

4-(Dimethylamino)pyridinium octaaqua-erbium(III) tetrachloride monohydrate

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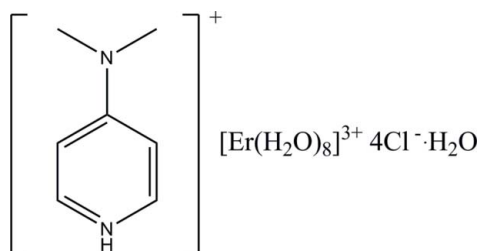
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Key indicators: single-crystal X-ray study; $T = 180$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.015; wR factor = 0.038; data-to-parameter ratio = 20.5.

In the title compound, $(\text{C}_7\text{H}_{11}\text{N}_2)[\text{Er}(\text{H}_2\text{O})_8]\text{Cl}_4 \cdot \text{H}_2\text{O}$, the asymmetric unit consists of one 4-(dimethylamino)pyridinium and one octaaquaerbium cation balanced by four Cl^- anions, and one water molecule. The 4-(dimethylamino)pyridinium cation is protonated at the pyridine N atom. The dimethylamino group (C/N/C) lies close to the plane of the pyridinium ring, making a dihedral angle of $4.5(3)^\circ$. In the crystal, the $[\text{Er}(\text{H}_2\text{O})_8]^{3+}$ cations are linked *via* $\text{O}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bonds, forming two-dimensional networks propagating in the *ab* plane. These networks are linked *via* $\text{O}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bonds, forming a three-dimensional network. The 4-(dimethylamino)pyridinium cations are located in the cavities and are linked to the framework *via* $\text{N}-\text{H}\cdots\text{Cl}$, $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds.

Related literature

For similar structures in this series involving 4-(dimethylamino)pyridinium, see: Benslimane *et al.* (2012*a,b*). For details of the Cambridge Structural Database, see: Allen (2002). For hydrogen-bond motifs see: Bernstein *et al.* (1995).



Experimental

Crystal data

$(\text{C}_7\text{H}_{11}\text{N}_2)[\text{Er}(\text{H}_2\text{O})_8]\text{Cl}_4 \cdot \text{H}_2\text{O}$
 $M_r = 594.38$
 Triclinic, $P\bar{1}$
 $a = 7.8775(3)$ Å
 $b = 9.3601(4)$ Å
 $c = 15.2593(6)$ Å
 $\alpha = 105.831(3)^\circ$
 $\beta = 101.498(3)^\circ$

$\gamma = 90.919(3)^\circ$
 $V = 1057.77(8)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 4.51$ mm⁻¹
 $T = 180$ K
 $0.35 \times 0.17 \times 0.09$ mm

Data collection

Agilent Xcalibur Sapphire1 diffractometer
 Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
 $T_{\min} = 0.415$, $T_{\max} = 0.666$

21843 measured reflections
 4315 independent reflections
 4110 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.015$
 $wR(F^2) = 0.038$
 $S = 1.12$
 4315 reflections

210 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.38$ e Å⁻³
 $\Delta\rho_{\min} = -0.84$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{Cl1}$	0.86	2.53	3.229 (2)	139
$\text{O1W}-\text{H1W}\cdots\text{Cl3}^{\text{i}}$	0.85	2.44	3.2686 (18)	165
$\text{O1W}-\text{H2W}\cdots\text{Cl3}^{\text{ii}}$	0.85	2.25	3.0874 (18)	171
$\text{O1}-\text{H11}\cdots\text{Cl4}^{\text{iii}}$	0.85	2.29	3.1036 (18)	160
$\text{O1}-\text{H12}\cdots\text{Cl1}$	0.85	2.24	3.0863 (17)	172
$\text{O2}-\text{H21}\cdots\text{Cl1}$	0.85	2.25	3.0708 (17)	164
$\text{O2}-\text{H22}\cdots\text{Cl2}$	0.84	2.31	3.1372 (17)	167
$\text{O3}-\text{H31}\cdots\text{O1W}$	0.85	1.82	2.671 (2)	177
$\text{O3}-\text{H32}\cdots\text{Cl3}$	0.84	2.37	3.1826 (17)	162
$\text{O4}-\text{H41}\cdots\text{Cl4}$	0.85	2.25	3.0925 (17)	169
$\text{O4}-\text{H42}\cdots\text{Cl2}$	0.85	2.23	3.0685 (16)	168
$\text{O5}-\text{H51}\cdots\text{Cl4}$	0.85	2.33	3.1469 (18)	160
$\text{O5}-\text{H52}\cdots\text{Cl2}^{\text{iv}}$	0.85	2.27	3.0819 (18)	161
$\text{O6}-\text{H61}\cdots\text{Cl4}^{\text{v}}$	0.85	2.27	3.1164 (17)	171
$\text{O6}-\text{H62}\cdots\text{Cl1}^{\text{vi}}$	0.85	2.25	3.0858 (17)	169
$\text{O7}-\text{H71}\cdots\text{Cl3}$	0.84	2.19	3.0304 (18)	173
$\text{O7}-\text{H72}\cdots\text{Cl1}^{\text{iv}}$	0.85	2.30	3.1132 (18)	159
$\text{O8}-\text{H81}\cdots\text{Cl4}^{\text{vii}}$	0.85	2.29	3.1377 (17)	173
$\text{O8}-\text{H82}\cdots\text{Cl2}^{\text{viii}}$	0.85	2.31	3.1464 (17)	166
$\text{C2}-\text{H2}\cdots\text{Cl3}^{\text{viii}}$	0.93	2.77	3.683 (3)	169
$\text{C3}-\text{H3}\cdots\text{O1W}^{\text{iii}}$	0.93	2.51	3.332 (3)	148
$\text{C6}-\text{H6B}\cdots\text{O4}^{\text{ii}}$	0.96	2.47	3.379 (3)	158

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP III* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2511).

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supporting information

Acta Cryst. (2012). E68, m1388–m1389 [doi:10.1107/S1600536812043048]

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S1. Comment

The title compound is part of a series of lanthanide complexes with the organic cation 4-(dimethylamino)pyridinium, for example: $(C_7H_{10}N_2)_2LaCl(H_2O)_8Cl_4 \cdot 3H_2O$ (I) (Benslimane *et al.*, 2012a) and $(C_7H_{10}N_2)_3[Nd_2Cl_4(H_2O)_{10}] \cdot Cl_5 \cdot 2H_2O$ (II) (Benslimane *et al.*, 2012b).

The title compound (III) contains an inorganic $[Er(H_2O)_8]^{3+}$ and an organic $(C_7H_{10}N_2)^+$ cation equilibrated by four Cl⁻ anions, and one lattice water molecule (Fig. 1). Atom Er1 is coordinated by eight water molecules with Er-O bond distances ranging from 2.2989 (15) to 2.3807 (15) Å. The $[Er(H_2O)_8]^{3+}$ cations are linked to the organic cations via Cl⁻ anions through intermolecular O-H...Cl and N-H...Cl hydrogen bonds. Each Cl⁻ anion acts as an acceptor of hydrogen bonds from the pyridinium groups and the water molecules. The water molecules, which act as bridging units between the cations, form cooperative infinite chains parallel to the (100) plane through O-H...Cl hydrogen bonds generating centrosymmetric $R^2_4(8)$ ring motives (Bernstein *et al.*, 1995), as shown in Fig. 2 and Table 1.

In the three compounds, (I) - (III), there is a decrease in the bond lengths of the metal-O(water) bonds, from 2.5101 (15) - 2.5632 (15) Å in (I), 2.404 (3) - 2.479 (4) Å in (II) and 2.2989 (15) - 2.3807 (15) Å in (III). This trend corresponds to the decreasing metallic radius of the lanthanide ion involved; La³⁺, Nd³⁺ and Er³⁺, respectively. In addition, the 4-(dimethylamino)pyridinium cation in the three compounds is protonated at the pyridine N atom. The N-C bond linking the dimethylamino substituent to the pyridinium ring is short, 1.321 (3), 1.324 (3) Å for (I), 1.330 (5), 1.2855 (2) Å for (II) and 1.331 (3) Å for (III), suggesting some delocalization in the cation. A search of the Cambridge Structural Database (CSD, V5.33, Update 4, August 2012; Allen, 2002) reveals similar structures incorporating the 4-(dimethylamino)-pyridinium cation for which the corresponding mean N-C distance is 1.34 (1) Å. The dimethylamino group lies close to the plane of the pyridinium ring, with dihedral angles of 3.5 (3) and 2.0 (3)° for (I), 1.6 (6)° and 6.5 (3)° for (II) and 4.5 (3)° for (III).

In conclusion, on the structural level the atomic arrangement in all three compounds, (I) - (III), consists of networks of alternating organic–inorganic layers. The chloride anions are located between these entities forming hydrogen bonds with the NH atoms of the 4-(dimethylamino)pyridinium cations and the water molecules. There are also C—H...Cl interactions present involving one of the 4-(dimethylamino)pyridinium cations. The result is the formation of three-dimensional supramolecular architectures.

S2. Experimental

4-(Dimethylamino)pyridine (1 mmol, 0.051g) and hydrochloric acid (1M) was added slowly to a solution of $ErCl_3 \cdot 6H_2O$ (1mmol, 0.08g). The mixture was refluxed at 353 K for about 1 h and then cooled to room temperature. Slow evaporation of the solvent at room temperature lead to the formation of pink plate-like crystals of the title compound.

S3. Refinement

The H-atoms of the coordinated water molecules were located in difference Fourier syntheses and were initially refined using distance restraints: O-H = 0.85 (2) Å, and H···H = 1.40 (2) Å, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. In the last cycles of refinement they were constrained to ride on their parent O atoms. The N-bound H atom was located in a difference Fourier map but like the C-bound H atoms it was included in calculated positions and treated as riding: N-H = 0.86 Å, C-H = 0.93 (aromatic), 0.96 (methyl), with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for the methyl groups and $1.2U_{\text{eq}}(\text{N,C})$ for the other H atoms.

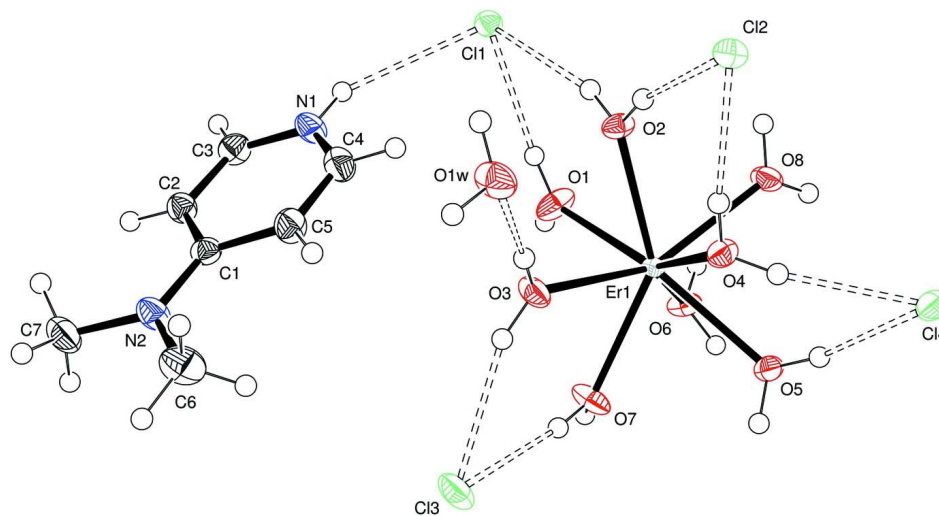
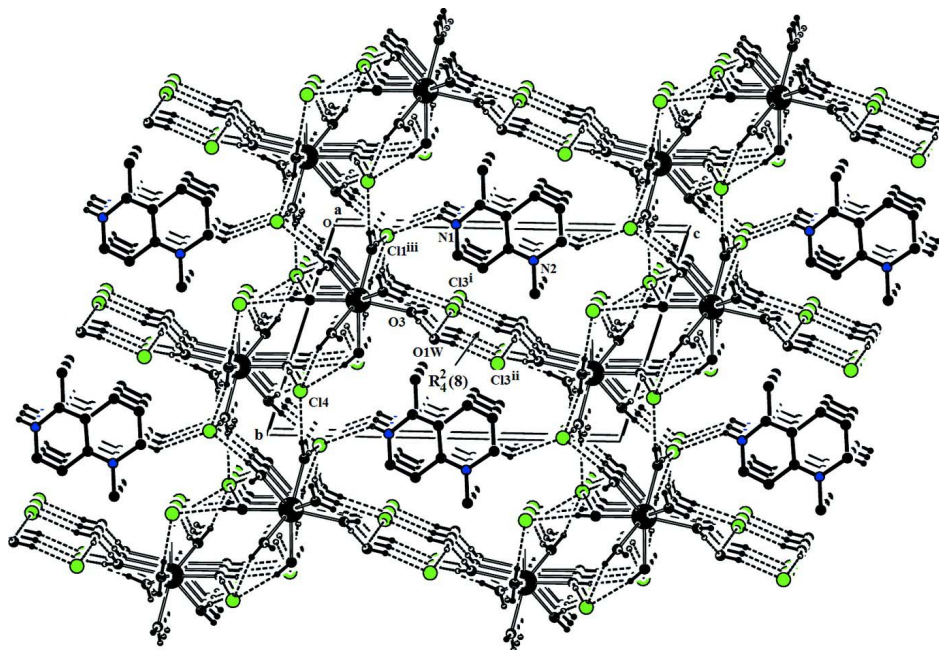


Figure 1

The molecular structure of the title compound, showing the atom-numbering. Displacement ellipsoids are drawn at the 50% probability level. The O-H···Cl and N-H···Cl hydrogen bonds are shown as double dashed lines.

**Figure 2**

A view of part of the crystal structure of the title compound lying parallel to (100), showing the formation of rings *via* O-H \cdots Cl and N-H \cdots Cl hydrogen-bonds. Hydrogen bonds are drawn as dashed lines [symmetry codes: (i) $x-1, y, z$; (ii) $-x+2, -y+1, -z+1$; (iii) $x+1, y, z$].

4-(Dimethylamino)pyridinium octaquaerbium(III) tetrachloride monohydrate

Crystal data

$(C_7H_{11}N_2)[Er(H_2O)_8]Cl_4 \cdot H_2O$

$M_r = 594.38$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 7.8775$ (3) Å

$b = 9.3601$ (4) Å

$c = 15.2593$ (6) Å

$\alpha = 105.831$ (3) $^\circ$

$\beta = 101.498$ (3) $^\circ$

$\gamma = 90.919$ (3) $^\circ$

$V = 1057.77$ (8) Å 3

$Z = 2$

$F(000) = 586$

$D_x = 1.866$ Mg m $^{-3}$

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

Cell parameters from 17643 reflections

$\theta = 2.8$ – 28.5 $^\circ$

$\mu = 4.51$ mm $^{-1}$

$T = 180$ K

Plate, pink

$0.35 \times 0.17 \times 0.09$ mm

Data collection

Agilent Xcalibur Sapphire1
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 8.2632 pixels mm $^{-1}$

ω scan

Absorption correction: multi-scan

(*CrysAlis PRO*; Agilent, 2011)

$T_{\min} = 0.415$, $T_{\max} = 0.666$

21843 measured reflections

4315 independent reflections

4110 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\max} = 26.4$ $^\circ$, $\theta_{\min} = 2.8$ $^\circ$

$h = -9 \rightarrow 9$

$k = -11 \rightarrow 11$

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.015$
 $wR(F^2) = 0.038$
 $S = 1.12$
 4315 reflections
 210 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0184P)^2 + 0.1863P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.013$
 $\Delta\rho_{\max} = 0.38 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.84 \text{ e } \text{\AA}^{-3}$

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.

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Er1	0.784214 (11)	0.328931 (10)	0.139815 (6)	0.01301 (4)
O1	0.6913 (2)	0.08907 (17)	0.13083 (13)	0.0290 (4)
H11	0.7409	0.0112	0.1094	0.043*
H12	0.5921	0.0645	0.1382	0.043*
O2	0.49910 (19)	0.33181 (16)	0.16570 (11)	0.0196 (3)
H21	0.4352	0.2530	0.1551	0.029*
H22	0.4382	0.4056	0.1716	0.029*
O3	0.8148 (2)	0.37949 (19)	0.29989 (11)	0.0246 (4)
H31	0.7391	0.4245	0.3275	0.037*
H32	0.9063	0.3747	0.3382	0.037*
O4	0.71203 (19)	0.58031 (16)	0.18827 (11)	0.0202 (3)
H41	0.7442	0.6380	0.1593	0.030*
H42	0.6119	0.6010	0.1983	0.030*
O5	0.9675 (2)	0.48121 (18)	0.09471 (12)	0.0231 (4)
H51	0.9316	0.5525	0.0728	0.035*
H52	1.0724	0.5045	0.1238	0.035*
O6	0.8996 (2)	0.16376 (17)	0.02461 (11)	0.0222 (3)
H61	0.9847	0.1931	0.0055	0.033*
H62	0.8278	0.1097	-0.0222	0.033*
O7	1.0635 (2)	0.27890 (19)	0.20245 (12)	0.0275 (4)
H71	1.1090	0.3133	0.2597	0.041*
H72	1.1158	0.2053	0.1770	0.041*
O8	0.6080 (2)	0.33727 (19)	0.00199 (11)	0.0253 (4)
H81	0.4987	0.3160	-0.0103	0.038*
H82	0.6398	0.3342	-0.0486	0.038*

N1	0.5425 (3)	-0.0329 (2)	0.34543 (14)	0.0269 (5)
H1	0.4717	-0.0651	0.2923	0.032*
N2	0.8825 (3)	0.1213 (2)	0.59717 (14)	0.0255 (4)
C1	0.7717 (3)	0.0707 (3)	0.51542 (16)	0.0205 (5)
C2	0.7091 (3)	-0.0813 (3)	0.47840 (17)	0.0228 (5)
H2	0.7453	-0.1490	0.5117	0.027*
C3	0.5969 (3)	-0.1280 (3)	0.39497 (17)	0.0250 (5)
H3	0.5568	-0.2279	0.3715	0.030*
C4	0.5976 (3)	0.1126 (3)	0.37797 (18)	0.0290 (6)
H4	0.5576	0.1769	0.3428	0.035*
C5	0.7091 (3)	0.1666 (3)	0.46032 (18)	0.0264 (5)
H5	0.7456	0.2674	0.4814	0.032*
C6	0.9502 (4)	0.2769 (3)	0.6311 (2)	0.0363 (6)
H6A	0.9889	0.3059	0.5822	0.054*
H6B	1.0459	0.2891	0.6832	0.054*
H6C	0.8602	0.3383	0.6504	0.054*
C7	0.9373 (3)	0.0284 (3)	0.65895 (18)	0.0331 (6)
H7A	0.8482	-0.0493	0.6484	0.050*
H7B	0.9571	0.0883	0.7226	0.050*
H7C	1.0427	-0.0150	0.6465	0.050*
Cl1	0.32218 (7)	0.03390 (6)	0.16034 (4)	0.01959 (11)
Cl2	0.33046 (7)	0.63783 (6)	0.19098 (4)	0.02174 (12)
Cl4	0.78967 (7)	0.76450 (6)	0.05870 (4)	0.02396 (12)
Cl3	1.20318 (8)	0.38429 (7)	0.41119 (4)	0.03275 (15)
O1W	0.5751 (2)	0.5134 (2)	0.38849 (12)	0.0326 (4)
H1W	0.4701	0.4892	0.3866	0.049*
H2W	0.6335	0.5310	0.4439	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Er1	0.01068 (5)	0.01438 (6)	0.01302 (6)	0.00048 (4)	0.00106 (4)	0.00335 (4)
O1	0.0269 (9)	0.0144 (8)	0.0502 (12)	0.0028 (7)	0.0212 (8)	0.0073 (8)
O2	0.0153 (8)	0.0132 (7)	0.0304 (9)	0.0007 (6)	0.0061 (7)	0.0052 (7)
O3	0.0201 (8)	0.0383 (10)	0.0147 (8)	0.0082 (7)	0.0020 (7)	0.0075 (7)
O4	0.0182 (8)	0.0181 (8)	0.0250 (9)	0.0000 (6)	0.0059 (7)	0.0062 (7)
O5	0.0150 (8)	0.0236 (9)	0.0343 (10)	0.0008 (6)	0.0043 (7)	0.0149 (8)
O6	0.0164 (8)	0.0263 (9)	0.0194 (8)	-0.0032 (6)	0.0059 (6)	-0.0024 (7)
O7	0.0196 (9)	0.0364 (10)	0.0200 (9)	0.0126 (7)	-0.0023 (7)	0.0014 (7)
O8	0.0152 (8)	0.0432 (11)	0.0168 (8)	0.0004 (7)	0.0002 (6)	0.0097 (8)
N1	0.0245 (11)	0.0337 (12)	0.0179 (10)	-0.0012 (9)	-0.0032 (8)	0.0052 (9)
N2	0.0265 (11)	0.0243 (11)	0.0207 (11)	-0.0009 (8)	-0.0026 (9)	0.0036 (9)
C1	0.0179 (11)	0.0228 (12)	0.0202 (12)	0.0011 (9)	0.0055 (9)	0.0042 (10)
C2	0.0237 (12)	0.0214 (12)	0.0229 (12)	0.0016 (9)	0.0032 (10)	0.0069 (10)
C3	0.0264 (13)	0.0210 (12)	0.0250 (13)	-0.0021 (10)	0.0045 (10)	0.0031 (10)
C4	0.0290 (14)	0.0299 (14)	0.0295 (14)	0.0029 (11)	0.0021 (11)	0.0136 (11)
C5	0.0301 (13)	0.0207 (12)	0.0285 (13)	-0.0004 (10)	0.0032 (11)	0.0091 (10)
C6	0.0373 (15)	0.0268 (14)	0.0338 (15)	-0.0051 (11)	-0.0026 (12)	-0.0021 (12)

C7	0.0323 (14)	0.0390 (16)	0.0246 (14)	0.0000 (12)	-0.0044 (11)	0.0108 (12)
Cl1	0.0179 (3)	0.0183 (3)	0.0215 (3)	-0.0010 (2)	0.0016 (2)	0.0057 (2)
Cl2	0.0182 (3)	0.0212 (3)	0.0242 (3)	0.0015 (2)	0.0031 (2)	0.0048 (2)
Cl4	0.0187 (3)	0.0194 (3)	0.0383 (3)	0.0041 (2)	0.0103 (2)	0.0123 (2)
Cl3	0.0335 (3)	0.0336 (3)	0.0244 (3)	-0.0001 (3)	-0.0101 (3)	0.0088 (3)
O1W	0.0283 (10)	0.0454 (11)	0.0188 (9)	0.0036 (8)	0.0020 (7)	0.0022 (8)

Geometric parameters (Å, °)

Er1—O8	2.2989 (15)	O8—H82	0.8517
Er1—O1	2.3097 (16)	N1—C3	1.341 (3)
Er1—O3	2.3195 (16)	N1—C4	1.347 (3)
Er1—O7	2.3263 (15)	N1—H1	0.8600
Er1—O5	2.3356 (15)	N2—C1	1.331 (3)
Er1—O6	2.3465 (15)	N2—C6	1.458 (3)
Er1—O2	2.3561 (15)	N2—C7	1.459 (3)
Er1—O4	2.3807 (15)	C1—C2	1.419 (3)
O1—H11	0.8493	C1—C5	1.420 (3)
O1—H12	0.8484	C2—C3	1.352 (3)
O2—H21	0.8455	C2—H2	0.9300
O2—H22	0.8425	C3—H3	0.9300
O3—H31	0.8495	C4—C5	1.344 (4)
O3—H32	0.8439	C4—H4	0.9300
O4—H41	0.8497	C5—H5	0.9300
O4—H42	0.8485	C6—H6A	0.9600
O5—H51	0.8522	C6—H6B	0.9600
O5—H52	0.8499	C6—H6C	0.9600
O6—H61	0.8514	C7—H7A	0.9600
O6—H62	0.8480	C7—H7B	0.9600
O7—H71	0.8439	C7—H7C	0.9600
O7—H72	0.8498	O1W—H1W	0.8471
O8—H81	0.8520	O1W—H2W	0.8491
O8—Er1—O1	95.94 (6)	Er1—O6—H61	120.3
O8—Er1—O3	146.14 (6)	Er1—O6—H62	117.0
O1—Er1—O3	86.60 (6)	H61—O6—H62	108.2
O8—Er1—O7	142.03 (6)	Er1—O7—H71	122.0
O1—Er1—O7	88.39 (6)	Er1—O7—H72	124.1
O3—Er1—O7	71.64 (6)	H71—O7—H72	111.0
O8—Er1—O5	81.09 (6)	Er1—O8—H81	122.4
O1—Er1—O5	146.98 (6)	Er1—O8—H82	126.5
O3—Er1—O5	114.04 (6)	H81—O8—H82	108.6
O7—Er1—O5	75.30 (6)	C3—N1—C4	120.7 (2)
O8—Er1—O6	75.79 (6)	C3—N1—H1	119.7
O1—Er1—O6	71.78 (6)	C4—N1—H1	119.7
O3—Er1—O6	135.91 (6)	C1—N2—C6	120.7 (2)
O7—Er1—O6	69.84 (6)	C1—N2—C7	122.8 (2)
O5—Er1—O6	75.65 (6)	C6—N2—C7	116.4 (2)

O8—Er1—O2	74.29 (6)	N2—C1—C2	122.3 (2)
O1—Er1—O2	71.93 (5)	N2—C1—C5	121.6 (2)
O3—Er1—O2	74.51 (6)	C2—C1—C5	116.2 (2)
O7—Er1—O2	141.61 (6)	C3—C2—C1	120.3 (2)
O5—Er1—O2	136.56 (5)	C3—C2—H2	119.9
O6—Er1—O2	129.45 (5)	C1—C2—H2	119.9
O8—Er1—O4	81.90 (6)	N1—C3—C2	121.2 (2)
O1—Er1—O4	141.90 (6)	N1—C3—H3	119.4
O3—Er1—O4	75.79 (6)	C2—C3—H3	119.4
O7—Er1—O4	116.47 (6)	C5—C4—N1	121.3 (2)
O5—Er1—O4	70.61 (5)	C5—C4—H4	119.3
O6—Er1—O4	141.89 (6)	N1—C4—H4	119.3
O2—Er1—O4	70.91 (5)	C4—C5—C1	120.4 (2)
Er1—O1—H11	125.4	C4—C5—H5	119.8
Er1—O1—H12	124.1	C1—C5—H5	119.8
H11—O1—H12	109.5	N2—C6—H6A	109.5
Er1—O2—H21	122.4	N2—C6—H6B	109.5
Er1—O2—H22	125.8	H6A—C6—H6B	109.5
H21—O2—H22	109.7	N2—C6—H6C	109.5
Er1—O3—H31	121.3	H6A—C6—H6C	109.5
Er1—O3—H32	126.0	H6B—C6—H6C	109.5
H31—O3—H32	111.3	N2—C7—H7A	109.5
Er1—O4—H41	115.9	N2—C7—H7B	109.5
Er1—O4—H42	121.1	H7A—C7—H7B	109.5
H41—O4—H42	108.9	N2—C7—H7C	109.5
Er1—O5—H51	122.7	H7A—C7—H7C	109.5
Er1—O5—H52	121.2	H7B—C7—H7C	109.5
H51—O5—H52	108.1	H1W—O1W—H2W	109.7

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1...C11	0.86	2.53	3.229 (2)	139
O1 <i>W</i> —H1 <i>W</i> ...C13 ⁱ	0.85	2.44	3.2686 (18)	165
O1 <i>W</i> —H2 <i>W</i> ...C13 ⁱⁱ	0.85	2.25	3.0874 (18)	171
O1—H11...C14 ⁱⁱⁱ	0.85	2.29	3.1036 (18)	160
O1—H12...C11	0.85	2.24	3.0863 (17)	172
O2—H21...C11	0.85	2.25	3.0708 (17)	164
O2—H22...C12	0.84	2.31	3.1372 (17)	167
O3—H31...O1 <i>W</i>	0.85	1.82	2.671 (2)	177
O3—H32...C13	0.84	2.37	3.1826 (17)	162
O4—H41...C14	0.85	2.25	3.0925 (17)	169
O4—H42...C12	0.85	2.23	3.0685 (16)	168
O5—H51...C14	0.85	2.33	3.1469 (18)	160
O5—H52...C12 ^{iv}	0.85	2.27	3.0819 (18)	161
O6—H61...C14 ^v	0.85	2.27	3.1164 (17)	171
O6—H62...C11 ^{vi}	0.85	2.25	3.0858 (17)	169
O7—H71...C13	0.84	2.19	3.0304 (18)	173

O7—H72···C11 ^{iv}	0.85	2.30	3.1132 (18)	159
O8—H81···C14 ^{vii}	0.85	2.29	3.1377 (17)	173
O8—H82···C12 ^{vii}	0.85	2.31	3.1464 (17)	166
C2—H2···C13 ^{viii}	0.93	2.77	3.683 (3)	169
C3—H3···O1 ⁱⁱⁱ	0.93	2.51	3.332 (3)	148
C6—H6B···O4 ⁱⁱ	0.96	2.47	3.379 (3)	158

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