0.55348 (10) | 0.0322 (7) | |
| H1WE | 0.351200 | 0.256916 | 0.567085 | 0.048* | |
| H1WF | 0.406991 | 0.243166 | 0.563275 | 0.048* | |
| O17W | 0.9242 (2) | 0.1000 (4) | 0.4650 (3) | 0.084 (3) | 0.810 (13) |

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|---|---|---|---|---|---|
| H17E | 0.953798 | 0.128045 | 0.469856 | 0.125* | 0.810 (13) |
| H17F | 0.932326 | 0.070075 | 0.441486 | 0.125* | 0.810 (13) |
| O3W | 0.31358 (10) | 0.45574 (16) | 0.36281 (10) | 0.0328 (7) | |
| H3WE | 0.317282 | 0.412308 | 0.347052 | 0.049* | |
| H3WF | 0.280852 | 0.472889 | 0.355052 | 0.049* | |
| O23W | 0.3721 (7) | 0.7829 (12) | 0.6466 (11) | 0.101 (6) | 0.268 (13) |
| H23E | 0.385269 | 0.798725 | 0.620035 | 0.151* | 0.268 (13) |
| H23F | 0.390731 | 0.804397 | 0.669369 | 0.151* | 0.268 (13) |
| O2W | 0.32994 (10) | 0.38489 (14) | 0.45206 (9) | 0.0262 (6) | |
| H2WE | 0.313484 | 0.409891 | 0.429402 | 0.039* | |
| H2WF | 0.304996 | 0.352951 | 0.462630 | 0.039* | |
| O21W | 0.2860 (5) | 0.6953 (5) | 0.6317 (4) | 0.068 (3) | 0.71 (2) |
| H21A | 0.281586 | 0.712810 | 0.660446 | 0.102* | 0.71 (2) |
| H21B | 0.271467 | 0.646363 | 0.633036 | 0.102* | 0.71 (2) |
| O19W | 0.83588 (15) | 0.1981 (2) | 0.43782 (14) | 0.0665 (11) | |
| H19C | 0.803121 | 0.179963 | 0.444289 | 0.100* | |
| H19D | 0.856591 | 0.182842 | 0.461129 | 0.100* | |
| O14W | 0.84558 (13) | 0.4649 (2) | 0.39566 (12) | 0.0575 (10) | |
| H14C | 0.810849 | 0.454316 | 0.401063 | 0.086* | |
| H14D | 0.863130 | 0.442404 | 0.417723 | 0.086* | |
| O6W | 0.29069 (18) | 0.7823 (3) | 0.11899 (16) | 0.0797 (13) | |
| H6WA | 0.291 (3) | 0.8322 (11) | 0.1154 (17) | 0.120* | |
| H6WB | 0.276 (3) | 0.765 (2) | 0.0934 (10) | 0.120* | |
| O16W | 0.64638 (11) | 0.52937 (15) | 0.13768 (10) | 0.0340 (7) | |
| H16A | 0.668857 | 0.547816 | 0.116851 | 0.051* | |
| H16B | 0.624094 | 0.498744 | 0.122059 | 0.051* | |
| O7W | 0.3860 (7) | 0.8012 (10) | 0.1658 (6) | 0.0459 (15)* | 0.179 (3) |
| H7WA | 0.355099 | 0.800048 | 0.148376 | 0.069* | 0.179 (3) |
| H7WB | 0.380089 | 0.780447 | 0.193037 | 0.069* | 0.179 (3) |
| O4W | 0.32609 (10) | 0.32259 (15) | 0.31050 (10) | 0.0313 (7) | |
| H4WE | 0.355673 | 0.332245 | 0.294487 | 0.047* | |
| H4WF | 0.300503 | 0.314226 | 0.289477 | 0.047* | |
| O8W | 0.3801 (3) | 0.7352 (5) | 0.1712 (3) | 0.0459 (15)* | 0.430 (3) |
| H8WA | 0.346164 | 0.745262 | 0.162848 | 0.069* | 0.430 (3) |
| H8WB | 0.377194 | 0.700095 | 0.193128 | 0.069* | 0.430 (3) |
| O18W | 0.9063 (10) | 0.1339 (17) | 0.4920 (13) | 0.085 (5) | 0.190 (13) |
| H18E | 0.936805 | 0.160753 | 0.490161 | 0.128* | 0.190 (13) |
| H18F | 0.898504 | 0.134003 | 0.521622 | 0.128* | 0.190 (13) |
| O9W | 0.3805 (4) | 0.7046 (5) | 0.1611 (3) | 0.0459 (15)* | 0.391 (3) |
| H9WA | 0.371171 | 0.666792 | 0.177675 | 0.069* | 0.391 (3) |
| H9WB | 0.352882 | 0.729641 | 0.148865 | 0.069* | 0.391 (3) |
| O5W | 0.8489 (5) | 0.6034 (6) | 0.3737 (4) | 0.043 (4) | 0.272 (8) |
| H5WE | 0.856544 | 0.554241 | 0.383207 | 0.065* | 0.272 (8) |
| H5WF | 0.817436 | 0.622181 | 0.383057 | 0.065* | 0.272 (8) |
| O10W | 0.40465 (11) | 0.54046 (15) | 0.38409 (10) | 0.0323 (7) | |
| H10A | 0.429569 | 0.504098 | 0.387889 | 0.048* | |
| H10B | 0.374939 | 0.515039 | 0.375738 | 0.048* | |
| O20W | 0.2621 (12) | 0.7059 (13) | 0.6121 (10) | 0.076 (5) | 0.29 (2) |

| | | | | | |
|---|---|---|---|---|---|
| H20C | 0.261675 | 0.669053 | 0.591025 | 0.114* | 0.29 (2) |
| H20D | 0.233016 | 0.734203 | 0.605775 | 0.114* | 0.29 (2) |
| O11W | 0.36283 (10) | 0.15384 (14) | 0.25786 (9) | 0.0272 (6) | |
| H11E | 0.358043 | 0.190848 | 0.237224 | 0.041* | |
| H11F | 0.330993 | 0.149829 | 0.271514 | 0.041* | |
| O22W | 0.3694 (3) | 0.7887 (5) | 0.6070 (5) | 0.103 (4) | 0.570 (14) |
| H22A | 0.342314 | 0.758387 | 0.615393 | 0.154* | 0.570 (14) |
| H22B | 0.399086 | 0.763617 | 0.615923 | 0.154* | 0.570 (14) |
| O12W | 0.41996 (11) | 0.37574 (16) | 0.26779 (11) | 0.0382 (7) | |
| H12E | 0.442509 | 0.394474 | 0.288857 | 0.057* | |
| H12F | 0.437690 | 0.336314 | 0.255707 | 0.057* | |
| O25W | 0.86965 (16) | 0.2593 (3) | 0.54626 (14) | 0.0892 (14) | |
| H25C | 0.842890 | 0.251026 | 0.565829 | 0.134* | |
| H25D | 0.897800 | 0.234455 | 0.558301 | 0.134* | |
| O13W | 0.36971 (13) | 0.25594 (17) | 0.18376 (12) | 0.0483 (8) | |
| H13C | 0.397488 | 0.249018 | 0.165131 | 0.072* | |
| H13D | 0.341148 | 0.260256 | 0.165221 | 0.072* | |
| O24W | 0.83946 (12) | 0.37567 (19) | 0.48225 (14) | 0.0638 (11) | |
| H24E | 0.847245 | 0.335749 | 0.500164 | 0.096* | |
| H24F | 0.808034 | 0.363338 | 0.469114 | 0.096* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pr1B | 0.01164 (10) | 0.01606 (10) | 0.01665 (10) | −0.00069 (8) | −0.00064 (8) | 0.00139 (8) |
| O1WB | 0.0286 (16) | 0.0493 (18) | 0.0353 (17) | −0.0073 (14) | 0.0040 (14) | 0.0136 (14) |
| O1B | 0.0118 (13) | 0.0263 (14) | 0.0427 (17) | 0.0032 (11) | −0.0012 (13) | 0.0008 (12) |
| O2WB | 0.0164 (13) | 0.0287 (14) | 0.0228 (14) | 0.0020 (11) | 0.0017 (11) | 0.0030 (11) |
| O2B | 0.0200 (15) | 0.0239 (15) | 0.083 (3) | 0.0007 (12) | 0.0232 (16) | 0.0093 (15) |
| O3WB | 0.0148 (13) | 0.0230 (14) | 0.0385 (17) | −0.0014 (11) | −0.0002 (12) | −0.0035 (12) |
| O3B | 0.0206 (14) | 0.0501 (18) | 0.0277 (16) | −0.0156 (13) | 0.0074 (13) | −0.0098 (13) |
| O4WB | 0.0199 (14) | 0.0379 (16) | 0.0268 (15) | −0.0019 (12) | −0.0010 (12) | −0.0058 (12) |
| O4B | 0.0163 (13) | 0.0201 (13) | 0.0294 (15) | −0.0034 (10) | −0.0044 (12) | 0.0006 (11) |
| O5WB | 0.0123 (12) | 0.0283 (14) | 0.0311 (15) | −0.0053 (11) | −0.0022 (12) | 0.0038 (11) |
| O5B | 0.0134 (12) | 0.0199 (13) | 0.0199 (13) | 0.0009 (10) | −0.0052 (11) | −0.0005 (10) |
| O6B | 0.0143 (13) | 0.0276 (14) | 0.0239 (14) | 0.0061 (11) | −0.0037 (11) | −0.0045 (11) |
| O7B | 0.0166 (14) | 0.0347 (16) | 0.0427 (18) | −0.0043 (12) | 0.0069 (13) | −0.0037 (13) |
| O8B | 0.0129 (13) | 0.0356 (15) | 0.0258 (15) | −0.0029 (11) | 0.0013 (12) | −0.0037 (12) |
| O9B | 0.0214 (14) | 0.0233 (14) | 0.0345 (16) | −0.0075 (11) | −0.0105 (13) | 0.0025 (12) |
| O10B | 0.0186 (14) | 0.0201 (14) | 0.0410 (17) | −0.0008 (11) | −0.0116 (13) | −0.0008 (12) |
| O11B | 0.0175 (14) | 0.0448 (17) | 0.0273 (16) | 0.0083 (12) | −0.0027 (12) | −0.0083 (13) |
| O12B | 0.0174 (14) | 0.0368 (16) | 0.0421 (18) | 0.0071 (12) | 0.0066 (13) | 0.0077 (13) |
| O13B | 0.0385 (16) | 0.0286 (15) | 0.0188 (14) | −0.0108 (12) | −0.0025 (13) | 0.0069 (11) |
| O14B | 0.0300 (15) | 0.0231 (14) | 0.0179 (14) | −0.0025 (11) | 0.0035 (12) | 0.0001 (11) |
| O15B | 0.0271 (15) | 0.0164 (13) | 0.0381 (17) | −0.0051 (12) | −0.0029 (13) | 0.0030 (11) |
| N1B | 0.0132 (15) | 0.0190 (16) | 0.0245 (18) | 0.0037 (13) | −0.0027 (14) | 0.0035 (13) |
| N4B | 0.0096 (14) | 0.0213 (16) | 0.0181 (16) | 0.0003 (12) | −0.0002 (13) | −0.0004 (12) |
| N5B | 0.0106 (14) | 0.0173 (15) | 0.0192 (16) | 0.0003 (12) | −0.0025 (13) | 0.0015 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N6B | 0.0135 (15) | 0.0148 (15) | 0.0231 (17) | −0.0038 (12) | −0.0030 (13) | 0.0044 (12) |
| N7B | 0.0120 (15) | 0.0162 (15) | 0.0317 (18) | 0.0019 (12) | −0.0027 (14) | 0.0050 (13) |
| N8B | 0.0119 (15) | 0.0145 (15) | 0.0302 (18) | −0.0006 (12) | −0.0008 (14) | 0.0016 (13) |
| N9B | 0.0145 (15) | 0.0129 (15) | 0.0259 (17) | 0.0009 (12) | −0.0036 (14) | 0.0005 (12) |
| N10B | 0.0153 (15) | 0.0126 (15) | 0.0206 (16) | −0.0009 (12) | −0.0030 (13) | −0.0015 (12) |
| N11B | 0.0144 (15) | 0.0130 (15) | 0.0251 (17) | 0.0026 (12) | 0.0042 (13) | 0.0029 (12) |
| N12B | 0.0152 (15) | 0.0190 (15) | 0.0187 (16) | 0.0029 (12) | −0.0002 (13) | −0.0029 (12) |
| N13B | 0.0142 (15) | 0.0232 (16) | 0.0184 (16) | −0.0010 (12) | 0.0019 (13) | −0.0017 (13) |
| N14B | 0.0144 (15) | 0.0228 (16) | 0.0210 (17) | −0.0023 (13) | 0.0029 (13) | −0.0018 (13) |
| N15B | 0.0153 (15) | 0.0247 (16) | 0.0188 (16) | 0.0020 (13) | −0.0011 (13) | −0.0032 (13) |
| N16B | 0.0160 (15) | 0.0236 (16) | 0.0206 (17) | 0.0022 (13) | 0.0030 (14) | 0.0040 (13) |
| N17B | 0.0163 (15) | 0.0181 (15) | 0.0192 (16) | −0.0033 (12) | −0.0020 (13) | 0.0019 (12) |
| N18B | 0.0157 (15) | 0.0197 (16) | 0.0241 (17) | −0.0006 (13) | −0.0009 (14) | 0.0049 (13) |
| N19B | 0.0126 (15) | 0.0153 (15) | 0.0216 (16) | −0.0036 (12) | −0.0008 (13) | 0.0015 (12) |
| N20B | 0.0149 (15) | 0.0190 (16) | 0.0250 (17) | −0.0010 (12) | −0.0009 (14) | 0.0015 (13) |
| N21B | 0.0122 (14) | 0.0141 (14) | 0.0168 (15) | 0.0009 (11) | −0.0030 (13) | −0.0014 (12) |
| N22B | 0.0118 (14) | 0.0191 (16) | 0.0202 (16) | −0.0001 (12) | 0.0019 (13) | −0.0015 (12) |
| N23B | 0.0132 (14) | 0.0135 (14) | 0.0169 (15) | 0.0015 (12) | −0.0022 (13) | 0.0002 (12) |
| N24B | 0.0123 (15) | 0.0228 (16) | 0.0217 (17) | −0.0004 (12) | −0.0009 (13) | −0.0062 (13) |
| N25B | 0.0125 (15) | 0.0189 (15) | 0.0186 (16) | 0.0045 (12) | 0.0032 (13) | −0.0040 (12) |
| N26B | 0.0135 (15) | 0.0190 (15) | 0.0166 (16) | −0.0003 (12) | 0.0020 (13) | −0.0020 (12) |
| N27B | 0.0119 (14) | 0.0161 (15) | 0.0193 (16) | 0.0017 (12) | −0.0012 (13) | −0.0047 (12) |
| C1B | 0.0125 (17) | 0.0111 (17) | 0.0186 (19) | −0.0010 (13) | 0.0022 (15) | −0.0029 (14) |
| C2B | 0.0134 (17) | 0.0112 (17) | 0.0200 (19) | −0.0005 (14) | −0.0016 (15) | −0.0018 (14) |
| C3B | 0.0159 (19) | 0.0117 (17) | 0.028 (2) | −0.0026 (14) | −0.0030 (17) | −0.0062 (15) |
| C4B | 0.0116 (17) | 0.0124 (17) | 0.024 (2) | 0.0023 (14) | 0.0023 (16) | −0.0033 (14) |
| C5B | 0.0145 (18) | 0.0152 (18) | 0.027 (2) | 0.0004 (14) | 0.0018 (16) | 0.0028 (15) |
| C6B | 0.0175 (19) | 0.0171 (19) | 0.033 (2) | −0.0042 (15) | −0.0089 (17) | 0.0037 (16) |
| C7B | 0.0160 (18) | 0.0143 (17) | 0.0202 (19) | 0.0004 (14) | −0.0007 (16) | 0.0011 (14) |
| C8B | 0.0138 (17) | 0.0163 (18) | 0.0166 (18) | 0.0032 (14) | 0.0005 (15) | 0.0028 (14) |
| C9B | 0.018 (2) | 0.020 (2) | 0.030 (2) | 0.0020 (16) | −0.0002 (18) | 0.0065 (16) |
| C10B | 0.0156 (19) | 0.0189 (19) | 0.0182 (19) | 0.0009 (15) | 0.0021 (16) | 0.0002 (15) |
| C11B | 0.0162 (18) | 0.0164 (18) | 0.0200 (19) | −0.0032 (14) | 0.0051 (16) | 0.0015 (14) |
| C12B | 0.0141 (18) | 0.0176 (18) | 0.0196 (19) | 0.0050 (14) | −0.0009 (16) | 0.0002 (14) |
| C13B | 0.0178 (18) | 0.0146 (18) | 0.0174 (19) | 0.0034 (14) | −0.0007 (16) | 0.0037 (14) |
| C14B | 0.0175 (18) | 0.0132 (17) | 0.0175 (19) | 0.0001 (14) | 0.0037 (16) | 0.0047 (14) |
| C15B | 0.0145 (19) | 0.024 (2) | 0.021 (2) | 0.0042 (16) | −0.0012 (16) | 0.0026 (16) |
| C16B | 0.0164 (19) | 0.0141 (18) | 0.027 (2) | −0.0030 (15) | 0.0010 (17) | 0.0021 (15) |
| C17B | 0.0147 (18) | 0.0171 (18) | 0.022 (2) | 0.0049 (14) | 0.0025 (16) | −0.0009 (15) |
| C18B | 0.0176 (19) | 0.023 (2) | 0.025 (2) | −0.0042 (15) | 0.0016 (17) | 0.0016 (16) |
| C19B | 0.0184 (18) | 0.0147 (18) | 0.0173 (19) | −0.0030 (14) | −0.0010 (16) | −0.0019 (14) |
| C20B | 0.0168 (18) | 0.0152 (18) | 0.0194 (19) | −0.0037 (14) | 0.0020 (16) | −0.0024 (14) |
| C21B | 0.0148 (18) | 0.0141 (17) | 0.0187 (19) | 0.0012 (14) | 0.0025 (16) | −0.0059 (14) |
| C22B | 0.018 (2) | 0.022 (2) | 0.024 (2) | −0.0058 (16) | −0.0028 (17) | −0.0006 (16) |
| C23B | 0.0208 (19) | 0.0208 (19) | 0.024 (2) | −0.0050 (15) | −0.0067 (17) | 0.0005 (16) |
| C24B | 0.0146 (17) | 0.0136 (17) | 0.0206 (19) | 0.0020 (14) | 0.0005 (15) | −0.0020 (14) |
| C25B | 0.0147 (17) | 0.0180 (18) | 0.0139 (18) | −0.0030 (14) | −0.0028 (15) | 0.0019 (14) |
| C26B | 0.0131 (17) | 0.0193 (18) | 0.0145 (18) | 0.0019 (14) | −0.0014 (15) | −0.0009 (14) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C27B | 0.0155 (18) | 0.0188 (19) | 0.0117 (17) | −0.0028 (15) | 0.0050 (15) | 0.0003 (14) |
| C28B | 0.0157 (19) | 0.029 (2) | 0.0185 (19) | −0.0003 (16) | −0.0027 (16) | −0.0002 (16) |
| C29B | 0.0122 (17) | 0.026 (2) | 0.019 (2) | 0.0048 (15) | −0.0043 (16) | −0.0017 (15) |
| C30B | 0.0141 (17) | 0.0156 (18) | 0.0165 (18) | −0.0005 (14) | 0.0026 (15) | 0.0017 (14) |
| C31B | 0.0163 (18) | 0.0168 (18) | 0.0202 (19) | 0.0039 (14) | 0.0039 (16) | 0.0013 (14) |
| C32B | 0.0144 (18) | 0.0160 (18) | 0.0208 (19) | −0.0002 (14) | 0.0038 (16) | 0.0015 (14) |
| C33B | 0.0131 (18) | 0.0135 (17) | 0.023 (2) | −0.0053 (14) | 0.0002 (16) | −0.0022 (14) |
| C34B | 0.0153 (18) | 0.0158 (18) | 0.0178 (19) | 0.0075 (15) | 0.0000 (16) | 0.0021 (14) |
| C35B | 0.0151 (18) | 0.0198 (19) | 0.0202 (19) | 0.0044 (15) | 0.0008 (16) | −0.0002 (15) |
| C36B | 0.0135 (18) | 0.0206 (19) | 0.022 (2) | −0.0061 (15) | 0.0016 (16) | −0.0049 (15) |
| Pr1A | 0.01196 (10) | 0.01339 (10) | 0.01629 (10) | 0.00072 (7) | −0.00024 (8) | −0.00015 (7) |
| O1A | 0.0175 (13) | 0.0225 (14) | 0.0331 (16) | 0.0061 (11) | −0.0009 (12) | 0.0010 (11) |
| O1WA | 0.0220 (14) | 0.0508 (18) | 0.0284 (16) | 0.0002 (13) | −0.0039 (13) | −0.0070 (13) |
| O2A | 0.0202 (14) | 0.0316 (16) | 0.0435 (18) | 0.0002 (12) | −0.0116 (14) | −0.0023 (13) |
| O2WA | 0.0275 (15) | 0.0387 (16) | 0.0222 (15) | 0.0133 (12) | −0.0001 (12) | 0.0067 (12) |
| O3WA | 0.0223 (14) | 0.0180 (14) | 0.0519 (19) | −0.0063 (11) | 0.0111 (14) | −0.0136 (12) |
| O3A | 0.0158 (14) | 0.0411 (16) | 0.0324 (16) | −0.0032 (12) | −0.0023 (13) | 0.0094 (13) |
| O4A | 0.0115 (13) | 0.0256 (14) | 0.0404 (17) | −0.0005 (11) | 0.0043 (12) | 0.0014 (12) |
| O4WA | 0.0187 (13) | 0.0242 (14) | 0.0265 (15) | −0.0014 (11) | 0.0000 (12) | 0.0035 (11) |
| O5WA | 0.0190 (13) | 0.0229 (13) | 0.0252 (14) | 0.0061 (11) | −0.0026 (12) | 0.0020 (11) |
| O5A | 0.0176 (13) | 0.0185 (13) | 0.0241 (14) | −0.0017 (10) | 0.0017 (12) | −0.0010 (10) |
| O6A | 0.0172 (13) | 0.0203 (13) | 0.0217 (14) | 0.0065 (11) | 0.0017 (11) | −0.0002 (10) |
| O7A | 0.0135 (13) | 0.0344 (15) | 0.0343 (16) | −0.0016 (11) | −0.0076 (12) | 0.0019 (12) |
| O8A | 0.0121 (13) | 0.0373 (16) | 0.0315 (16) | −0.0004 (11) | −0.0043 (12) | 0.0045 (12) |
| O9A | 0.0208 (15) | 0.0464 (18) | 0.0349 (17) | −0.0139 (13) | 0.0083 (13) | −0.0118 (13) |
| O10A | 0.0187 (14) | 0.0229 (14) | 0.0322 (16) | 0.0000 (11) | 0.0071 (12) | −0.0056 (11) |
| O11A | 0.0240 (14) | 0.0324 (15) | 0.0290 (16) | 0.0104 (12) | 0.0042 (13) | 0.0016 (12) |
| O12A | 0.0192 (14) | 0.0340 (15) | 0.0253 (15) | 0.0094 (12) | −0.0025 (12) | −0.0016 (12) |
| O13A | 0.0350 (16) | 0.0160 (13) | 0.0246 (15) | 0.0037 (11) | −0.0073 (13) | 0.0001 (11) |
| O14A | 0.0235 (14) | 0.0151 (13) | 0.0265 (15) | 0.0006 (11) | −0.0045 (12) | −0.0002 (11) |
| O15A | 0.091 (3) | 0.0393 (18) | 0.0288 (18) | 0.0010 (17) | −0.0338 (19) | 0.0013 (14) |
| N1A | 0.0325 (19) | 0.0226 (18) | 0.0197 (18) | −0.0064 (15) | −0.0063 (15) | 0.0017 (14) |
| N4A | 0.0167 (15) | 0.0188 (16) | 0.0221 (17) | 0.0027 (12) | −0.0010 (14) | 0.0006 (13) |
| N5A | 0.0132 (15) | 0.0244 (17) | 0.0222 (17) | −0.0024 (13) | 0.0001 (14) | −0.0028 (13) |
| N6A | 0.0162 (15) | 0.0192 (16) | 0.0194 (16) | −0.0036 (12) | 0.0015 (13) | −0.0014 (12) |
| N7A | 0.0168 (16) | 0.0209 (16) | 0.0235 (17) | −0.0005 (13) | 0.0025 (14) | −0.0027 (13) |
| N8A | 0.0162 (16) | 0.0192 (16) | 0.0304 (18) | −0.0032 (13) | −0.0024 (14) | 0.0000 (13) |
| N9A | 0.0161 (15) | 0.0156 (15) | 0.0240 (17) | 0.0006 (12) | 0.0004 (14) | −0.0026 (12) |
| N10A | 0.0135 (15) | 0.0164 (15) | 0.0251 (17) | −0.0013 (12) | 0.0018 (13) | −0.0038 (13) |
| N11A | 0.0141 (15) | 0.0214 (16) | 0.0250 (17) | −0.0003 (13) | −0.0025 (14) | 0.0015 (13) |
| N12A | 0.0131 (15) | 0.0204 (16) | 0.0219 (17) | −0.0003 (12) | 0.0022 (13) | −0.0003 (13) |
| N13A | 0.0151 (15) | 0.0211 (16) | 0.0195 (16) | −0.0009 (12) | 0.0003 (13) | 0.0010 (13) |
| N14A | 0.0161 (16) | 0.0227 (16) | 0.0242 (17) | −0.0016 (13) | −0.0017 (14) | 0.0043 (13) |
| N15A | 0.0161 (16) | 0.0238 (16) | 0.0199 (17) | 0.0020 (13) | 0.0025 (14) | 0.0006 (13) |
| N16A | 0.0115 (15) | 0.0227 (16) | 0.0206 (16) | 0.0010 (12) | −0.0007 (13) | −0.0038 (13) |
| N17A | 0.0115 (15) | 0.0236 (16) | 0.0197 (16) | −0.0009 (12) | −0.0001 (13) | 0.0021 (13) |
| N18A | 0.0133 (15) | 0.0248 (16) | 0.0179 (16) | 0.0001 (12) | 0.0001 (13) | −0.0010 (13) |
| N19A | 0.0125 (15) | 0.0178 (15) | 0.0272 (18) | −0.0029 (12) | −0.0025 (14) | −0.0009 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N20A | 0.0143 (15) | 0.0221 (16) | 0.0236 (17) | −0.0022 (13) | −0.0034 (14) | 0.0004 (13) |
| N21A | 0.0139 (15) | 0.0160 (15) | 0.0221 (16) | −0.0012 (12) | 0.0008 (13) | −0.0012 (12) |
| N22A | 0.0113 (14) | 0.0229 (16) | 0.0188 (16) | −0.0016 (12) | −0.0017 (13) | 0.0018 (13) |
| N23A | 0.0124 (14) | 0.0170 (15) | 0.0176 (16) | −0.0025 (12) | 0.0024 (13) | −0.0017 (12) |
| N24A | 0.0104 (14) | 0.0200 (16) | 0.0214 (17) | −0.0005 (12) | −0.0004 (13) | −0.0001 (12) |
| N25A | 0.0125 (14) | 0.0180 (15) | 0.0156 (15) | 0.0037 (12) | −0.0001 (13) | −0.0004 (12) |
| N26A | 0.0121 (15) | 0.0196 (16) | 0.0207 (16) | −0.0001 (12) | −0.0005 (13) | 0.0008 (12) |
| N27A | 0.0146 (15) | 0.0178 (15) | 0.0190 (16) | 0.0039 (12) | 0.0016 (13) | 0.0024 (12) |
| C1A | 0.0189 (19) | 0.0153 (18) | 0.0188 (19) | 0.0025 (14) | −0.0009 (16) | 0.0044 (14) |
| C2A | 0.0166 (18) | 0.0164 (18) | 0.021 (2) | −0.0005 (14) | −0.0016 (16) | 0.0018 (15) |
| C3A | 0.0202 (19) | 0.0155 (18) | 0.021 (2) | −0.0027 (15) | 0.0060 (17) | 0.0036 (15) |
| C4A | 0.0168 (19) | 0.0175 (19) | 0.027 (2) | −0.0028 (15) | −0.0015 (17) | 0.0002 (15) |
| C5A | 0.0176 (19) | 0.023 (2) | 0.019 (2) | 0.0007 (15) | −0.0028 (16) | 0.0012 (15) |
| C6A | 0.0188 (19) | 0.021 (2) | 0.025 (2) | −0.0049 (15) | 0.0100 (17) | −0.0041 (16) |
| C7A | 0.0173 (18) | 0.0217 (19) | 0.0175 (19) | −0.0014 (15) | 0.0010 (16) | −0.0002 (15) |
| C8A | 0.0185 (19) | 0.0222 (19) | 0.0140 (18) | 0.0005 (15) | 0.0004 (16) | −0.0046 (15) |
| C9A | 0.019 (2) | 0.025 (2) | 0.022 (2) | −0.0030 (16) | 0.0019 (17) | −0.0025 (16) |
| C10A | 0.0175 (19) | 0.023 (2) | 0.0151 (18) | −0.0015 (15) | −0.0027 (16) | −0.0021 (15) |
| C11A | 0.0168 (18) | 0.0216 (19) | 0.0188 (19) | −0.0023 (15) | −0.0010 (16) | −0.0032 (15) |
| C12A | 0.0145 (18) | 0.0210 (19) | 0.026 (2) | 0.0019 (15) | 0.0025 (16) | −0.0003 (15) |
| C13A | 0.0163 (18) | 0.0184 (18) | 0.021 (2) | 0.0013 (15) | 0.0022 (16) | −0.0038 (15) |
| C14A | 0.0163 (18) | 0.0170 (18) | 0.022 (2) | −0.0011 (15) | 0.0027 (16) | −0.0031 (15) |
| C15A | 0.019 (2) | 0.0198 (19) | 0.023 (2) | 0.0026 (15) | −0.0001 (17) | −0.0015 (15) |
| C16A | 0.0158 (18) | 0.0182 (19) | 0.022 (2) | −0.0024 (15) | 0.0006 (16) | −0.0021 (15) |
| C17A | 0.0194 (19) | 0.0178 (19) | 0.027 (2) | 0.0054 (15) | 0.0023 (17) | 0.0062 (16) |
| C18A | 0.0131 (18) | 0.0235 (19) | 0.021 (2) | −0.0068 (15) | 0.0010 (16) | −0.0002 (15) |
| C19A | 0.0185 (19) | 0.0178 (18) | 0.021 (2) | 0.0000 (15) | −0.0004 (16) | 0.0040 (15) |
| C20A | 0.0170 (18) | 0.0167 (18) | 0.0174 (19) | −0.0019 (14) | 0.0002 (16) | 0.0061 (14) |
| C21A | 0.020 (2) | 0.0133 (18) | 0.026 (2) | 0.0030 (15) | −0.0030 (17) | 0.0094 (15) |
| C22A | 0.0118 (18) | 0.0241 (19) | 0.0175 (19) | −0.0045 (15) | 0.0033 (16) | 0.0035 (15) |
| C23A | 0.0171 (19) | 0.026 (2) | 0.023 (2) | −0.0039 (16) | 0.0070 (17) | −0.0033 (16) |
| C24A | 0.0153 (18) | 0.0179 (19) | 0.028 (2) | 0.0008 (15) | −0.0042 (17) | 0.0071 (15) |
| C25A | 0.0122 (17) | 0.0242 (19) | 0.0132 (18) | −0.0039 (15) | 0.0001 (15) | 0.0028 (14) |
| C26A | 0.0124 (17) | 0.0234 (19) | 0.0137 (18) | −0.0019 (15) | −0.0014 (15) | −0.0004 (14) |
| C27A | 0.0126 (18) | 0.0219 (19) | 0.0125 (17) | −0.0021 (14) | −0.0031 (15) | 0.0019 (14) |
| C28A | 0.0150 (19) | 0.029 (2) | 0.0167 (19) | −0.0025 (16) | 0.0019 (16) | −0.0005 (15) |
| C29A | 0.0142 (18) | 0.025 (2) | 0.0177 (19) | 0.0034 (15) | 0.0019 (16) | −0.0038 (15) |
| C30A | 0.0110 (17) | 0.0176 (18) | 0.0195 (19) | −0.0026 (14) | −0.0028 (15) | −0.0019 (14) |
| C31A | 0.0130 (17) | 0.0153 (18) | 0.0214 (19) | 0.0008 (14) | −0.0023 (16) | −0.0031 (14) |
| C32A | 0.0146 (18) | 0.0123 (17) | 0.0205 (19) | 0.0002 (14) | −0.0021 (16) | −0.0024 (14) |
| C33A | 0.0126 (17) | 0.0103 (17) | 0.023 (2) | −0.0024 (14) | −0.0039 (16) | −0.0017 (14) |
| C34A | 0.019 (2) | 0.0172 (18) | 0.022 (2) | 0.0062 (15) | −0.0017 (17) | −0.0047 (15) |
| C35A | 0.0158 (18) | 0.0202 (19) | 0.022 (2) | 0.0058 (15) | −0.0027 (16) | 0.0002 (15) |
| C36A | 0.0109 (17) | 0.0207 (19) | 0.023 (2) | −0.0019 (14) | −0.0013 (16) | 0.0003 (15) |
| O16B | 0.039 (2) | 0.116 (3) | 0.062 (3) | 0.015 (2) | 0.004 (2) | 0.026 (2) |
| O17B | 0.063 (2) | 0.0304 (19) | 0.120 (4) | −0.0052 (17) | 0.014 (2) | 0.015 (2) |
| O18B | 0.071 (3) | 0.061 (2) | 0.090 (3) | 0.005 (2) | 0.000 (2) | 0.012 (2) |
| N2B | 0.037 (2) | 0.033 (2) | 0.074 (3) | 0.0101 (19) | 0.008 (2) | 0.005 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O19B | 0.0298 (15) | 0.0346 (16) | 0.0304 (16) | −0.0038 (13) | 0.0062 (13) | 0.0059 (12) |
| O20B | 0.058 (2) | 0.0225 (16) | 0.047 (2) | 0.0055 (14) | 0.0009 (17) | −0.0018 (13) |
| O21B | 0.0202 (14) | 0.0467 (18) | 0.0298 (16) | 0.0010 (13) | 0.0048 (13) | −0.0004 (13) |
| N3B | 0.0278 (19) | 0.032 (2) | 0.0149 (16) | −0.0007 (15) | −0.0062 (15) | 0.0015 (14) |
| O19A | 0.0395 (18) | 0.0464 (18) | 0.0409 (19) | −0.0217 (15) | −0.0048 (15) | 0.0045 (15) |
| O20A | 0.059 (2) | 0.0227 (16) | 0.0452 (19) | −0.0012 (14) | −0.0025 (17) | −0.0048 (13) |
| O21A | 0.0336 (18) | 0.0471 (19) | 0.056 (2) | 0.0099 (15) | 0.0060 (16) | −0.0039 (16) |
| N3A | 0.0308 (19) | 0.0277 (19) | 0.0186 (17) | −0.0026 (15) | 0.0007 (15) | −0.0011 (14) |
| O16A | 0.0315 (18) | 0.066 (2) | 0.074 (3) | −0.0070 (16) | −0.0174 (19) | 0.0213 (19) |
| O17A | 0.072 (3) | 0.051 (2) | 0.073 (3) | −0.005 (2) | 0.005 (2) | −0.0041 (19) |
| O18A | 0.0312 (17) | 0.063 (2) | 0.0327 (18) | 0.0064 (16) | 0.0012 (14) | 0.0125 (15) |
| N2A | 0.0233 (19) | 0.053 (2) | 0.033 (2) | −0.0084 (18) | 0.0037 (17) | 0.0140 (18) |
| O15W | 0.0251 (15) | 0.0420 (17) | 0.0403 (18) | −0.0014 (13) | −0.0071 (14) | −0.0045 (14) |
| O1W | 0.0324 (16) | 0.0225 (14) | 0.0418 (18) | 0.0032 (12) | 0.0070 (14) | 0.0011 (12) |
| O17W | 0.033 (3) | 0.094 (5) | 0.124 (6) | −0.009 (3) | 0.005 (3) | 0.046 (4) |
| O3W | 0.0174 (14) | 0.0448 (17) | 0.0361 (17) | 0.0048 (12) | −0.0038 (13) | 0.0002 (13) |
| O23W | 0.038 (7) | 0.111 (9) | 0.154 (13) | 0.011 (7) | 0.007 (10) | 0.013 (11) |
| O2W | 0.0188 (13) | 0.0245 (14) | 0.0353 (16) | −0.0014 (11) | −0.0041 (12) | 0.0022 (12) |
| O21W | 0.070 (6) | 0.066 (4) | 0.069 (6) | −0.020 (4) | 0.024 (5) | −0.012 (4) |
| O19W | 0.059 (2) | 0.060 (2) | 0.081 (3) | −0.0130 (18) | 0.036 (2) | −0.013 (2) |
| O14W | 0.0380 (19) | 0.085 (3) | 0.049 (2) | 0.0254 (17) | −0.0152 (17) | −0.0354 (19) |
| O6W | 0.054 (3) | 0.102 (3) | 0.083 (3) | −0.006 (3) | −0.017 (2) | 0.024 (3) |
| O16W | 0.0255 (15) | 0.0321 (16) | 0.0445 (18) | −0.0042 (12) | 0.0037 (14) | −0.0033 (13) |
| O4W | 0.0185 (14) | 0.0427 (17) | 0.0325 (16) | 0.0001 (12) | −0.0091 (13) | 0.0033 (13) |
| O18W | 0.028 (8) | 0.094 (10) | 0.134 (11) | −0.007 (8) | 0.021 (9) | 0.045 (9) |
| O5W | 0.056 (8) | 0.040 (7) | 0.035 (7) | −0.008 (6) | 0.011 (6) | −0.007 (5) |
| O10W | 0.0260 (15) | 0.0349 (16) | 0.0359 (17) | −0.0024 (12) | −0.0043 (13) | 0.0050 (13) |
| O20W | 0.082 (11) | 0.070 (7) | 0.076 (11) | −0.003 (8) | 0.019 (8) | −0.026 (8) |
| O11W | 0.0243 (14) | 0.0309 (15) | 0.0264 (15) | 0.0040 (12) | 0.0037 (12) | 0.0001 (12) |
| O22W | 0.032 (4) | 0.116 (6) | 0.160 (11) | −0.011 (4) | −0.011 (6) | 0.072 (7) |
| O12W | 0.0298 (16) | 0.0336 (16) | 0.051 (2) | 0.0051 (13) | 0.0021 (15) | 0.0091 (14) |
| O25W | 0.054 (2) | 0.160 (4) | 0.053 (3) | −0.008 (3) | 0.005 (2) | 0.026 (3) |
| O13W | 0.0425 (19) | 0.0503 (19) | 0.052 (2) | −0.0060 (15) | −0.0046 (17) | 0.0181 (16) |
| O24W | 0.0298 (18) | 0.056 (2) | 0.106 (3) | −0.0114 (16) | −0.006 (2) | 0.014 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Pr1A—O1WA | 2.544 (2) | Pr1B—O1WB | 2.553 (3) |
| Pr1A—O2WA | 2.449 (3) | Pr1B—O2WB | 2.438 (2) |
| Pr1A—O3WA | 2.442 (2) | Pr1B—O3WB | 2.448 (2) |
| Pr1B—O4WB | 2.527 (3) | Pr1B—O4WB | 2.527 (3) |
| Pr1A—O5A | 2.493 (2) | Pr1B—O5B | 2.519 (2) |
| Pr1A—O5WA | 2.483 (2) | Pr1B—O5WB | 2.476 (2) |
| Pr1A—O6A | 2.466 (2) | Pr1B—O6B | 2.460 (2) |
| Pr1A—O13A | 2.571 (2) | Pr1B—O13B | 2.651 (3) |
| Pr1A—O14A | 2.613 (2) | Pr1B—O14B | 2.572 (2) |
| | | | |
| O2WA—Pr1A—O1WA | 68.01 (9) | O2WB—Pr1B—O13B | 68.61 (8) |

| | | | |
|---|---|---|---|
| O2WA—Pr1A—O4WA | 77.25 (8) | O2WB—Pr1B—O3WB | 84.55 (8) |
| O2WA—Pr1A—O5WA | 67.92 (8) | O2WB—Pr1B—O6B | 96.37 (8) |
| O2WA—Pr1A—O6A | 84.64 (8) | O2WB—Pr1B—O1WB | 67.77 (9) |
| O3WA—Pr1A—O1WA | 73.57 (9) | O2WB—Pr1B—O5WB | 71.46 (8) |
| O3WA—Pr1A—O2WA | 93.13 (9) | O3WB—Pr1B—O5WB | 71.21 (8) |
| O3WA—Pr1A—O5WA | 70.71 (8) | O3WB—Pr1B—O5B | 78.97 (8) |
| O3WA—Pr1A—O5A | 77.35 (8) | O3WB—Pr1B—O4WB | 76.07 (9) |
| O3WA—Pr1A—O13A | 73.92 (8) | O3WB—Pr1B—O1WB | 71.69 (9) |
| O4WA—Pr1A—O13A | 88.91 (8) | O3WB—Pr1B—O1WB | 71.69 (9) |
| O4WA—Pr1A—O14A | 65.33 (8) | O4WB—Pr1B—O14B | 65.36 (8) |
| O5WA—Pr1A—O4WA | 71.24 (8) | O5B—Pr1B—O4WB | 70.75 (8) |
| O5WA—Pr1A—O13A | 70.72 (8) | O5B—Pr1B—O1WB | 71.12 (9) |
| O5A—Pr1A—O1WA | 72.17 (8) | O5WB—Pr1B—O4WB | 69.88 (8) |
| O5A—Pr1A—O13A | 76.26 (8) | O5WB—Pr1B—O14B | 82.62 (8) |
| O5A—Pr1A—O14A | 71.00 (8) | O5WB—Pr1B—O13B | 71.53 (8) |
| O6A—Pr1A—O1WA | 74.26 (8) | O6B—Pr1B—O1WB | 75.85 (9) |
| O6A—Pr1A—O4WA | 70.85 (8) | O6B—Pr1B—O5B | 77.22 (8) |
| O6A—Pr1A—O5A | 82.86 (8) | O6B—Pr1B—O14B | 71.49 (8) |
| O6A—Pr1A—O14A | 78.55 (7) | O6B—Pr1B—O13B | 71.15 (8) |
| O13A—Pr1A—O14A | 49.19 (7) | O14B—Pr1B—O13B | 48.49 (8) |

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|---|---|---|---|
| Pr1B—O13B—N1B—O15B | −171.1 (3) | Pr1A—O14A—N1A—O15A | 177.0 (3) |
| Pr1B—O13B—N1B—O14B | 6.9 (3) | Pr1A—O14A—N1A—O13A | −1.7 (3) |
| Pr1B—O14B—N1B—O15B | 170.8 (2) | Pr1A—O13A—N1A—O15A | −177.0 (3) |
| Pr1B—O14B—N1B—O13B | −7.1 (3) | Pr1A—O13A—N1A—O14A | 1.7 (3) |
| C4B—N5B—C1B—N4B | 110.1 (3) | C4A—N5A—C1A—N4A | −108.5 (3) |
| C35B—N5B—C1B—N4B | −85.0 (4) | C35A—N5A—C1A—N4A | 79.6 (4) |
| C4B—N5B—C1B—C2B | −1.6 (3) | C4A—N5A—C1A—C2A | 3.1 (4) |
| C35B—N5B—C1B—C2B | 163.2 (3) | C35A—N5A—C1A—C2A | −168.9 (3) |
| C3B—N4B—C1B—N5B | −116.9 (3) | C3A—N4A—C1A—N5A | 118.6 (3) |
| C36B—N4B—C1B—N5B | 65.3 (4) | C36A—N4A—C1A—N5A | −68.1 (4) |
| C3B—N4B—C1B—C2B | −4.6 (3) | C3A—N4A—C1A—C2A | 6.8 (4) |
| C36B—N4B—C1B—C2B | 177.5 (3) | C36A—N4A—C1A—C2A | −179.9 (3) |
| C3B—N7B—C2B—N6B | 104.4 (3) | C3A—N7A—C2A—N6A | −108.1 (3) |
| C6B—N7B—C2B—N6B | −67.2 (4) | C6A—N7A—C2A—N6A | 67.4 (4) |
| C3B—N7B—C2B—C1B | −6.0 (4) | C3A—N7A—C2A—C1A | 3.2 (4) |
| C6B—N7B—C2B—C1B | −177.6 (3) | C6A—N7A—C2A—C1A | 178.7 (3) |
| C4B—N6B—C2B—N7B | −117.7 (3) | C4A—N6A—C2A—N7A | 118.9 (3) |
| C5B—N6B—C2B—N7B | 82.5 (4) | C5A—N6A—C2A—N7A | −84.5 (4) |
| C4B—N6B—C2B—C1B | −7.0 (3) | C4A—N6A—C2A—C1A | 7.6 (4) |
| C5B—N6B—C2B—C1B | −166.8 (3) | C5A—N6A—C2A—C1A | 164.2 (3) |
| N5B—C1B—C2B—N7B | 125.2 (3) | N5A—C1A—C2A—N7A | −126.2 (3) |
| N4B—C1B—C2B—N7B | 6.0 (3) | N4A—C1A—C2A—N7A | −5.7 (3) |
| N5B—C1B—C2B—N6B | 4.9 (3) | N5A—C1A—C2A—N6A | −6.1 (3) |
| N4B—C1B—C2B—N6B | −114.2 (3) | N4A—C1A—C2A—N6A | 114.3 (3) |
| C2B—N7B—C3B—O1B | −179.6 (3) | C36A—N4A—C3A—O1A | −3.0 (5) |
| C6B—N7B—C3B—O1B | −7.6 (5) | C1A—N4A—C3A—O1A | 170.5 (3) |
| C2B—N7B—C3B—N4B | 3.4 (4) | C36A—N4A—C3A—N7A | −178.6 (3) |

| | | | |
|---|---|---|---|
| C6B—N7B—C3B—N4B | 175.4 (3) | C1A—N4A—C3A—N7A | −5.1 (4) |
| C36B—N4B—C3B—O1B | 2.0 (5) | C6A—N7A—C3A—O1A | 9.7 (5) |
| C1B—N4B—C3B—O1B | −175.9 (3) | C2A—N7A—C3A—O1A | −174.7 (3) |
| C36B—N4B—C3B—N7B | 179.0 (3) | C6A—N7A—C3A—N4A | −174.8 (3) |
| C1B—N4B—C3B—N7B | 1.1 (4) | C2A—N7A—C3A—N4A | 0.9 (4) |
| C5B—N6B—C4B—O9B | −10.9 (5) | C5A—N6A—C4A—O9A | 16.0 (6) |
| C2B—N6B—C4B—O9B | −171.4 (3) | C2A—N6A—C4A—O9A | 173.4 (3) |
| C5B—N6B—C4B—N5B | 166.8 (3) | C5A—N6A—C4A—N5A | −163.4 (3) |
| C2B—N6B—C4B—N5B | 6.3 (4) | C2A—N6A—C4A—N5A | −6.0 (4) |
| C1B—N5B—C4B—O9B | 175.1 (3) | C1A—N5A—C4A—O9A | −177.8 (3) |
| C35B—N5B—C4B—O9B | 10.0 (5) | C35A—N5A—C4A—O9A | −5.8 (6) |
| C1B—N5B—C4B—N6B | −2.7 (4) | C1A—N5A—C4A—N6A | 1.6 (4) |
| C35B—N5B—C4B—N6B | −167.8 (3) | C35A—N5A—C4A—N6A | 173.7 (3) |
| C10B—N9B—C5B—N6B | −110.6 (4) | C10A—N9A—C5A—N6A | 111.7 (4) |
| C7B—N9B—C5B—N6B | 79.2 (4) | C7A—N9A—C5A—N6A | −79.4 (4) |
| C4B—N6B—C5B—N9B | 108.8 (3) | C4A—N6A—C5A—N9A | −111.3 (4) |
| C2B—N6B—C5B—N9B | −93.0 (4) | C2A—N6A—C5A—N9A | 94.1 (4) |
| C9B—N8B—C6B—N7B | 107.3 (4) | C9A—N8A—C6A—N7A | −106.1 (4) |
| C7B—N8B—C6B—N7B | −94.4 (4) | C7A—N8A—C6A—N7A | 93.4 (4) |
| C3B—N7B—C6B—N8B | −94.6 (4) | C3A—N7A—C6A—N8A | 100.6 (4) |
| C2B—N7B—C6B—N8B | 76.4 (4) | C2A—N7A—C6A—N8A | −74.5 (4) |
| C9B—N8B—C7B—N9B | −111.9 (3) | C10A—N9A—C7A—N8A | −116.5 (3) |
| C6B—N8B—C7B—N9B | 87.9 (4) | C5A—N9A—C7A—N8A | 73.4 (4) |
| C9B—N8B—C7B—C8B | −0.8 (4) | C10A—N9A—C7A—C8A | −5.2 (4) |
| C6B—N8B—C7B—C8B | −160.9 (3) | C5A—N9A—C7A—C8A | −175.3 (3) |
| C10B—N9B—C7B—N8B | 116.1 (3) | C9A—N8A—C7A—N9A | 109.0 (3) |
| C5B—N9B—C7B—N8B | −72.8 (4) | C6A—N8A—C7A—N9A | −88.8 (4) |
| C10B—N9B—C7B—C8B | 4.4 (4) | C9A—N8A—C7A—C8A | −2.2 (4) |
| C5B—N9B—C7B—C8B | 175.6 (3) | C6A—N8A—C7A—C8A | 159.9 (3) |
| C10B—N10B—C8B—N11B | −110.4 (3) | C10A—N10A—C8A—N11A | 110.6 (3) |
| C11B—N10B—C8B—N11B | 81.1 (4) | C11A—N10A—C8A—N11A | −80.3 (4) |
| C10B—N10B—C8B—C7B | 1.1 (4) | C10A—N10A—C8A—C7A | −1.0 (4) |
| C11B—N10B—C8B—C7B | −167.5 (3) | C11A—N10A—C8A—C7A | 168.1 (3) |
| C9B—N11B—C8B—N10B | 118.2 (3) | C9A—N11A—C8A—N10A | −113.7 (3) |
| C12B—N11B—C8B—N10B | −78.8 (4) | C12A—N11A—C8A—N10A | 77.3 (4) |
| C9B—N11B—C8B—C7B | 6.4 (4) | C9A—N11A—C8A—C7A | −2.0 (4) |
| C12B—N11B—C8B—C7B | 169.4 (3) | C12A—N11A—C8A—C7A | −170.9 (3) |
| N8B—C7B—C8B—N10B | −122.6 (3) | N9A—C7A—C8A—N10A | 3.5 (3) |
| N9B—C7B—C8B—N10B | −3.1 (3) | N8A—C7A—C8A—N10A | 122.3 (3) |
| N8B—C7B—C8B—N11B | −3.3 (3) | N9A—C7A—C8A—N11A | −116.4 (3) |
| N9B—C7B—C8B—N11B | 116.2 (3) | N8A—C7A—C8A—N11A | 2.4 (3) |
| C6B—N8B—C9B—O2B | −14.3 (6) | C12A—N11A—C9A—O2A | −9.4 (6) |
| C7B—N8B—C9B—O2B | −174.5 (4) | C8A—N11A—C9A—O2A | −178.2 (4) |
| C6B—N8B—C9B—N11B | 165.0 (3) | C12A—N11A—C9A—N8A | 169.5 (3) |
| C7B—N8B—C9B—N11B | 4.8 (4) | C8A—N11A—C9A—N8A | 0.7 (4) |
| C12B—N11B—C9B—O2B | 9.1 (6) | C6A—N8A—C9A—O2A | 17.7 (6) |
| C8B—N11B—C9B—O2B | 172.1 (4) | C7A—N8A—C9A—O2A | 180.0 (4) |
| C12B—N11B—C9B—N8B | −170.1 (3) | C6A—N8A—C9A—N11A | −161.2 (3) |

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| C8B—N11B—C9B—N8B | −7.2 (4) | C7A—N8A—C9A—N11A | 1.1 (4) |
| C5B—N9B—C10B—O10B | 4.6 (6) | C5A—N9A—C10A—O10A | −4.9 (6) |
| C7B—N9B—C10B—O10B | 175.7 (4) | C7A—N9A—C10A—O10A | −174.8 (3) |
| C5B—N9B—C10B—N10B | −175.0 (3) | C5A—N9A—C10A—N10A | 174.7 (3) |
| C7B—N9B—C10B—N10B | −3.9 (4) | C7A—N9A—C10A—N10A | 4.8 (4) |
| C11B—N10B—C10B—O10B | −9.4 (6) | C8A—N10A—C10A—O10A | 177.4 (3) |
| C8B—N10B—C10B—O10B | −178.0 (3) | C11A—N10A—C10A—O10A | 8.2 (6) |
| C11B—N10B—C10B—N9B | 170.2 (3) | C8A—N10A—C10A—N9A | −2.2 (4) |
| C8B—N10B—C10B—N9B | 1.6 (4) | C11A—N10A—C10A—N9A | −171.4 (3) |
| C10B—N10B—C11B—N12B | 105.6 (4) | C16A—N12A—C11A—N10A | 93.6 (4) |
| C8B—N10B—C11B—N12B | −87.0 (4) | C13A—N12A—C11A—N10A | −82.1 (4) |
| C16B—N12B—C11B—N10B | −101.7 (4) | C10A—N10A—C11A—N12A | −105.1 (4) |
| C13B—N12B—C11B—N10B | 82.6 (4) | C8A—N10A—C11A—N12A | 87.0 (4) |
| C9B—N11B—C12B—N13B | −112.7 (4) | C15A—N13A—C12A—N11A | −115.7 (3) |
| C8B—N11B—C12B—N13B | 86.1 (4) | C13A—N13A—C12A—N11A | 89.9 (4) |
| C15B—N13B—C12B—N11B | 108.2 (4) | C9A—N11A—C12A—N13A | 105.9 (4) |
| C13B—N13B—C12B—N11B | −88.0 (4) | C8A—N11A—C12A—N13A | −86.3 (4) |
| C15B—N13B—C13B—N12B | −115.3 (3) | C16A—N12A—C13A—N13A | −101.8 (3) |
| C12B—N13B—C13B—N12B | 79.4 (4) | C11A—N12A—C13A—N13A | 74.3 (4) |
| C15B—N13B—C13B—C14B | −4.2 (4) | C16A—N12A—C13A—C14A | 9.5 (4) |
| C12B—N13B—C13B—C14B | −169.5 (3) | C11A—N12A—C13A—C14A | −174.4 (3) |
| C16B—N12B—C13B—N13B | 107.9 (3) | C15A—N13A—C13A—N12A | 124.0 (3) |
| C11B—N12B—C13B—N13B | −76.0 (4) | C12A—N13A—C13A—N12A | −79.4 (4) |
| C16B—N12B—C13B—C14B | −3.2 (3) | C15A—N13A—C13A—C14A | 12.7 (4) |
| C11B—N12B—C13B—C14B | 172.9 (3) | C12A—N13A—C13A—C14A | 169.2 (3) |
| C16B—N15B—C14B—N14B | −116.4 (3) | C15A—N14A—C14A—N15A | −103.3 (4) |
| C18B—N15B—C14B—N14B | 68.0 (4) | C17A—N14A—C14A—N15A | 68.5 (4) |
| C16B—N15B—C14B—C13B | −4.8 (4) | C15A—N14A—C14A—C13A | 8.0 (4) |
| C18B—N15B—C14B—C13B | 179.6 (3) | C17A—N14A—C14A—C13A | 179.7 (3) |
| C15B—N14B—C14B—N15B | 107.6 (3) | C16A—N15A—C14A—N14A | 122.4 (3) |
| C17B—N14B—C14B—N15B | −78.4 (4) | C18A—N15A—C14A—N14A | −78.7 (4) |
| C15B—N14B—C14B—C13B | −4.0 (4) | C16A—N15A—C14A—C13A | 11.1 (4) |
| C17B—N14B—C14B—C13B | 169.9 (3) | C18A—N15A—C14A—C13A | 170.0 (3) |
| N13B—C13B—C14B—N15B | −115.4 (3) | N12A—C13A—C14A—N14A | −132.1 (3) |
| N12B—C13B—C14B—N15B | 4.6 (3) | N13A—C13A—C14A—N14A | −11.9 (3) |
| N13B—C13B—C14B—N14B | 4.7 (3) | N12A—C13A—C14A—N15A | −11.7 (3) |
| N12B—C13B—C14B—N14B | 124.6 (3) | N13A—C13A—C14A—N15A | 108.5 (3) |
| C13B—N13B—C15B—O3B | −176.1 (3) | C17A—N14A—C15A—O3A | 10.3 (6) |
| C12B—N13B—C15B—O3B | −10.8 (5) | C14A—N14A—C15A—O3A | −177.9 (3) |
| C13B—N13B—C15B—N14B | 1.9 (4) | C17A—N14A—C15A—N13A | −172.2 (3) |
| C12B—N13B—C15B—N14B | 167.2 (3) | C14A—N14A—C15A—N13A | −0.4 (4) |
| C17B—N14B—C15B—O3B | 5.6 (6) | C12A—N13A—C15A—O3A | 12.2 (5) |
| C14B—N14B—C15B—O3B | 179.6 (3) | C13A—N13A—C15A—O3A | 169.2 (3) |
| C17B—N14B—C15B—N13B | −172.4 (3) | C12A—N13A—C15A—N14A | −165.3 (3) |
| C14B—N14B—C15B—N13B | 1.6 (4) | C13A—N13A—C15A—N14A | −8.3 (4) |
| C14B—N15B—C16B—O11B | −174.3 (3) | C13A—N12A—C16A—O11A | 178.8 (3) |
| C18B—N15B—C16B—O11B | 1.4 (6) | C11A—N12A—C16A—O11A | 2.5 (5) |
| C14B—N15B—C16B—N12B | 2.9 (4) | C13A—N12A—C16A—N15A | −2.9 (4) |

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|---|---|---|---|
| C18B—N15B—C16B—N12B | 178.6 (3) | C11A—N12A—C16A—N15A | −179.2 (3) |
| C11B—N12B—C16B—O11B | 1.5 (5) | C14A—N15A—C16A—O11A | 172.6 (3) |
| C13B—N12B—C16B—O11B | 177.7 (3) | C18A—N15A—C16A—O11A | 13.2 (5) |
| C11B—N12B—C16B—N15B | −175.7 (3) | C14A—N15A—C16A—N12A | −5.7 (4) |
| C13B—N12B—C16B—N15B | 0.5 (4) | C18A—N15A—C16A—N12A | −165.1 (3) |
| C15B—N14B—C17B—N17B | −91.9 (4) | C15A—N14A—C17A—N17A | 88.9 (4) |
| C14B—N14B—C17B—N17B | 94.7 (4) | C14A—N14A—C17A—N17A | −82.0 (4) |
| C21B—N17B—C17B—N14B | 92.7 (4) | C21A—N17A—C17A—N14A | −101.1 (4) |
| C19B—N17B—C17B—N14B | −81.9 (4) | C19A—N17A—C17A—N14A | 94.4 (4) |
| C16B—N15B—C18B—N16B | 100.9 (4) | C22A—N16A—C18A—N15A | 96.8 (4) |
| C14B—N15B—C18B—N16B | −83.9 (4) | C19A—N16A—C18A—N15A | −82.5 (4) |
| C22B—N16B—C18B—N15B | −100.7 (4) | C16A—N15A—C18A—N16A | −109.6 (4) |
| C19B—N16B—C18B—N15B | 95.7 (4) | C14A—N15A—C18A—N16A | 93.4 (4) |
| C21B—N17B—C19B—N16B | −109.0 (3) | C22A—N16A—C19A—N17A | −110.8 (3) |
| C17B—N17B—C19B—N16B | 66.0 (4) | C18A—N16A—C19A—N17A | 68.6 (4) |
| C21B—N17B—C19B—C20B | 1.8 (4) | C22A—N16A—C19A—C20A | 1.0 (4) |
| C17B—N17B—C19B—C20B | 176.8 (3) | C18A—N16A—C19A—C20A | −179.6 (3) |
| C22B—N16B—C19B—N17B | 116.9 (3) | C21A—N17A—C19A—N16A | 114.8 (3) |
| C18B—N16B—C19B—N17B | −78.1 (4) | C17A—N17A—C19A—N16A | −79.4 (4) |
| C22B—N16B—C19B—C20B | 5.8 (4) | C21A—N17A—C19A—C20A | 3.3 (4) |
| C18B—N16B—C19B—C20B | 170.9 (3) | C17A—N17A—C19A—C20A | 169.1 (3) |
| C22B—N18B—C20B—N19B | −108.2 (3) | C22A—N18A—C20A—N19A | 112.4 (3) |
| C23B—N18B—C20B—N19B | 82.1 (4) | C23A—N18A—C20A—N19A | −82.5 (4) |
| C22B—N18B—C20B—C19B | 3.1 (4) | C22A—N18A—C20A—C19A | 1.5 (4) |
| C23B—N18B—C20B—C19B | −166.5 (3) | C23A—N18A—C20A—C19A | 166.6 (3) |
| C21B—N19B—C20B—N18B | 119.1 (3) | C21A—N19A—C20A—N18A | −114.1 (3) |
| C24B—N19B—C20B—N18B | −76.9 (4) | C24A—N19A—C20A—N18A | 77.8 (4) |
| C21B—N19B—C20B—C19B | 7.4 (4) | C21A—N19A—C20A—C19A | −2.9 (4) |
| C24B—N19B—C20B—C19B | 171.4 (3) | C24A—N19A—C20A—C19A | −171.0 (3) |
| N17B—C19B—C20B—N18B | −124.9 (3) | N16A—C19A—C20A—N18A | −1.4 (3) |
| N16B—C19B—C20B—N18B | −5.1 (3) | N17A—C19A—C20A—N18A | 118.6 (3) |
| N17B—C19B—C20B—N19B | −5.3 (3) | N16A—C19A—C20A—N19A | −120.3 (3) |
| N16B—C19B—C20B—N19B | 114.5 (3) | N17A—C19A—C20A—N19A | −0.2 (3) |
| C24B—N19B—C21B—O4B | 5.6 (5) | C19A—N17A—C21A—O4A | 173.6 (3) |
| C20B—N19B—C21B—O4B | 169.8 (3) | C17A—N17A—C21A—O4A | 7.6 (5) |
| C24B—N19B—C21B—N17B | −170.8 (3) | C19A—N17A—C21A—N19A | −5.3 (4) |
| C20B—N19B—C21B—N17B | −6.6 (4) | C17A—N17A—C21A—N19A | −171.4 (3) |
| C17B—N17B—C21B—O4B | 11.2 (5) | C24A—N19A—C21A—O4A | −5.5 (5) |
| C19B—N17B—C21B—O4B | −173.7 (3) | C20A—N19A—C21A—O4A | −173.8 (3) |
| C17B—N17B—C21B—N19B | −172.3 (3) | C24A—N19A—C21A—N17A | 173.4 (3) |
| C19B—N17B—C21B—N19B | 2.8 (4) | C20A—N19A—C21A—N17A | 5.1 (4) |
| C23B—N18B—C22B—O12B | −8.8 (6) | C19A—N16A—C22A—O12A | −178.9 (3) |
| C20B—N18B—C22B—O12B | −178.6 (3) | C18A—N16A—C22A—O12A | 1.7 (5) |
| C23B—N18B—C22B—N16B | 170.2 (3) | C19A—N16A—C22A—N18A | −0.1 (4) |
| C20B—N18B—C22B—N16B | 0.4 (4) | C18A—N16A—C22A—N18A | −179.5 (3) |
| C18B—N16B—C22B—O12B | 9.6 (6) | C20A—N18A—C22A—O12A | 177.8 (3) |
| C19B—N16B—C22B—O12B | 174.8 (3) | C23A—N18A—C22A—O12A | 12.6 (5) |
| C18B—N16B—C22B—N18B | −169.4 (3) | C20A—N18A—C22A—N16A | −0.9 (4) |

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| C19B—N16B—C22B—N18B | −4.2 (4) | C23A—N18A—C22A—N16A | −166.1 (3) |
| C22B—N18B—C23B—N20B | 103.4 (4) | C28A—N20A—C23A—N18A | 109.9 (4) |
| C20B—N18B—C23B—N20B | −88.1 (4) | C25A—N20A—C23A—N18A | −83.9 (4) |
| C28B—N20B—C23B—N18B | −108.8 (4) | C22A—N18A—C23A—N20A | −107.5 (4) |
| C25B—N20B—C23B—N18B | 83.7 (4) | C20A—N18A—C23A—N20A | 88.9 (4) |
| C21B—N19B—C24B—N21B | −114.2 (3) | C21A—N19A—C24A—N21A | 109.7 (4) |
| C20B—N19B—C24B—N21B | 83.4 (4) | C20A—N19A—C24A—N21A | −83.4 (4) |
| C27B—N21B—C24B—N19B | 116.2 (3) | C27A—N21A—C24A—N19A | −109.3 (4) |
| C25B—N21B—C24B—N19B | −89.3 (4) | C25A—N21A—C24A—N19A | 86.9 (4) |
| C28B—N20B—C25B—N21B | 110.8 (3) | C28A—N20A—C25A—N21A | −114.8 (3) |
| C23B—N20B—C25B—N21B | −80.5 (4) | C23A—N20A—C25A—N21A | 77.7 (4) |
| C28B—N20B—C25B—C26B | −0.6 (4) | C28A—N20A—C25A—C26A | −3.2 (4) |
| C23B—N20B—C25B—C26B | 168.1 (3) | C23A—N20A—C25A—C26A | −170.7 (3) |
| C27B—N21B—C25B—N20B | −117.5 (3) | C27A—N21A—C25A—N20A | 113.5 (3) |
| C24B—N21B—C25B—N20B | 85.3 (4) | C24A—N21A—C25A—N20A | −81.1 (4) |
| C27B—N21B—C25B—C26B | −6.3 (4) | C27A—N21A—C25A—C26A | 1.8 (4) |
| C24B—N21B—C25B—C26B | −163.4 (3) | C24A—N21A—C25A—C26A | 167.2 (3) |
| C27B—N23B—C26B—N22B | 108.9 (3) | C27A—N23A—C26A—N22A | −111.0 (3) |
| C30B—N23B—C26B—N22B | −75.4 (4) | C30A—N23A—C26A—N22A | 78.4 (4) |
| C27B—N23B—C26B—C25B | −2.6 (4) | C27A—N23A—C26A—C25A | 0.8 (4) |
| C30B—N23B—C26B—C25B | 173.1 (3) | C30A—N23A—C26A—C25A | −169.8 (3) |
| C28B—N22B—C26B—N23B | −119.8 (3) | C28A—N22A—C26A—N23A | 118.3 (3) |
| C29B—N22B—C26B—N23B | 83.6 (4) | C29A—N22A—C26A—N23A | −76.4 (4) |
| C28B—N22B—C26B—C25B | −8.7 (4) | C28A—N22A—C26A—C25A | 6.8 (4) |
| C29B—N22B—C26B—C25B | −165.2 (3) | C29A—N22A—C26A—C25A | 172.1 (3) |
| N20B—C25B—C26B—N23B | 124.2 (3) | N20A—C25A—C26A—N23A | −121.4 (3) |
| N21B—C25B—C26B—N23B | 5.1 (3) | N21A—C25A—C26A—N23A | −1.5 (3) |
| N20B—C25B—C26B—N22B | 5.4 (3) | N20A—C25A—C26A—N22A | −2.0 (3) |
| N21B—C25B—C26B—N22B | −113.6 (3) | N21A—C25A—C26A—N22A | 117.9 (3) |
| Pr1B—O5B—C27B—N23B | 54.7 (6) | Pr1A—O5A—C27A—N23A | −28.3 (7) |
| Pr1B—O5B—C27B—N21B | −126.2 (4) | Pr1A—O5A—C27A—N21A | 152.9 (3) |
| C30B—N23B—C27B—O5B | 2.4 (5) | C30A—N23A—C27A—O5A | −8.2 (5) |
| C26B—N23B—C27B—O5B | 178.0 (3) | C26A—N23A—C27A—O5A | −178.6 (3) |
| C30B—N23B—C27B—N21B | −176.8 (3) | C30A—N23A—C27A—N21A | 170.8 (3) |
| C26B—N23B—C27B—N21B | −1.2 (4) | C26A—N23A—C27A—N21A | 0.3 (4) |
| C24B—N21B—C27B—O5B | −17.6 (5) | C24A—N21A—C27A—O5A | 12.2 (5) |
| C25B—N21B—C27B—O5B | −174.3 (3) | C25A—N21A—C27A—O5A | 177.6 (3) |
| C24B—N21B—C27B—N23B | 161.6 (3) | C24A—N21A—C27A—N23A | −166.8 (3) |
| C25B—N21B—C27B—N23B | 4.9 (4) | C25A—N21A—C27A—N23A | −1.4 (4) |
| C25B—N20B—C28B—O7B | 174.6 (3) | C29A—N22A—C28A—O7A | 4.6 (6) |
| C23B—N20B—C28B—O7B | 6.0 (6) | C26A—N22A—C28A—O7A | 170.1 (4) |
| C25B—N20B—C28B—N22B | −4.8 (4) | C29A—N22A—C28A—N20A | −174.5 (3) |
| C23B—N20B—C28B—N22B | −173.4 (3) | C26A—N22A—C28A—N20A | −9.0 (4) |
| C29B—N22B—C28B—O7B | −14.2 (6) | C25A—N20A—C28A—O7A | −171.6 (4) |
| C26B—N22B—C28B—O7B | −170.7 (4) | C23A—N20A—C28A—O7A | −3.9 (6) |
| C29B—N22B—C28B—N20B | 165.2 (3) | C25A—N20A—C28A—N22A | 7.6 (4) |
| C26B—N22B—C28B—N20B | 8.7 (4) | C23A—N20A—C28A—N22A | 175.2 (3) |
| C34B—N24B—C29B—N22B | −104.7 (4) | C28A—N22A—C29A—N24A | −110.0 (4) |

| | | | |
|---|---|---|---|
| C31B—N24B—C29B—N22B | 82.0 (4) | C26A—N22A—C29A—N24A | 86.2 (4) |
| C28B—N22B—C29B—N24B | 112.1 (4) | C34A—N24A—C29A—N22A | 111.2 (3) |
| C26B—N22B—C29B—N24B | −93.9 (4) | C31A—N24A—C29A—N22A | −88.7 (4) |
| C27B—N23B—C30B—N25B | −100.6 (4) | C27A—N23A—C30A—N25A | 100.4 (4) |
| C26B—N23B—C30B—N25B | 84.2 (4) | C26A—N23A—C30A—N25A | −90.1 (4) |
| C33B—N25B—C30B—N23B | 90.8 (4) | C33A—N25A—C30A—N23A | −98.8 (4) |
| C31B—N25B—C30B—N23B | −91.8 (4) | C31A—N25A—C30A—N23A | 88.1 (4) |
| C33B—N25B—C31B—N24B | −104.3 (3) | C33A—N25A—C31A—N24A | 109.5 (3) |
| C30B—N25B—C31B—N24B | 78.1 (4) | C30A—N25A—C31A—N24A | −76.7 (4) |
| C33B—N25B—C31B—C32B | 6.2 (4) | C33A—N25A—C31A—C32A | −1.7 (3) |
| C30B—N25B—C31B—C32B | −171.4 (3) | C30A—N25A—C31A—C32A | 172.1 (3) |
| C34B—N24B—C31B—N25B | 117.5 (3) | C34A—N24A—C31A—N25A | −119.0 (3) |
| C29B—N24B—C31B—N25B | −68.6 (4) | C29A—N24A—C31A—N25A | 79.1 (4) |
| C34B—N24B—C31B—C32B | 7.1 (4) | C34A—N24A—C31A—C32A | −8.3 (4) |
| C29B—N24B—C31B—C32B | −179.0 (3) | C29A—N24A—C31A—C32A | −170.2 (3) |
| C34B—N26B—C32B—N27B | −108.0 (3) | C34A—N26A—C32A—N27A | 111.7 (3) |
| C35B—N26B—C32B—N27B | 69.7 (4) | C35A—N26A—C32A—N27A | −71.1 (4) |
| C34B—N26B—C32B—C31B | 3.2 (4) | C34A—N26A—C32A—C31A | −0.3 (3) |
| C35B—N26B—C32B—C31B | −179.1 (3) | C35A—N26A—C32A—C31A | 176.9 (3) |
| C33B—N27B—C32B—N26B | 117.4 (3) | C33A—N27A—C32A—N26A | −116.2 (3) |
| C36B—N27B—C32B—N26B | −88.2 (4) | C36A—N27A—C32A—N26A | 79.9 (4) |
| C33B—N27B—C32B—C31B | 6.2 (4) | C33A—N27A—C32A—C31A | −4.4 (3) |
| C36B—N27B—C32B—C31B | 160.6 (3) | C36A—N27A—C32A—C31A | −168.4 (3) |
| N25B—C31B—C32B—N26B | −125.6 (3) | N25A—C31A—C32A—N26A | 123.7 (3) |
| N24B—C31B—C32B—N26B | −5.9 (3) | N24A—C31A—C32A—N26A | 4.9 (3) |
| N25B—C31B—C32B—N27B | −7.1 (3) | N25A—C31A—C32A—N27A | 3.5 (3) |
| N24B—C31B—C32B—N27B | 112.6 (3) | N24A—C31A—C32A—N27A | −115.3 (3) |
| Pr1B—O6B—C33B—N27B | 154.6 (6) | Pr1A—O6A—C33A—N25A | 36.4 (7) |
| Pr1B—O6B—C33B—N25B | −25.9 (10) | Pr1A—O6A—C33A—N27A | −145.6 (4) |
| C32B—N27B—C33B—O6B | 177.0 (3) | C31A—N25A—C33A—O6A | 177.1 (3) |
| C36B—N27B—C33B—O6B | 22.4 (5) | C30A—N25A—C33A—O6A | 3.5 (5) |
| C32B—N27B—C33B—N25B | −2.6 (4) | C31A—N25A—C33A—N27A | −1.1 (4) |
| C36B—N27B—C33B—N25B | −157.1 (3) | C30A—N25A—C33A—N27A | −174.7 (3) |
| C31B—N25B—C33B—O6B | 177.8 (3) | C36A—N27A—C33A—O6A | −10.6 (5) |
| C30B—N25B—C33B—O6B | −4.5 (5) | C32A—N27A—C33A—O6A | −174.6 (3) |
| C31B—N25B—C33B—N27B | −2.7 (4) | C36A—N27A—C33A—N25A | 167.7 (3) |
| C30B—N25B—C33B—N27B | 175.0 (3) | C32A—N27A—C33A—N25A | 3.6 (4) |
| C35B—N26B—C34B—O8B | 6.5 (5) | C29A—N24A—C34A—O8A | −7.8 (5) |
| C32B—N26B—C34B—O8B | −175.9 (3) | C31A—N24A—C34A—O8A | −170.1 (3) |
| C35B—N26B—C34B—N24B | −176.6 (3) | C29A—N24A—C34A—N26A | 170.7 (3) |
| C32B—N26B—C34B—N24B | 1.1 (4) | C31A—N24A—C34A—N26A | 8.4 (4) |
| C29B—N24B—C34B—O8B | −2.5 (5) | C35A—N26A—C34A—O8A | −3.5 (5) |
| C31B—N24B—C34B—O8B | 171.5 (3) | C32A—N26A—C34A—O8A | 173.6 (3) |
| C29B—N24B—C34B—N26B | −179.5 (3) | C35A—N26A—C34A—N24A | 177.9 (3) |
| C31B—N24B—C34B—N26B | −5.5 (4) | C32A—N26A—C34A—N24A | −4.9 (4) |
| C34B—N26B—C35B—N5B | 99.8 (4) | C34A—N26A—C35A—N5A | −100.1 (4) |
| C32B—N26B—C35B—N5B | −77.7 (4) | C32A—N26A—C35A—N5A | 83.1 (4) |
| C4B—N5B—C35B—N26B | −99.0 (4) | C4A—N5A—C35A—N26A | 95.3 (4) |

| | | | |
|---|---|---|---|
| C1B—N5B—C35B—N26B | 97.7 (4) | C1A—N5A—C35A—N26A | −93.5 (4) |
| C3B—N4B—C36B—N27B | 106.5 (4) | C33A—N27A—C36A—N4A | 106.2 (4) |
| C1B—N4B—C36B—N27B | −75.9 (4) | C32A—N27A—C36A—N4A | −91.7 (4) |
| C33B—N27B—C36B—N4B | −110.8 (4) | C3A—N4A—C36A—N27A | −107.0 (4) |
| C32B—N27B—C36B—N4B | 97.2 (4) | C1A—N4A—C36A—N27A | 80.4 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*WB*—H1*WA*···O3*B* | 0.90 | 2.50 | 3.378 (4) | 169 |
| O2*WB*—H2*WA*···O11*W*$^{i}$ | 0.87 | 1.85 | 2.674 (3) | 157 |
| O2*WB*—H2*WB*···O1*B* | 0.87 | 2.07 | 2.865 (3) | 150 |
| O2*WB*—H2*WB*···O2*B* | 0.87 | 2.46 | 2.894 (4) | 111 |
| O3*WB*—H3*WA*···O2*W*$^{i}$ | 0.87 | 1.88 | 2.709 (4) | 158 |
| O3*WB*—H3*WB*···O4*B* | 0.87 | 1.89 | 2.710 (3) | 156 |
| O4*WB*—H4*WA*···O1*W*$^{i}$ | 0.87 | 2.01 | 2.729 (4) | 139 |
| O4*WB*—H4*WB*···O10*A*$^{ii}$ | 0.87 | 2.48 | 3.211 (3) | 142 |
| O4*WB*—H4*WB*···O11*A*$^{ii}$ | 0.87 | 2.60 | 3.206 (3) | 127 |
| O5*WB*—H5*WA*···O11*A*$^{ii}$ | 0.87 | 2.08 | 2.798 (4) | 140 |
| O5*WB*—H5*WA*···O12*A*$^{ii}$ | 0.87 | 2.44 | 3.018 (3) | 124 |
| O5*WB*—H5*WB*···O4*W*$^{i}$ | 0.87 | 1.86 | 2.712 (4) | 167 |
| O1*WA*—H1*WC*···O2*A* | 0.86 | 2.41 | 3.251 (4) | 167 |
| O1*WA*—H1*WD*···O7*W*$^{c}$ | 0.85 | 1.99 | 2.749 (17) | 148 |
| O1*WA*—H1*WD*···O8*W*$^{a}$ | 0.85 | 2.25 | 2.751 (9) | 118 |
| O2*WA*—H2*WC*···O1*A* | 0.87 | 1.80 | 2.667 (3) | 179 |
| O2*WA*—H2*WD*···O19*W*$^{iii}$ | 0.87 | 1.95 | 2.723 (4) | 147 |
| O3*WA*—H3*WC*···O4*A* | 0.87 | 1.87 | 2.723 (3) | 166 |
| O3*WA*—H3*WD*···O16*W* | 0.87 | 1.93 | 2.733 (4) | 153 |
| O4*WA*—H4*WC*···O10*B*$^{iv}$ | 0.87 | 2.05 | 2.905 (3) | 167 |
| O4*WA*—H4*WD*···O14*W*$^{iii}$ | 0.85 | 1.93 | 2.743 (4) | 159 |
| O5*WA*—H5*WC*···O19*W*$^{iii}$ | 0.87 | 1.93 | 2.766 (5) | 159 |
| O5*WA*—H5*WD*···O9*B*$^{iv}$ | 0.87 | 1.97 | 2.676 (3) | 137 |
| O15*W*—H15*A*···O3*A* | 0.87 | 1.97 | 2.837 (4) | 174 |
| O15*W*—H15*B*···O16*B* | 0.87 | 2.19 | 3.019 (5) | 159 |
| O15*W*—H15*B*···O18*B* | 0.87 | 2.39 | 3.128 (5) | 143 |
| O15*W*—H15*B*···N2*B* | 0.87 | 2.53 | 3.394 (5) | 173 |
| O1*W*—H1*WE*···O21*B* | 0.87 | 1.92 | 2.768 (4) | 165 |
| O1*W*—H1*WF*···O16*A* | 0.87 | 1.89 | 2.750 (4) | 170 |
| O17*W*$^{b}$—H17*E*$^{b}$···O2*A*$^{v}$ | 0.87 | 2.07 | 2.913 (6) | 163 |
| O17*W*$^{b}$—H17*F*$^{b}$···O3*A*$^{v}$ | 0.87 | 2.46 | 3.045 (9) | 126 |
| O3*W*—H3*WE*···O4*W* | 0.87 | 1.86 | 2.734 (4) | 177 |
| O3*W*—H3*WF*···O8*A*$^{vi}$ | 0.87 | 1.98 | 2.764 (3) | 150 |
| O2*W*—H2*WE*···O9*A*$^{vi}$ | 0.87 | 2.41 | 3.047 (3) | 131 |
| O2*W*—H2*WE*···O3*W* | 0.87 | 2.06 | 2.850 (4) | 151 |
| O2*W*—H2*WF*···O10*A*$^{vi}$ | 0.87 | 1.96 | 2.822 (3) | 173 |
| O21*W*$^{a}$—H21*A*$^{a}$···O10*B* | 0.88 | 2.41 | 3.181 (9) | 145 |
| O21*W*$^{a}$—H21*B*$^{a}$···O11*B* | 0.90 | 2.36 | 3.213 (9) | 157 |
| O21*W*$^{a}$—H21*B*$^{a}$···O12*B* | 0.90 | 2.60 | 3.127 (10) | 118 |

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|---|---|---|---|---|
| O19*W*—H19*C*···O7*B*$^{i}$ | 0.87 | 2.29 | 2.856 (4) | 123 |
| O19*W*—H19*C*···O8*B*$^{i}$ | 0.87 | 2.28 | 2.939 (4) | 132 |
| O19*W*—H19*D*···O17*W*$^{b}$ | 0.87 | 2.16 | 2.813 (7) | 132 |
| O19*W*—H19*D*···O18*W*$^{a}$ | 0.87 | 1.70 | 2.54 (2) | 160 |
| O14*W*—H14*C*···O11*B*$^{i}$ | 0.87 | 2.42 | 2.870 (4) | 112 |
| O14*W*—H14*C*···O12*B*$^{i}$ | 0.87 | 2.21 | 3.024 (4) | 156 |
| O14*W*—H14*D*···O24*W* | 0.85 | 2.25 | 2.913 (5) | 135 |
| O6*W*—H6*WA*···O9*A* | 0.86 (2) | 2.29 (2) | 3.101 (5) | 159 (4) |
| O6*W*—H6*WB*···O10*A* | 0.87 (2) | 2.31 (2) | 3.117 (5) | 155 (4) |
| O16*W*—H16*A*···O8*B*$^{iv}$ | 0.87 | 2.17 | 3.014 (4) | 163 |
| O16*W*—H16*B*···O15*W* | 0.87 | 1.93 | 2.723 (4) | 152 |
| O7*W*$^{c}$—H7*WA*$^{c}$···O6*W* | 0.89 | 1.79 | 2.673 (17) | 170 |
| O4*W*—H4*WE*···O12*W* | 0.87 | 1.89 | 2.744 (4) | 166 |
| O4*W*—H4*WF*···O7*A*$^{vi}$ | 0.87 | 1.91 | 2.777 (3) | 177 |
| O8*W*$^{a}$—H8*WA*$^{a}$···O6*W* | 0.87 | 1.93 | 2.737 (9) | 153 |
| O8*W*$^{a}$—H8*WB*$^{a}$···N21*A* | 0.87 | 2.66 | 3.316 (9) | 133 |
| O18*W*$^{a}$—H18*E*$^{a}$···O2*A*$^{v}$ | 0.87 | 2.08 | 2.94 (2) | 171 |
| O18*W*$^{a}$—H18*F*$^{a}$···O25*W* | 0.87 | 2.35 | 2.79 (4) | 111 |
| O9*W*$^{b}$—H9*WA*$^{b}$···N19*A* | 0.83 | 2.69 | 3.411 (10) | 146 |
| O9*W*$^{b}$—H9*WB*$^{b}$···O6*W* | 0.86 | 1.94 | 2.805 (10) | 177 |
| O5*W*—H5*WE*···O14*W* | 0.90 | 1.58 | 2.440 (11) | 158 |
| O5*W*—H5*WF*···O20*B*$^{i}$ | 0.87 | 1.99 | 2.786 (12) | 151 |
| O10*W*—H10*A*···O4*B*$^{i}$ | 0.87 | 2.21 | 2.981 (3) | 148 |
| O10*W*—H10*B*···O3*W* | 0.87 | 1.83 | 2.697 (4) | 175 |
| O20*W*$^{b}$—H20*C*$^{b}$···O12*B* | 0.87 | 2.00 | 2.86 (2) | 167 |
| O20*W*$^{b}$—H20*D*$^{b}$···O5*WA*$^{vii}$ | 0.87 | 2.38 | 3.00 (2) | 128 |
| O20*W*$^{b}$—H20*D*$^{b}$···O19*W*$^{i}$ | 0.87 | 2.37 | 3.20 (4) | 160 |
| O11*W*—H11*E*···O13*W* | 0.87 | 1.91 | 2.749 (4) | 161 |
| O11*W*—H11*F*···O12*A*$^{vi}$ | 0.87 | 1.90 | 2.755 (4) | 168 |
| O22*W*$^{a}$—H22*A*$^{a}$···O21*W*$^{a}$ | 0.87 | 1.80 | 2.670 (11) | 179 |
| O22*W*$^{a}$—H22*B*$^{a}$···O1*WB* | 0.87 | 1.93 | 2.763 (8) | 161 |
| O12*W*—H12*E*···O3*B*$^{i}$ | 0.87 | 2.05 | 2.913 (4) | 169 |
| O12*W*—H12*F*···O2*B*$^{i}$ | 0.87 | 2.15 | 2.918 (4) | 147 |
| O25*W*—H25*C*···O21*A* | 0.87 | 2.02 | 2.872 (5) | 166 |
| O25*W*—H25*D*···O18*B*$^{viii}$ | 0.87 | 2.09 | 2.953 (6) | 170 |
| O13*W*—H13*C*···O17*B* | 0.87 | 2.03 | 2.884 (5) | 165 |
| O13*W*—H13*D*···O21*A*$^{ix}$ | 0.87 | 1.96 | 2.800 (4) | 163 |
| O24*W*—H24*E*···O25*W* | 0.87 | 1.93 | 2.790 (5) | 171 |
| O24*W*—H24*F*···O12*B*$^{i}$ | 0.87 | 2.17 | 2.839 (4) | 133 |

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