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# Poly[[diaqua(3-carboxy-5-nitrobenzoato)(μ-5-nitrobenzene-1,3-dicarboxylato)neodymium(III)] 2.5-hydrate]

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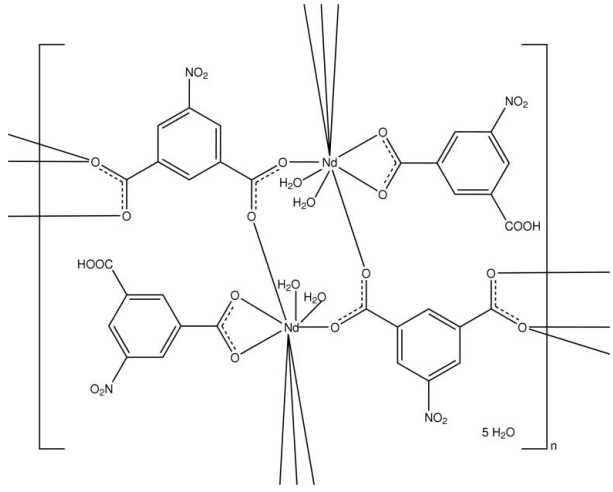
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; disorder in main residue; $R$ factor = 0.018; $wR$ factor = 0.057; data-to-parameter ratio = 14.8.

In the title compound, $\{[Nd(C_8H_3NO_6)(C_8H_4NO_6)(H_2O)_2]\cdot 2.5H_2O\}_n$, the $Nd^{III}$ ion is nine-coordinated by seven O atoms from five carboxylate groups and two water molecules. The $[Nd(C_8H_3NO_6)(H_2O)_2]^{2+}$ units are bridged by 5-nitroisophthalate dianions, forming polymeric sheets parallel to the *ab* plane. The polymeric sheets are linked into a three-dimensional network by O—H···O and C—H···O hydrogen bonds, and $\pi$–$\pi$ interactions [centroid–centroid distance = 3.5533 (11) Å]. The 5-nitroisophthalate(1−) anion is disordered over three positions with an occupancy ratio of 0.68:0.23:0.09. Two of the uncoordinated water molecules are disordered over two positions, with occupancy ratios of 0.722 (15):0.278 (15) and 0.279 (6):0.221 (6), respectively.

## Related literature

For related structures, see: Ye *et al.* (2008); Eddaoudi *et al.* (2001); Bünzli & Choppin (1989); Huang *et al.* (2008); Cui *et al.* (2002); Yan *et al.* (2005); Ren *et al.* (2006); Li *et al.* (2005). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).




## Experimental

### Crystal data

$[Nd(C_8H_3NO_6)(C_8H_4NO_6)(H_2O)_2]\cdot 2.5H_2O$
$M_r$ = 644.55
Triclinic, $P\overline{1}$
$a$ = 9.5748 (1) Å
$b$ = 10.4634 (1) Å
$c$ = 13.3285 (2) Å
$\alpha$ = 69.279 (1)°
$\beta$ = 71.753 (1)°
$\gamma$ = 66.046 (1)°
$V$ = 1118.71 (2) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 2.41 mm$^{-1}$
$T$ = 100 K
0.35 × 0.24 × 0.13 mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.484, $T_{max}$ = 0.742
22527 measured reflections
5879 independent reflections
5725 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.019

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.057
$S$ = 1.21
5879 reflections
398 parameters
115 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.77 e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Nd1—O7 | 2.3302 (13) | Nd1—O2*W* | 2.4775 (15) |
| Nd1—O8$^{i}$ | 2.4214 (14) | Nd1—O2 | 2.5223 (13) |
| Nd1—O10$^{ii}$ | 2.4481 (14) | Nd1—O1 | 2.5743 (14) |
| Nd1—O1*W* | 2.4612 (14) | Nd1—O10$^{iii}$ | 2.9332 (14) |
| Nd1—O9$^{iii}$ | 2.4708 (13) | | |

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

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O5$A$—H5$A$···O3$W^{iv}$ | 0.84 | 1.76 | 2.596 (5) | 178 |
| O1$W$—H1$W$1···O2$^{v}$ | 0.74 | 1.99 | 2.731 (3) | 175 |
| O1$W$—H2$W$1···O4$WA$ | 0.94 | 2.00 | 2.849 (4) | 149 |
| O2$W$—H1$W$2···O4$WA$ | 0.84 | 1.86 | 2.667 (3) | 159 |
| O2$W$—H2$W$2···O1$^{i}$ | 0.82 | 2.06 | 2.874 (3) | 172 |
| O3$W$—H1$W$3···O11$^{vi}$ | 0.91 | 2.56 | 3.246 (3) | 132 |
| O3$W$—H1$W$3···O12$^{vi}$ | 0.91 | 2.05 | 2.902 (3) | 156 |
| O3$W$—H2$W$3···O9$^{iii}$ | 0.96 | 1.76 | 2.688 (2) | 162 |
| O4$WA$—H2$W$4···O3$W$ | 0.85 | 2.51 | 3.118 (6) | 130 |
| C12—H12$A$···O1$^{ii}$ | 0.95 | 2.41 | 3.351 (2) | 169 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2868).

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# supporting information

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# Poly[[diaqua(3-carboxy-5-nitrobenzoato)(μ-5-nitrobenzene-1,3-dicarboxylato)neodymium(III)] 2.5-hydrate]

**Nurul-Nadia Raime, Rohana Adnan, Mohd Mustaqim Rosli and Hoong-Kun Fun**

## S1. Comment

The research on the assembly of lanthanide coordination networks has increased over the years (Ye *et al.*, 2008; Eddaoudi *et al.*, 2001). Lanthanide provide opportunities for the discovery of unusual network topologies (Bünzli & Choppin, 1989; Huang *et al.*, 2008; Cui *et al.*, 2002) due to its high and variable coordination numbers and flexible coordination environments (Yan *et al.*, 2005).

5- Nitroisophthalic acid (**nia**) has two carboxylic groups which may be completely or partially deprotonated and thus produces versatile coordination modes with lanthanide ions. Moreover, the existence of nitro group as an electron-withdrawing group has profound impacts on the electron density of the whole ligand, and thereby different physical phenomena can be produced (Ren *et al.*, 2006; Li *et al.*, 2005). In this paper, we report the crystal structure of a polymeric coordination complex formed from hydrothermal reaction between trivalent neodymium ion and nitro-isophthalic acid.

The asymmetric unit of the title polymeric compound is shown in Fig. 1. In the crystal structure, each $Nd^{III}$ ion adopts a nine-coordination environment being coordinated by two O atoms from two water molecules and seven O atoms from five carboxylate groups. The Nd—O distances range from 2.3302 (13) to 2.9332 (14) Å for carboxylate groups and 2.4612 (14) and 2.4775 (15) Å, respectively for O1W and O2W (Table 1). The nitro group attached to the C1-C6 benzene ring is slightly twisted, with a dihedral angle of 12.2 (3)° for the major disorder component A [ 9(1)° for B and 3(1)° for C]. The nitro group attached to the C9-C14 benzene ring is twisted by a dihedral angle of 21.2 (1)°. The dihedral angles between C1-C6 benzene rings and planes of carboxyl groups in disorder components A, B and C are 5.8 (5)°, 9(1)° and 29 (1)°, respectively. The adjacent $[Nd(C_8H_3NO_6)(H_2O)_2]^{2+}$ units are bridged by 5-nitroisophthalate dianions to form polymeric sheets parallel to the *ab* plane (Fig. 2).

The polymeric sheets are linked into a three-dimensional network (Fig. 3) by O—H···O and C—H···O hydrogen bonds (Table 2). There also exist a *π*–*π* interaction between the C9–C14 benzene rings at (x, y, z) and (-x, 2-y, 1-z), with a centroid-to-centroid distance of 3.5533 (11) Å.

## S2. Experimental

A mixture of 5-nitroisophthalic acid (0.4243 g, 2.0 mmol), sodium hydroxide (0.140 g, 3.5 mmol) and distilled water (30 ml) was heated till boiling. The solution was left to cool to room temperature before neodymium(III) nitrate hexahydrate salt, $Nd(NO_3).6H_2O$ (0.4380 g, 1.0 mmol) was added to it. The pH of the mixture was controlled to be between 3–4 by adding 1 *M* NaOH or 1 *M* $HNO_3$. Subsequently the solution was poured into a 40 ml Teflon tube, which was then sealed and heated at 403 K for 3 d. Upon cooling to room temperature, light purple crystals of the title compound were obtained which were filtered, washed with distilled water and left to dry in air.

### S3. Refinement

The 5-nitroisophthalate(1-) anion is disordered over three positions with an occupancy ratio of 0.683 (7):0.234 (7):0.087 (7) which was fixed at 0.68:0.23:0.09 for the final refinement. The two minor disorder components B and C were refined isotropically; a common $U_{iso}$ was used for the disorder component C. In all disorder components, the C1—C6 benzene ring is constrained to a regular hexagon with d = 1.39 Å. Atom O4W and hemihydrate O5W are also disordered over two positions, with occupancies of 0.722 (15) and 0.278 (15), and 0.279 (6) and 0.221 (6) respectively. For the disordered 5-nitroisophthalate(1-) anion, similarity restraints were applied. The O atoms of the uncoordinated water molecules are restrained so that their $U_{ij}$ components approximate to isotropic behavior. H atoms for O1W, O2W, O3W and O4WB were located in a difference Fourier map and refined as riding with the parent atom with $U_{iso}$(H) = 1.5$U_{eq}$(O). The rest of H atoms were positioned geometrically and refined using a riding model, with C-H = 0.95 Å, O-H = 0.84 Å and $U_{iso}$ = 1.2$_{eq}$(C) and 1.5$_{eq}$(O).

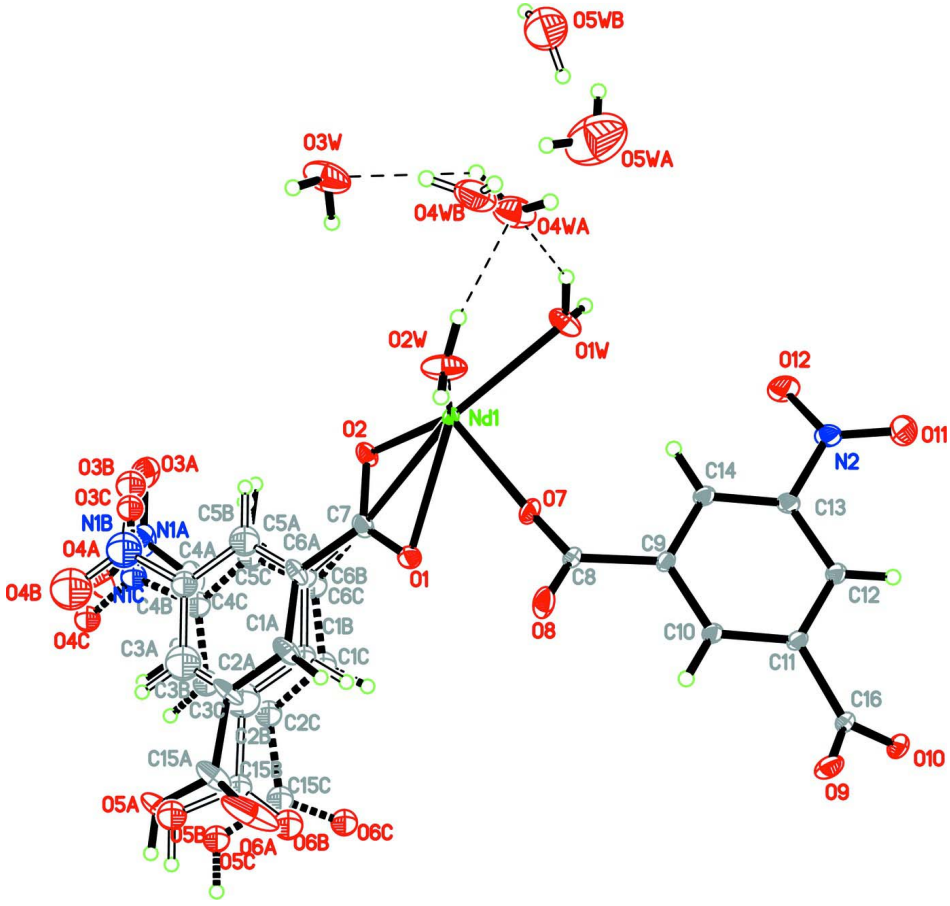


**Figure 1**

The asymetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level. All disorder components are shown. Hydrogen bonds are shown as dashed lines.

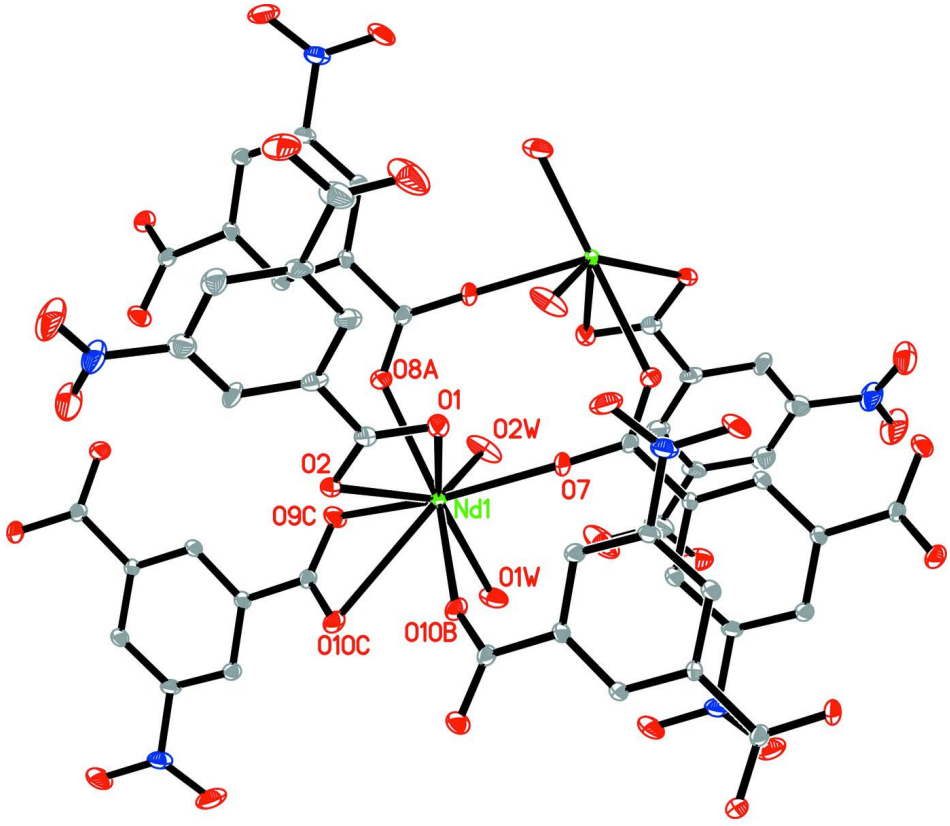


**Figure 2**

Part of the polymeric sheet, showing the coordination environment of $Nd^{III}$ ion. Displacement ellipsoids are drawn at the 50% probability level. Only major disorder components are shown. Uncoordinated water molecules and H atoms have been omitted for clarity. Symmetry codes: (A) -x, 1-y, 1-z ; (B) -x, 2-y, 1-z; (c) 1+x, -1+y, z.

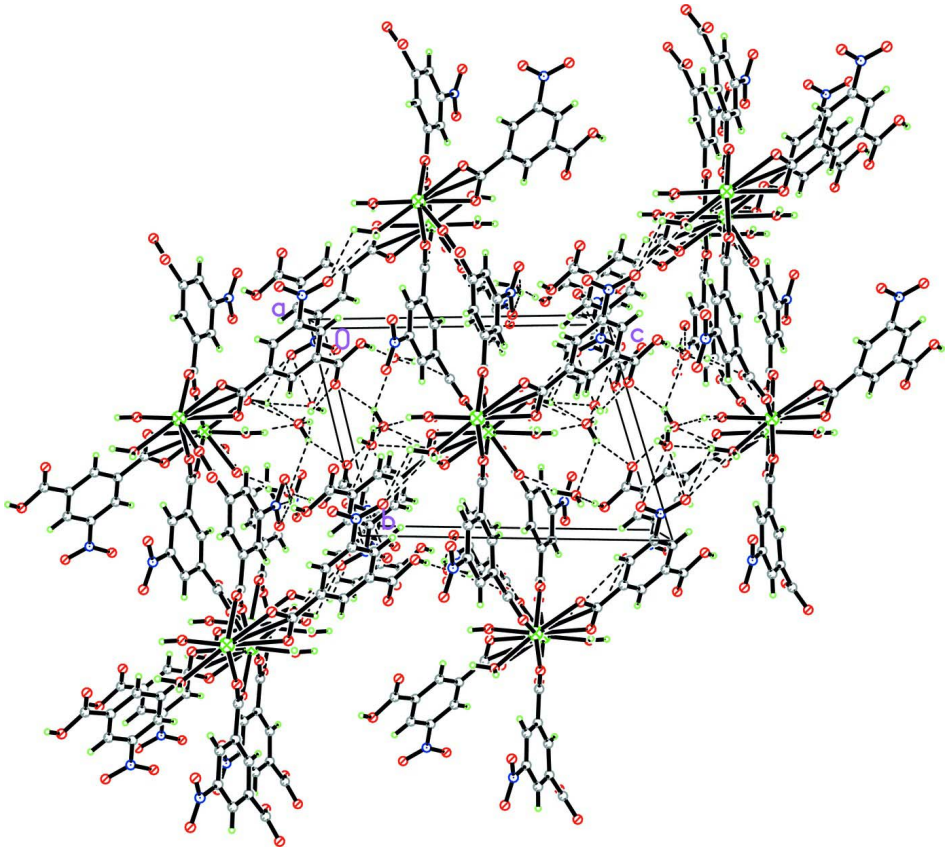

**Figure 3**

The crystal packing of the title compound, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines. Only major disorder components are shown.

**Poly[[diaqua(3-carboxy-5-nitrobenzoato)(*μ*-5-nitrobenzene-1,3- dicarboxylato)neodymium(III)] 2.5-hydrate]**

*Crystal data*

$[Nd(C_8H_3NO_6)(C_8H_4NO_6)(H_2O)_2]\cdot 2.5H_2O$
$M_r = 644.55$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.5748$ (1) Å
$b = 10.4634$ (1) Å
$c = 13.3285$ (2) Å
$\alpha = 69.279$ (1)°
$\beta = 71.753$ (1)°
$\gamma = 66.046$ (1)°
$V = 1118.71$ (2) Å$^3$
$Z = 2$
$F(000) = 636$
$D_x = 1.913$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9930 reflections
$\theta = 2.7$–$29.0$°
$\mu = 2.41$ mm$^{-1}$
$T = 100$ K
Plate, purple
0.35 × 0.24 × 0.13 mm

*Data collection*

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.484$, $T_{max} = 0.742$
22527 measured reflections
5879 independent reflections
5725 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.019
$\theta_{max}$ = 29.0°, $\theta_{min}$ = 1.7°
$h$ = −13→13
$k$ = −14→14
$l$ = −18→18

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.057
$S$ = 1.21
5879 reflections
398 parameters
115 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2 + 0.5091P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.77 e Å$^{-3}$

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness of fit $S$ are based on $F^2$, conventional $R$-factors $R$ are based on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating $R$-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^2$ are statistically about twice as large as those based on $F$, and $R$- factors based on ALL data will be even larger.

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Nd1 | 0.285572 (9) | 0.468414 (9) | 0.486911 (7) | 0.01037 (4) | |
| O3A | 0.5272 (5) | −0.1271 (4) | 0.9533 (3) | 0.0330 (9) | 0.68 |
| O4A | 0.3769 (4) | −0.1558 (3) | 1.1135 (2) | 0.0463 (8) | 0.68 |
| O5A | −0.1663 (5) | 0.1114 (5) | 1.1553 (3) | 0.0263 (8) | 0.68 |
| H5A | −0.2601 | 0.1301 | 1.1875 | 0.039* | 0.68 |
| O6A | −0.2644 (3) | 0.3037 (5) | 1.0252 (3) | 0.0605 (13) | 0.68 |
| N1A | 0.4039 (6) | −0.0919 (4) | 1.0164 (3) | 0.0297 (7) | 0.68 |
| C1A | 0.0383 (3) | 0.2754 (4) | 0.8934 (3) | 0.0205 (8) | 0.68 |
| H1AA | −0.0439 | 0.3572 | 0.8654 | 0.025* | 0.68 |
| C2A | 0.0078 (3) | 0.1835 (5) | 0.9962 (3) | 0.0198 (8) | 0.68 |
| C3A | 0.1281 (4) | 0.0639 (4) | 1.0372 (2) | 0.0238 (9) | 0.68 |
| H3AA | 0.1072 | 0.0011 | 1.1075 | 0.029* | 0.68 |
| C4A | 0.2789 (4) | 0.0361 (3) | 0.9754 (3) | 0.0245 (8) | 0.68 |
| C5A | 0.3094 (3) | 0.1279 (4) | 0.8726 (3) | 0.0189 (9) | 0.68 |
| H5AA | 0.4125 | 0.1089 | 0.8304 | 0.023* | 0.68 |
| C6A | 0.1891 (4) | 0.2476 (4) | 0.8316 (3) | 0.0165 (13) | 0.68 |
| C15A | −0.1548 (5) | 0.2079 (7) | 1.0602 (3) | 0.0268 (9) | 0.68 |
| O3B | 0.4896 (15) | −0.1413 (17) | 0.9604 (13) | 0.027 (3)* | 0.23 |
| O4B | 0.3076 (14) | −0.1937 (12) | 1.0907 (9) | 0.056 (3)* | 0.23 |
| O5B | −0.1948 (16) | 0.1468 (13) | 1.1445 (11) | 0.025 (3)* | 0.23 |

| | | | | | |
|---|---|---|---|---|---|
| H5B | −0.2852 | 0.1742 | 1.1814 | 0.037* | 0.23 |
| O6B | −0.2641 (10) | 0.3699 (8) | 1.0410 (7) | 0.0257 (18)* | 0.23 |
| N1B | 0.3557 (15) | −0.1115 (12) | 1.0079 (10) | 0.040 (3)* | 0.23 |
| C1B | 0.0367 (14) | 0.3066 (10) | 0.8974 (11) | 0.016 (3)* | 0.23 |
| H1BA | −0.0349 | 0.4004 | 0.8737 | 0.019* | 0.23 |
| C2B | −0.0066 (12) | 0.2128 (14) | 0.9957 (11) | 0.038 (5)* | 0.23 |
| C3B | 0.0982 (14) | 0.0756 (13) | 1.0304 (10) | 0.039 (5)* | 0.23 |
| H3BA | 0.0686 | 0.0115 | 1.0976 | 0.046* | 0.23 |
| C4B | 0.2463 (12) | 0.0322 (10) | 0.9668 (10) | 0.021 (3)* | 0.23 |
| C5B | 0.2896 (12) | 0.1260 (15) | 0.8684 (10) | 0.028 (4)* | 0.23 |
| H5BA | 0.3907 | 0.0963 | 0.8249 | 0.033* | 0.23 |
| C6B | 0.1848 (16) | 0.2632 (14) | 0.8337 (10) | 0.016 (4)* | 0.23 |
| C15B | −0.1695 (13) | 0.2567 (12) | 1.0630 (10) | 0.019 (3)* | 0.23 |
| O3C | 0.449 (2) | −0.130 (3) | 0.9824 (19) | 0.0208 (13)* | 0.09 |
| O4C | 0.272 (2) | −0.1538 (18) | 1.1276 (12) | 0.0208 (13)* | 0.09 |
| O5C | −0.2380 (19) | 0.2386 (18) | 1.1423 (12) | 0.0208 (13)* | 0.09 |
| H5C | −0.3302 | 0.2675 | 1.1873 | 0.025* | 0.09 |
| O6C | −0.2201 (18) | 0.4585 (14) | 1.0575 (13) | 0.0208 (13)* | 0.09 |
| N1C | 0.318 (2) | −0.0826 (18) | 1.0374 (14) | 0.0208 (13)* | 0.09 |
| C1C | 0.0294 (19) | 0.3429 (15) | 0.9028 (13) | 0.0208 (13)* | 0.09 |
| H1CA | −0.0355 | 0.4382 | 0.8740 | 0.025* | 0.09 |
| C2C | −0.0198 (15) | 0.2637 (16) | 1.0071 (12) | 0.0208 (13)* | 0.09 |
| C3C | 0.0750 (18) | 0.1244 (16) | 1.0493 (11) | 0.0208 (13)* | 0.09 |
| H3CA | 0.0414 | 0.0702 | 1.1206 | 0.025* | 0.09 |
| C4C | 0.2191 (19) | 0.0642 (16) | 0.9873 (14) | 0.0208 (13)* | 0.09 |
| C5C | 0.2683 (19) | 0.143 (2) | 0.8830 (15) | 0.0208 (13)* | 0.09 |
| H5CA | 0.3668 | 0.1023 | 0.8406 | 0.025* | 0.09 |
| C6C | 0.173 (2) | 0.283 (2) | 0.8408 (12) | 0.0208 (13)* | 0.09 |
| C15C | −0.174 (2) | 0.3312 (17) | 1.0721 (15) | 0.0208 (13)* | 0.09 |
| O1 | 0.11719 (16) | 0.45727 (15) | 0.68090 (11) | 0.0170 (3) | |
| O2 | 0.36376 (16) | 0.31566 (15) | 0.66785 (11) | 0.0165 (3) | |
| O7 | 0.05148 (16) | 0.65931 (14) | 0.46945 (12) | 0.0176 (3) | |
| O8 | −0.19586 (17) | 0.73727 (15) | 0.45331 (13) | 0.0209 (3) | |
| O9 | −0.49580 (16) | 1.26834 (15) | 0.42188 (12) | 0.0188 (3) | |
| O10 | −0.37511 (16) | 1.38214 (14) | 0.45852 (11) | 0.0157 (3) | |
| O11 | 0.1860 (2) | 1.24682 (18) | 0.22910 (16) | 0.0325 (4) | |
| O12 | 0.32156 (17) | 1.02380 (18) | 0.29539 (14) | 0.0253 (3) | |
| N2 | 0.19668 (19) | 1.12233 (19) | 0.28241 (14) | 0.0178 (3) | |
| C7 | 0.2251 (2) | 0.3495 (2) | 0.72073 (15) | 0.0155 (3) | |
| C8 | −0.0736 (2) | 0.75718 (19) | 0.44717 (14) | 0.0122 (3) | |
| C9 | −0.0762 (2) | 0.91156 (18) | 0.41124 (14) | 0.0107 (3) | |
| C10 | −0.2178 (2) | 1.02243 (19) | 0.42723 (14) | 0.0115 (3) | |
| H10A | −0.3122 | 1.0009 | 0.4554 | 0.014* | |
| C11 | −0.2213 (2) | 1.16466 (19) | 0.40205 (14) | 0.0113 (3) | |
| C12 | −0.0849 (2) | 1.19940 (19) | 0.35355 (14) | 0.0124 (3) | |
| H12A | −0.0861 | 1.2963 | 0.3343 | 0.015* | |
| C13 | 0.0528 (2) | 1.0867 (2) | 0.33446 (14) | 0.0129 (3) | |
| C14 | 0.0619 (2) | 0.94284 (19) | 0.36509 (14) | 0.0124 (3) | |

| | | | | | |
|---|---|---|---|---|---|
| H14A | 0.1593 | 0.8681 | 0.3549 | 0.015* | |
| C16 | −0.3728 (2) | 1.27944 (19) | 0.42875 (14) | 0.0127 (3) | |
| O1W | 0.39421 (17) | 0.62127 (17) | 0.31765 (11) | 0.0214 (3) | |
| H1W1 | 0.4595 | 0.6422 | 0.3181 | 0.032* | |
| H2W1 | 0.4207 | 0.6070 | 0.2475 | 0.032* | |
| O2W | 0.20344 (18) | 0.4620 (2) | 0.33051 (13) | 0.0285 (4) | |
| H1W2 | 0.2599 | 0.4648 | 0.2674 | 0.043* | |
| H2W2 | 0.1146 | 0.4785 | 0.3245 | 0.043* | |
| O3W | 0.5412 (2) | 0.1731 (2) | 0.24946 (15) | 0.0377 (4) | |
| H1W3 | 0.4742 | 0.1364 | 0.2425 | 0.057* | |
| H2W3 | 0.5221 | 0.1903 | 0.3193 | 0.057* | |
| O4WA | 0.4139 (3) | 0.5063 (6) | 0.1473 (2) | 0.0342 (12) | 0.722 (15) |
| H1W4 | 0.3780 | 0.5660 | 0.0913 | 0.051* | 0.722 (15) |
| H2W4 | 0.4716 | 0.4275 | 0.1301 | 0.051* | 0.722 (15) |
| O4WB | 0.4055 (9) | 0.4415 (15) | 0.1312 (8) | 0.037 (3) | 0.278 (15) |
| H3W4 | 0.3704 | 0.4757 | 0.0809 | 0.056* | 0.278 (15) |
| H4W4 | 0.4353 | 0.3561 | 0.1412 | 0.056* | 0.278 (15) |
| O5WA | 0.6107 (14) | 0.5930 (14) | 0.0951 (10) | 0.082 (4) | 0.279 (6) |
| H1W5 | 0.7059 | 0.5714 | 0.0630 | 0.123* | 0.279 (6) |
| H2W5 | 0.5861 | 0.5169 | 0.1155 | 0.123* | 0.279 (6) |
| O5WB | 0.9195 (14) | 0.4364 (12) | 0.0923 (8) | 0.051 (3) | 0.221 (6) |
| H3W5 | 0.8615 | 0.4864 | 0.1375 | 0.077* | 0.221 (6) |
| H4W5 | 1.0037 | 0.3835 | 0.1152 | 0.077* | 0.221 (6) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Nd1 | 0.00707 (6) | 0.00691 (6) | 0.01558 (6) | −0.00155 (4) | −0.00089 (3) | −0.00326 (4) |
| O3A | 0.038 (2) | 0.0212 (16) | 0.0264 (15) | −0.0010 (16) | −0.0073 (15) | −0.0004 (11) |
| O4A | 0.064 (2) | 0.0291 (15) | 0.0201 (12) | −0.0069 (14) | −0.0055 (13) | 0.0107 (10) |
| O5A | 0.0263 (18) | 0.037 (2) | 0.0144 (13) | −0.0199 (18) | 0.0051 (12) | −0.0027 (14) |
| O6A | 0.0223 (14) | 0.103 (3) | 0.0277 (14) | −0.0250 (18) | −0.0064 (11) | 0.0225 (18) |
| N1A | 0.043 (2) | 0.0183 (15) | 0.0194 (14) | −0.0077 (16) | −0.0092 (15) | 0.0041 (11) |
| C1A | 0.0177 (17) | 0.027 (2) | 0.0192 (16) | −0.0148 (15) | −0.0041 (11) | −0.0003 (16) |
| C2A | 0.0189 (16) | 0.034 (2) | 0.0095 (14) | −0.0193 (14) | −0.0011 (10) | 0.0016 (13) |
| C3A | 0.036 (2) | 0.0240 (19) | 0.0128 (14) | −0.0182 (16) | −0.0061 (15) | 0.0037 (11) |
| C4A | 0.035 (2) | 0.0231 (19) | 0.0186 (16) | −0.0142 (16) | −0.0103 (16) | 0.0006 (12) |
| C5A | 0.0233 (17) | 0.0150 (17) | 0.0155 (15) | −0.0079 (14) | −0.0039 (13) | 0.0010 (11) |
| C6A | 0.018 (2) | 0.019 (2) | 0.0147 (17) | −0.0128 (14) | −0.0026 (10) | 0.0009 (12) |
| C15A | 0.0245 (18) | 0.044 (3) | 0.0150 (16) | −0.0223 (19) | −0.0037 (12) | 0.0009 (17) |
| O1 | 0.0127 (6) | 0.0151 (6) | 0.0183 (6) | −0.0033 (5) | −0.0015 (5) | −0.0018 (5) |
| O2 | 0.0112 (6) | 0.0155 (6) | 0.0192 (6) | −0.0062 (5) | −0.0027 (5) | 0.0014 (5) |
| O7 | 0.0123 (6) | 0.0091 (6) | 0.0256 (7) | 0.0005 (5) | −0.0037 (5) | −0.0026 (5) |
| O8 | 0.0148 (7) | 0.0110 (6) | 0.0374 (8) | −0.0051 (5) | −0.0068 (6) | −0.0047 (6) |
| O9 | 0.0096 (6) | 0.0161 (7) | 0.0311 (7) | −0.0019 (5) | −0.0015 (5) | −0.0117 (6) |
| O10 | 0.0170 (6) | 0.0099 (6) | 0.0203 (6) | −0.0039 (5) | −0.0009 (5) | −0.0072 (5) |
| O11 | 0.0217 (8) | 0.0195 (8) | 0.0512 (10) | −0.0135 (6) | 0.0080 (7) | −0.0089 (7) |
| O12 | 0.0092 (6) | 0.0269 (8) | 0.0378 (8) | −0.0053 (6) | 0.0001 (6) | −0.0111 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N2 | 0.0120 (7) | 0.0190 (8) | 0.0244 (8) | −0.0080 (6) | 0.0022 (6) | −0.0099 (6) |
| C7 | 0.0139 (8) | 0.0152 (9) | 0.0172 (8) | −0.0072 (7) | −0.0030 (6) | −0.0014 (6) |
| C8 | 0.0118 (8) | 0.0086 (7) | 0.0145 (7) | −0.0024 (6) | −0.0007 (6) | −0.0040 (6) |
| C9 | 0.0091 (7) | 0.0079 (7) | 0.0143 (7) | −0.0014 (6) | −0.0028 (6) | −0.0030 (6) |
| C10 | 0.0081 (7) | 0.0107 (8) | 0.0150 (7) | −0.0027 (6) | −0.0014 (6) | −0.0039 (6) |
| C11 | 0.0085 (7) | 0.0097 (8) | 0.0148 (7) | −0.0014 (6) | −0.0018 (6) | −0.0048 (6) |
| C12 | 0.0111 (8) | 0.0109 (8) | 0.0155 (7) | −0.0041 (6) | −0.0008 (6) | −0.0048 (6) |
| C13 | 0.0094 (8) | 0.0139 (8) | 0.0168 (7) | −0.0057 (6) | 0.0003 (6) | −0.0059 (6) |
| C14 | 0.0086 (7) | 0.0121 (8) | 0.0155 (7) | −0.0023 (6) | −0.0013 (6) | −0.0048 (6) |
| C16 | 0.0113 (8) | 0.0089 (8) | 0.0155 (7) | −0.0024 (6) | −0.0001 (6) | −0.0038 (6) |
| O1W | 0.0170 (7) | 0.0319 (8) | 0.0164 (6) | −0.0145 (6) | −0.0027 (5) | −0.0008 (6) |
| O2W | 0.0138 (7) | 0.0522 (11) | 0.0270 (7) | −0.0106 (7) | −0.0007 (6) | −0.0222 (7) |
| O3W | 0.0305 (9) | 0.0669 (13) | 0.0304 (8) | −0.0311 (9) | 0.0039 (7) | −0.0205 (9) |
| O4WA | 0.0301 (14) | 0.046 (3) | 0.0198 (11) | −0.0101 (13) | −0.0026 (9) | −0.0065 (11) |
| O4WB | 0.027 (3) | 0.045 (5) | 0.030 (3) | −0.013 (3) | 0.005 (3) | −0.005 (4) |
| O5WA | 0.072 (6) | 0.091 (7) | 0.103 (7) | −0.024 (5) | −0.012 (5) | −0.058 (6) |
| O5WB | 0.063 (6) | 0.052 (6) | 0.045 (5) | −0.022 (5) | −0.011 (4) | −0.017 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Nd1—O7 | 2.3302 (13) | C1C—C2C | 1.39 |
| Nd1—O8$^{i}$ | 2.4214 (14) | C1C—C6C | 1.39 |
| Nd1—O10$^{ii}$ | 2.4481 (14) | C1C—H1CA | 0.95 |
| Nd1—O1W | 2.4612 (14) | C2C—C3C | 1.39 |
| Nd1—O9$^{iii}$ | 2.4708 (13) | C2C—C15C | 1.486 (13) |
| Nd1—O2W | 2.4775 (15) | C3C—C4C | 1.39 |
| Nd1—O2 | 2.5223 (13) | C3C—H3CA | 0.95 |
| Nd1—O1 | 2.5743 (14) | C4C—C5C | 1.39 |
| Nd1—C7 | 2.8822 (18) | C5C—C6C | 1.39 |
| Nd1—O10$^{iii}$ | 2.9332 (14) | C5C—H5CA | 0.95 |
| Nd1—C16$^{iii}$ | 3.0749 (18) | C6C—C7 | 1.512 (12) |
| O3A—N1A | 1.218 (6) | O1—C7 | 1.263 (2) |
| O4A—N1A | 1.228 (4) | O2—C7 | 1.263 (2) |
| O5A—C15A | 1.317 (5) | O7—C8 | 1.258 (2) |
| O5A—H5A | 0.84 | O8—C8 | 1.243 (2) |
| O6A—C15A | 1.202 (6) | O8—Nd1$^{i}$ | 2.4214 (14) |
| N1A—C4A | 1.454 (4) | O9—C16 | 1.263 (2) |
| C1A—C2A | 1.39 | O9—Nd1$^{iv}$ | 2.4708 (13) |
| C1A—C6A | 1.39 | O10—C16 | 1.261 (2) |
| C1A—H1AA | 0.95 | O10—Nd1$^{ii}$ | 2.4482 (14) |
| C2A—C3A | 1.39 | O10—Nd1$^{iv}$ | 2.9332 (14) |
| C2A—C15A | 1.489 (4) | O11—N2 | 1.222 (2) |
| C3A—C4A | 1.39 | O12—N2 | 1.235 (2) |
| C3A—H3AA | 0.95 | N2—C13 | 1.468 (2) |
| C4A—C5A | 1.39 | C8—C9 | 1.505 (2) |
| C5A—C6A | 1.39 | C9—C14 | 1.391 (2) |
| C5A—H5AA | 0.95 | C9—C10 | 1.395 (2) |
| C6A—C7 | 1.518 (3) | C10—C11 | 1.393 (2) |

| | | | |
|---|---|---|---|
| O3B—N1B | 1.203 (14) | C10—H10A | 0.95 |
| O4B—N1B | 1.225 (12) | C11—C12 | 1.395 (2) |
| O5B—C15B | 1.319 (13) | C11—C16 | 1.496 (2) |
| O5B—H5B | 0.84 | C12—C13 | 1.390 (2) |
| O6B—C15B | 1.166 (12) | C12—H12A | 0.95 |
| N1B—C4B | 1.469 (11) | C13—C14 | 1.386 (3) |
| C1B—C2B | 1.39 | C14—H14A | 0.95 |
| C1B—C6B | 1.39 | C16—Nd1$^{iv}$ | 3.0749 (18) |
| C1B—H1BA | 0.95 | O1W—H1W1 | 0.74 |
| C2B—C3B | 1.39 | O1W—H2W1 | 0.94 |
| C2B—C15B | 1.511 (11) | O2W—H1W2 | 0.84 |
| C3B—C4B | 1.39 | O2W—H2W2 | 0.82 |
| C3B—H3BA | 0.95 | O3W—H1W3 | 0.91 |
| C4B—C5B | 1.39 | O3W—H2W3 | 0.96 |
| C5B—C6B | 1.39 | O4WA—H1W4 | 0.85 |
| C5B—H5BA | 0.95 | O4WA—H2W4 | 0.85 |
| C6B—C7 | 1.480 (9) | O4WB—H3W4 | 0.75 |
| O3C—N1C | 1.239 (16) | O4WB—H4W4 | 0.79 |
| O4C—N1C | 1.223 (15) | O5WA—H1W5 | 0.85 |
| O5C—C15C | 1.294 (15) | O5WA—H2W5 | 0.85 |
| O5C—H5C | 0.90 | O5WB—H3W5 | 0.85 |
| O6C—C15C | 1.184 (16) | O5WB—H4W5 | 0.85 |
| N1C—C4C | 1.481 (13) | | |

| | | | |
|---|---|---|---|
| O7—Nd1—O8$^{i}$ | 100.76 (5) | C5B—C6B—C1B | 120.0 |
| O7—Nd1—O10$^{ii}$ | 88.82 (5) | C5B—C6B—C7 | 118.1 (8) |
| O8$^{i}$—Nd1—O10$^{ii}$ | 145.95 (5) | C1B—C6B—C7 | 121.1 (8) |
| O7—Nd1—O1W | 84.42 (5) | O6B—C15B—O5B | 124.3 (11) |
| O8$^{i}$—Nd1—O1W | 139.99 (5) | O6B—C15B—C2B | 124.3 (10) |
| O10$^{ii}$—Nd1—O1W | 72.98 (5) | O5B—C15B—C2B | 111.2 (10) |
| O7—Nd1—O9$^{iii}$ | 151.36 (5) | C15C—O5C—H5C | 121.2 |
| O8$^{i}$—Nd1—O9$^{iii}$ | 73.06 (5) | O4C—N1C—O3C | 121.9 (17) |
| O10$^{ii}$—Nd1—O9$^{iii}$ | 112.18 (5) | O4C—N1C—C4C | 121.7 (16) |
| O1W—Nd1—O9$^{iii}$ | 83.59 (5) | O3C—N1C—C4C | 116.4 (15) |
| O7—Nd1—O2W | 74.02 (5) | C2C—C1C—C6C | 120.0 |
| O8$^{i}$—Nd1—O2W | 72.51 (6) | C2C—C1C—H1CA | 120.0 |
| O10$^{ii}$—Nd1—O2W | 141.22 (5) | C6C—C1C—H1CA | 120.0 |
| O1W—Nd1—O2W | 70.97 (5) | C3C—C2C—C1C | 120.0 |
| O9$^{iii}$—Nd1—O2W | 77.50 (5) | C3C—C2C—C15C | 121.1 (10) |
| O7—Nd1—O2 | 123.94 (5) | C1C—C2C—C15C | 118.9 (10) |
| O8$^{i}$—Nd1—O2 | 72.14 (5) | C4C—C3C—C2C | 120.0 |
| O10$^{ii}$—Nd1—O2 | 75.40 (5) | C4C—C3C—H3CA | 120.0 |
| O1W—Nd1—O2 | 136.59 (5) | C2C—C3C—H3CA | 120.0 |
| O9$^{iii}$—Nd1—O2 | 81.61 (5) | C3C—C4C—C5C | 120.0 |
| O2W—Nd1—O2 | 142.83 (6) | C3C—C4C—N1C | 117.9 (11) |
| O7—Nd1—O1 | 73.37 (5) | C5C—C4C—N1C | 122.1 (11) |
| O8$^{i}$—Nd1—O1 | 70.84 (5) | C6C—C5C—C4C | 120.0 |
| O10$^{ii}$—Nd1—O1 | 81.06 (5) | C6C—C5C—H5CA | 120.0 |

| | | | |
|---|---|---|---|
| O1W—Nd1—O1 | 146.05 (5) | C4C—C5C—H5CA | 120.0 |
| O9$^{iii}$—Nd1—O1 | 127.22 (5) | C5C—C6C—C1C | 120.0 |
| O2W—Nd1—O1 | 124.29 (5) | C5C—C6C—C7 | 115.6 (10) |
| O2—Nd1—O1 | 51.38 (4) | C1C—C6C—C7 | 123.6 (10) |
| O7—Nd1—C7 | 99.34 (5) | O6C—C15C—O5C | 128.0 (16) |
| O8$^{i}$—Nd1—C7 | 65.51 (5) | O6C—C15C—C2C | 118.1 (14) |
| O10$^{ii}$—Nd1—C7 | 80.77 (5) | O5C—C15C—C2C | 113.8 (14) |
| O1W—Nd1—C7 | 153.43 (5) | C7—O1—Nd1 | 90.75 (11) |
| O9$^{iii}$—Nd1—C7 | 102.98 (5) | C7—O2—Nd1 | 93.16 (11) |
| O2W—Nd1—C7 | 135.46 (6) | C8—O7—Nd1 | 171.21 (13) |
| O2—Nd1—C7 | 25.94 (5) | C8—O8—Nd1$^{i}$ | 136.37 (12) |
| O1—Nd1—C7 | 25.99 (5) | C16—O9—Nd1$^{iv}$ | 106.33 (11) |
| O7—Nd1—O10$^{iii}$ | 146.58 (4) | C16—O10—Nd1$^{ii}$ | 160.39 (12) |
| O8$^{i}$—Nd1—O10$^{iii}$ | 112.58 (4) | C16—O10—Nd1$^{iv}$ | 84.27 (11) |
| O10$^{ii}$—Nd1—O10$^{iii}$ | 64.92 (5) | Nd1$^{ii}$—O10—Nd1$^{iv}$ | 115.08 (5) |
| O1W—Nd1—O10$^{iii}$ | 68.84 (4) | O11—N2—O12 | 124.08 (17) |
| O9$^{iii}$—Nd1—O10$^{iii}$ | 47.27 (4) | O11—N2—C13 | 118.38 (17) |
| O2W—Nd1—O10$^{iii}$ | 113.16 (4) | O12—N2—C13 | 117.54 (16) |
| O2—Nd1—O10$^{iii}$ | 71.17 (4) | O2—C7—O1 | 122.11 (17) |
| O1—Nd1—O10$^{iii}$ | 119.02 (4) | O2—C7—C6B | 120.1 (5) |
| C7—Nd1—O10$^{iii}$ | 96.50 (5) | O1—C7—C6B | 117.7 (5) |
| O7—Nd1—C16$^{iii}$ | 159.88 (5) | O2—C7—C6C | 125.0 (7) |
| O8$^{i}$—Nd1—C16$^{iii}$ | 92.18 (5) | O1—C7—C6C | 112.3 (7) |
| O10$^{ii}$—Nd1—C16$^{iii}$ | 88.96 (5) | O2—C7—C6A | 117.2 (2) |
| O1W—Nd1—C16$^{iii}$ | 75.82 (5) | O1—C7—C6A | 120.5 (2) |
| O9$^{iii}$—Nd1—C16$^{iii}$ | 23.21 (5) | O2—C7—Nd1 | 60.91 (9) |
| O2W—Nd1—C16$^{iii}$ | 95.64 (5) | O1—C7—Nd1 | 63.26 (10) |
| O2—Nd1—C16$^{iii}$ | 74.63 (5) | C6B—C7—Nd1 | 166.1 (8) |
| O1—Nd1—C16$^{iii}$ | 125.93 (4) | C6C—C7—Nd1 | 171.4 (11) |
| C7—Nd1—C16$^{iii}$ | 100.03 (5) | C6A—C7—Nd1 | 160.6 (3) |
| O10$^{iii}$—Nd1—C16$^{iii}$ | 24.08 (4) | O8—C8—O7 | 125.51 (17) |
| C15A—O5A—H5A | 109.5 | O8—C8—C9 | 117.18 (16) |
| O3A—N1A—O4A | 124.8 (4) | O7—C8—C9 | 117.30 (16) |
| O3A—N1A—C4A | 118.3 (3) | C14—C9—C10 | 120.32 (16) |
| O4A—N1A—C4A | 116.9 (4) | C14—C9—C8 | 120.22 (15) |
| C2A—C1A—C6A | 120.0 | C10—C9—C8 | 119.44 (16) |
| C2A—C1A—H1AA | 120.0 | C11—C10—C9 | 120.31 (16) |
| C6A—C1A—H1AA | 120.0 | C11—C10—H10A | 119.8 |
| C3A—C2A—C1A | 120.0 | C9—C10—H10A | 119.8 |
| C3A—C2A—C15A | 119.6 (3) | C10—C11—C12 | 120.42 (16) |
| C1A—C2A—C15A | 120.3 (3) | C10—C11—C16 | 119.21 (16) |
| C4A—C3A—C2A | 120.0 | C12—C11—C16 | 120.37 (16) |
| C4A—C3A—H3AA | 120.0 | C13—C12—C11 | 117.41 (16) |
| C2A—C3A—H3AA | 120.0 | C13—C12—H12A | 121.3 |
| C3A—C4A—C5A | 120.0 | C11—C12—H12A | 121.3 |
| C3A—C4A—N1A | 120.1 (3) | C14—C13—C12 | 123.58 (16) |
| C5A—C4A—N1A | 119.9 (3) | C14—C13—N2 | 118.54 (16) |
| C4A—C5A—C6A | 120.0 | C12—C13—N2 | 117.84 (16) |

| | | | |
|---|---|---|---|
| C4A—C5A—H5AA | 120.0 | C13—C14—C9 | 117.75 (16) |
| C6A—C5A—H5AA | 120.0 | C13—C14—H14A | 121.1 |
| C5A—C6A—C1A | 120.0 | C9—C14—H14A | 121.1 |
| C5A—C6A—C7 | 119.4 (2) | O10—C16—O9 | 122.04 (17) |
| C1A—C6A—C7 | 120.6 (2) | O10—C16—C11 | 119.94 (16) |
| O6A—C15A—O5A | 124.1 (4) | O9—C16—C11 | 118.02 (16) |
| O6A—C15A—C2A | 122.3 (3) | O10—C16—Nd1$^{iv}$ | 71.65 (10) |
| O5A—C15A—C2A | 113.5 (4) | O9—C16—Nd1$^{iv}$ | 50.45 (9) |
| C15B—O5B—H5B | 109.5 | C11—C16—Nd1$^{iv}$ | 167.91 (13) |
| O3B—N1B—O4B | 123.1 (13) | Nd1—O1W—H1W1 | 118.6 |
| O3B—N1B—C4B | 118.3 (12) | Nd1—O1W—H2W1 | 125.6 |
| O4B—N1B—C4B | 118.5 (12) | H1W1—O1W—H2W1 | 102.4 |
| C2B—C1B—C6B | 120.0 | Nd1—O2W—H1W2 | 123.6 |
| C2B—C1B—H1BA | 120.0 | Nd1—O2W—H2W2 | 127.6 |
| C6B—C1B—H1BA | 120.0 | H1W2—O2W—H2W2 | 106.9 |
| C3B—C2B—C1B | 120.0 | H1W3—O3W—H2W3 | 115.1 |
| C3B—C2B—C15B | 119.6 (8) | H1W4—O4WA—H2W4 | 107.4 |
| C1B—C2B—C15B | 120.3 (8) | H1W4—O4WA—H3W4 | 54.4 |
| C2B—C3B—C4B | 120.0 | H2W4—O4WA—H3W4 | 64.4 |
| C2B—C3B—H3BA | 120.0 | H1W4—O4WB—H2W4 | 97.0 |
| C4B—C3B—H3BA | 120.0 | H1W4—O4WB—H3W4 | 60.6 |
| C3B—C4B—C5B | 120.0 | H2W4—O4WB—H3W4 | 123.4 |
| C3B—C4B—N1B | 118.5 (9) | H1W4—O4WB—H4W4 | 164.0 |
| C5B—C4B—N1B | 121.5 (9) | H2W4—O4WB—H4W4 | 79.4 |
| C6B—C5B—C4B | 120.0 | H3W4—O4WB—H4W4 | 108.3 |
| C6B—C5B—H5BA | 120.0 | H1W5—O5WA—H2W5 | 107.4 |
| C4B—C5B—H5BA | 120.0 | H3W5—O5WB—H4W5 | 107.7 |

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|---|---|---|---|
| C6A—C1A—C2A—C3A | 0.0 | C5B—C6B—C7—Nd1 | 73 (2) |
| C6A—C1A—C2A—C15A | −176.5 (5) | C1B—C6B—C7—Nd1 | −96 (2) |
| C1A—C2A—C3A—C4A | 0.0 | C5C—C6C—C7—O2 | −25.6 (17) |
| C15A—C2A—C3A—C4A | 176.6 (5) | C1C—C6C—C7—O2 | 164.7 (10) |
| C2A—C3A—C4A—C5A | 0.0 | C5C—C6C—C7—O1 | 163.1 (9) |
| C2A—C3A—C4A—N1A | −177.8 (4) | C1C—C6C—C7—O1 | −6.7 (19) |
| O3A—N1A—C4A—C3A | 167.1 (4) | C5C—C6C—C7—C6B | 33 (8) |
| O4A—N1A—C4A—C3A | −13.6 (6) | C1C—C6C—C7—C6B | −137 (10) |
| O3A—N1A—C4A—C5A | −10.7 (6) | C5C—C6C—C7—C6A | 36 (3) |
| O4A—N1A—C4A—C5A | 168.6 (4) | C1C—C6C—C7—C6A | −134 (5) |
| C3A—C4A—C5A—C6A | 0.0 | C5A—C6A—C7—O2 | 3.6 (4) |
| N1A—C4A—C5A—C6A | 177.8 (4) | C1A—C6A—C7—O2 | −178.3 (3) |
| C4A—C5A—C6A—C1A | 0.0 | C5A—C6A—C7—O1 | 178.6 (2) |
| C4A—C5A—C6A—C7 | 178.2 (5) | C1A—C6A—C7—O1 | −3.2 (5) |
| C2A—C1A—C6A—C5A | 0.0 | C5A—C6A—C7—C6B | −117 (7) |
| C2A—C1A—C6A—C7 | −178.2 (5) | C1A—C6A—C7—C6B | 61 (7) |
| C3A—C2A—C15A—O6A | −174.7 (5) | C5A—C6A—C7—C6C | −122 (4) |
| C1A—C2A—C15A—O6A | 1.8 (8) | C1A—C6A—C7—C6C | 56 (4) |
| C3A—C2A—C15A—O5A | 2.6 (6) | C5A—C6A—C7—Nd1 | 82.8 (6) |
| C1A—C2A—C15A—O5A | 179.2 (4) | C1A—C6A—C7—Nd1 | −99.0 (5) |

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| C6B—C1B—C2B—C3B | 0.0 | O7—Nd1—C7—O2 | −162.80 (11) |
| C6B—C1B—C2B—C15B | −177.4 (17) | O8$^{i}$—Nd1—C7—O2 | 99.56 (12) |
| C1B—C2B—C3B—C4B | 0.0 | O10$^{ii}$—Nd1—C7—O2 | −75.54 (11) |
| C15B—C2B—C3B—C4B | 177.4 (17) | O1W—Nd1—C7—O2 | −66.56 (17) |
| C2B—C3B—C4B—C5B | 0.0 | O9$^{iii}$—Nd1—C7—O2 | 35.26 (12) |
| C2B—C3B—C4B—N1B | 177.8 (12) | O2W—Nd1—C7—O2 | 120.53 (12) |
| O3B—N1B—C4B—C3B | −170.2 (14) | O1—Nd1—C7—O2 | −164.04 (19) |
| O4B—N1B—C4B—C3B | 7.7 (19) | O10$^{iii}$—Nd1—C7—O2 | −12.32 (12) |
| O3B—N1B—C4B—C5B | 8 (2) | C16$^{iii}$—Nd1—C7—O2 | 11.75 (12) |
| O4B—N1B—C4B—C5B | −174.5 (13) | O7—Nd1—C7—O1 | 1.25 (12) |
| C3B—C4B—C5B—C6B | 0.0 | O8$^{i}$—Nd1—C7—O1 | −96.39 (12) |
| N1B—C4B—C5B—C6B | −177.8 (12) | O10$^{ii}$—Nd1—C7—O1 | 88.51 (11) |
| C4B—C5B—C6B—C1B | 0.0 | O1W—Nd1—C7—O1 | 97.48 (15) |
| C4B—C5B—C6B—C7 | −169.7 (17) | O9$^{iii}$—Nd1—C7—O1 | −160.70 (11) |
| C2B—C1B—C6B—C5B | 0.0 | O2W—Nd1—C7—O1 | −75.42 (13) |
| C2B—C1B—C6B—C7 | 169.3 (17) | O2—Nd1—C7—O1 | 164.04 (19) |
| C3B—C2B—C15B—O6B | 178.9 (11) | O10$^{iii}$—Nd1—C7—O1 | 151.72 (11) |
| C1B—C2B—C15B—O6B | −4 (2) | C16$^{iii}$—Nd1—C7—O1 | 175.79 (11) |
| C3B—C2B—C15B—O5B | −6.3 (17) | O7—Nd1—C7—C6B | 99 (2) |
| C1B—C2B—C15B—O5B | 171.1 (13) | O8$^{i}$—Nd1—C7—C6B | 1 (2) |
| C6C—C1C—C2C—C3C | 0.0 | O10$^{ii}$—Nd1—C7—C6B | −174 (2) |
| C6C—C1C—C2C—C15C | 179.4 (19) | O1W—Nd1—C7—C6B | −165 (2) |
| C1C—C2C—C3C—C4C | 0.0 | O9$^{iii}$—Nd1—C7—C6B | −63 (2) |
| C15C—C2C—C3C—C4C | −179 (2) | O2W—Nd1—C7—C6B | 22 (2) |
| C2C—C3C—C4C—C5C | 0.0 | O2—Nd1—C7—C6B | −98 (2) |
| C2C—C3C—C4C—N1C | 178 (2) | O1—Nd1—C7—C6B | 98 (2) |
| O4C—N1C—C4C—C3C | 5 (3) | O10$^{iii}$—Nd1—C7—C6B | −111 (2) |
| O3C—N1C—C4C—C3C | −176 (2) | C16$^{iii}$—Nd1—C7—C6B | −86 (2) |
| O4C—N1C—C4C—C5C | −177 (2) | O7—Nd1—C7—C6A | 107.5 (5) |
| O3C—N1C—C4C—C5C | 2 (3) | O8$^{i}$—Nd1—C7—C6A | 9.9 (5) |
| C3C—C4C—C5C—C6C | 0.0 | O10$^{ii}$—Nd1—C7—C6A | −165.2 (5) |
| N1C—C4C—C5C—C6C | −178 (2) | O1W—Nd1—C7—C6A | −156.2 (5) |
| C4C—C5C—C6C—C1C | 0.0 | O9$^{iii}$—Nd1—C7—C6A | −54.4 (5) |
| C4C—C5C—C6C—C7 | −170 (2) | O2W—Nd1—C7—C6A | 30.9 (5) |
| C2C—C1C—C6C—C5C | 0.0 | O2—Nd1—C7—C6A | −89.7 (5) |
| C2C—C1C—C6C—C7 | 169 (2) | O1—Nd1—C7—C6A | 106.3 (5) |
| C3C—C2C—C15C—O6C | 149.3 (18) | O10$^{iii}$—Nd1—C7—C6A | −102.0 (5) |
| C1C—C2C—C15C—O6C | −30 (3) | C16$^{iii}$—Nd1—C7—C6A | −77.9 (5) |
| C3C—C2C—C15C—O5C | −28 (3) | Nd1$^{i}$—O8—C8—O7 | 4.0 (3) |
| C1C—C2C—C15C—O5C | 152.6 (16) | Nd1$^{i}$—O8—C8—C9 | −175.30 (12) |
| O7—Nd1—O1—C7 | −178.71 (12) | O8—C8—C9—C14 | −156.86 (17) |
| O8$^{i}$—Nd1—O1—C7 | 73.22 (11) | O7—C8—C9—C14 | 23.8 (2) |
| O10$^{ii}$—Nd1—O1—C7 | −87.26 (11) | O8—C8—C9—C10 | 24.8 (2) |
| O1W—Nd1—O1—C7 | −127.43 (12) | O7—C8—C9—C10 | −154.54 (17) |
| O9$^{iii}$—Nd1—O1—C7 | 23.86 (13) | C14—C9—C10—C11 | −3.1 (3) |
| O2W—Nd1—O1—C7 | 124.75 (12) | C8—C9—C10—C11 | 175.22 (15) |
| O2—Nd1—O1—C7 | −8.85 (11) | C9—C10—C11—C12 | 4.5 (3) |
| O10$^{iii}$—Nd1—O1—C7 | −32.57 (12) | C9—C10—C11—C16 | −174.87 (16) |

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| C16$^{iii}$—Nd1—O1—C7 | −5.12 (13) | C10—C11—C12—C13 | −1.6 (3) |
| O7—Nd1—O2—C7 | 20.60 (13) | C16—C11—C12—C13 | 177.77 (16) |
| O8$^{i}$—Nd1—O2—C7 | −70.53 (12) | C11—C12—C13—C14 | −2.8 (3) |
| O10$^{ii}$—Nd1—O2—C7 | 99.01 (12) | C11—C12—C13—N2 | 179.38 (16) |
| O1W—Nd1—O2—C7 | 143.33 (11) | O11—N2—C13—C14 | 160.22 (19) |
| O9$^{iii}$—Nd1—O2—C7 | −145.35 (12) | O12—N2—C13—C14 | −19.7 (3) |
| O2W—Nd1—O2—C7 | −89.17 (13) | O11—N2—C13—C12 | −21.9 (3) |
| O1—Nd1—O2—C7 | 8.87 (11) | O12—N2—C13—C12 | 158.19 (17) |
| O10$^{iii}$—Nd1—O2—C7 | 167.05 (12) | C12—C13—C14—C9 | 4.1 (3) |
| C16$^{iii}$—Nd1—O2—C7 | −168.00 (12) | N2—C13—C14—C9 | −178.07 (16) |
| Nd1—O2—C7—O1 | −16.8 (2) | C10—C9—C14—C13 | −1.1 (3) |
| Nd1—O2—C7—C6B | 164.1 (9) | C8—C9—C14—C13 | −179.40 (16) |
| Nd1—O2—C7—C6C | 172.6 (13) | Nd1$^{ii}$—O10—C16—O9 | 173.8 (3) |
| Nd1—O2—C7—C6A | 158.1 (3) | Nd1$^{iv}$—O10—C16—O9 | 2.76 (17) |
| Nd1—O1—C7—O2 | 16.47 (19) | Nd1$^{ii}$—O10—C16—C11 | −5.2 (5) |
| Nd1—O1—C7—C6B | −164.4 (9) | Nd1$^{iv}$—O10—C16—C11 | −176.24 (15) |
| Nd1—O1—C7—C6C | −171.9 (12) | Nd1$^{ii}$—O10—C16—Nd1$^{iv}$ | 171.0 (4) |
| Nd1—O1—C7—C6A | −158.3 (3) | Nd1$^{iv}$—O9—C16—O10 | −3.4 (2) |
| C5B—C6B—C7—O2 | −17.0 (11) | Nd1$^{iv}$—O9—C16—C11 | 175.62 (12) |
| C1B—C6B—C7—O2 | 173.5 (8) | C10—C11—C16—O10 | 145.14 (17) |
| C5B—C6B—C7—O1 | 163.9 (5) | C12—C11—C16—O10 | −34.2 (2) |
| C1B—C6B—C7—O1 | −5.6 (16) | C10—C11—C16—O9 | −33.9 (2) |
| C5B—C6B—C7—C6C | −143 (9) | C12—C11—C16—O9 | 146.75 (17) |
| C1B—C6B—C7—C6C | 47 (8) | C10—C11—C16—Nd1$^{iv}$ | −17.6 (7) |
| C5B—C6B—C7—C6A | 45 (7) | C12—C11—C16—Nd1$^{iv}$ | 163.1 (5) |
| C1B—C6B—C7—C6A | −124 (8) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O5*A*—H5*A*···O3*W*$^{v}$ | 0.84 | 1.76 | 2.596 (5) | 178 |
| O1*W*—H1*W*1···O2$^{vi}$ | 0.74 | 1.99 | 2.731 (3) | 175 |
| O1*W*—H2*W*1···O4*WA* | 0.94 | 2.00 | 2.849 (4) | 149 |
| O2*W*—H1*W*2···O4*WA* | 0.84 | 1.86 | 2.667 (3) | 159 |
| O2*W*—H2*W*2···O1$^{i}$ | 0.82 | 2.06 | 2.874 (3) | 172 |
| O3*W*—H1*W*3···O11$^{vii}$ | 0.91 | 2.56 | 3.246 (3) | 132 |
| O3*W*—H1*W*3···O12$^{vii}$ | 0.91 | 2.05 | 2.902 (3) | 156 |
| O3*W*—H2*W*3···O9$^{iii}$ | 0.96 | 1.76 | 2.688 (2) | 162 |
| O4*WA*—H2*W*4···O3*W* | 0.85 | 2.51 | 3.118 (6) | 130 |
| C12—H12*A*···O1$^{ii}$ | 0.95 | 2.41 | 3.351 (2) | 169 |

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