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Poly[hydronium [μ-(ethylenediaminetetraacetato-$\kappa^8N,N',O,O',O'',O''':O''',O''''$)erbate(III)] monohydrate]

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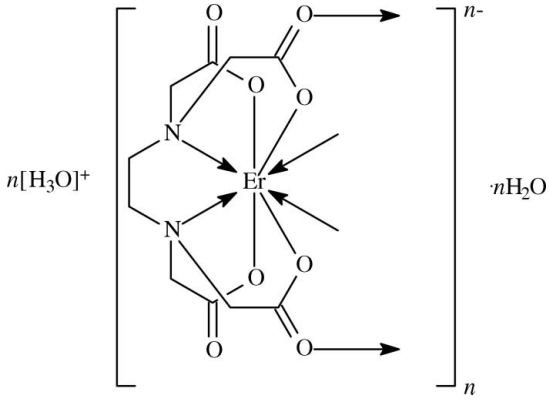
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(O–C) = 0.005 Å; H-atom completeness 71%; disorder in main residue; R factor = 0.022; wR factor = 0.055; data-to-parameter ratio = 10.4.

The erbium(III) atom in the title compound, $\{(H_3O)[Er(C_{10}H_{12}N_2O_8)]\cdot H_2O\}_n$, is N,N',O,O',O'',O'''-chelated by the ethylenediaminetetraacetate tetraanion. It is also linked to the O atoms of two other tetraaanions in the polyanionic layer. The metal atom, which lies on a special position of site symmetry m, exists in a square-antiprismatic geometry. The tetraanion is disordered across a mirror plane. The oxonium cation and water molecule are disordered in a ratio of 2:1; they occupy the space between adjacent layers.

Related literature

For related literature, see: Allen (2002); Filippova *et al.* (1977); Polynova *et al.* (1986).



Experimental

Crystal data

$(H_3O)[Er(C_{10}H_{12}N_2O_8)]\cdot H_2O$
M_r = 492.52
Orthorhombic, *Pbcm*
a = 6.5783 (1) Å
b = 12.8191 (2) Å
c = 18.4454 (3) Å
V = 1555.46 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.45 mm^{-1}
T = 295 (2) K
0.28 × 0.25 × 0.17 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.397, T_{max} = 0.516
(expected range = 0.305–0.396)
13530 measured reflections
1844 independent reflections
1625 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.055
S = 1.05
1844 reflections
178 parameters
127 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

Table 1
Selected bond lengths (Å).

Er1—O1	2.305 (3)	Er1—O4′^{ii}	2.297 (5)
Er1—O3	2.307 (4)	Er1—N1	2.574 (6)
Er1—O4^{i}	2.314 (4)	Er1—N1′	2.582 (6)
Er1—O3′	2.281 (4)		

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2139).

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supplementary materials

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Poly[hydronium [μ-(ethylenediaminetetraacetato-$\kappa^8N,N',O,O',O'',O''':O'''',O''''')$erbate(III)] monohydrate]

X.-L. You, L.-H. Wang and S. W. Ng

Comment

The edta tetraanion chelates a large number of lanthanide atoms (CSD Version 5.28, November 2006; Allen, 2002); among these are several examples of $[edta\text{-}Ln]^-$ anions whose negative charge is balanced by a unipositive cation. One erbium(III) derivative has an ammonium cation as the counterion; the metal atom itself exists in an eight-coordinate environment, and the water-coordinated cation, anion and solvent water molecules are linked through hydrogen bonds into a three-dimensional network structure (Filippova *et al.*, 1977; Polynova *et al.*, 1986). A hydrothermal synthesis yields the expected $[edta\text{-}Er]^-$ as a hydronium monohydrate (Fig. 1). The edta chelates the metal atom, and it also functions as a bridge to link adjacent anions into a polyanionic layer. The disordered hydronium cation and water molecules occupy the space between the layers; the metal shows a square-antiprismatic coordination (Fig. 2).

Experimental

Erbium(III) oxide (0.163 g, 0.5 mmol), edta (0.286 g, 0.8 mmol) and perchloric acid (0.385 mmol) were dissolved in methanol (5 ml) and water (5 ml). This solution was sealed in a Teflon-lined, stainless-steel autoclave (20 ml capacity) and heated to 433 K for 4 days. It was cooled to room temperature at 5 K h^{-1} to obtain colorless block-shaped crystals. CH&N elemental analysis. Calc. for $C_{10}H_{17}ErN_2O_{10}$: C 24.38, H 3.48, N 5.69%. Found 24.20, H 3.50, N 5.66%.

Refinement

The edta tetraanion is disordered across a mirror plane; only atoms O1, O2 and C1 have full site occupany, the other atoms having 0.5 occupancy. For the disordered atoms, the C—O distances were restrained to 1.25±0.01 Å, the C—N distances to 1.45±0.01 Å and the C—C distances to 1.50±0.01 Å. The displacement parameters of the ordered and disordered C, N and O atoms were restrained to be nearly isotropic.

Together with the $[(C_{10}H_{12}N_2O_8)Er]$ monoanion, the formula unit has one hydronium ion and one water molecule. Because *Z* is 4, as well as the fact that O3o and O1w both lie on general positions, these two O atoms are disordered; the sum of their site occupancies should be unity. The occupancies refined to 0.67 (1) and 0.33 (1), and were then fixed at these values. The 'o' and 'w' labels are arbitrary and do not imply that O3o is the hydronium and O1w the water O atoms. Their H atoms could not be placed in any chemically sensible positions.

The carbon-bound H atoms were placed at calculated positions (C—H 0.97 Å), and they were included in the refinement in the riding model approximation with U_{iso}(H) set equal to 1.2U_{eq}(C).

Figures

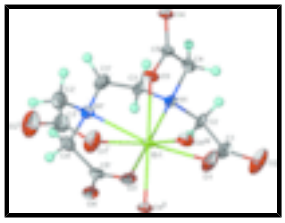

Fig. 1. A view of a portion of the polyanionic structure (I). Displacement ellipsoids are drawn at the 50% probability level, and H atoms are shown as spheres of arbitrary radius. Symmetry codes are as given in the Table. The disordered hydronium ion and water molecule are not shown.

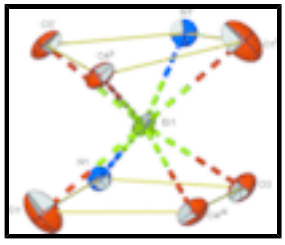

Fig. 2. Square-antiprismatic geometry of Er. Symmetry codes are as given in the Table.

Poly[hydronium [μ-(ethylenediaminetetraacetato- $\kappa^8N,N',O,O',O'',O''':O'''',O''''')$erbate(III)] monohydrate]

Crystal data

$(H_3O)[Er(C_{10}H_{12}N_2O_8)]\cdot H_2O$	$F_{000} = 956$
$M_r = 492.52$	$D_x = 2.103$ Mg m^{-3}
Orthorhombic, *Pbcm*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2c 2b	Cell parameters from 4071 reflections
a = 6.5783 (1) Å	θ = 3.4–27.6º
b = 12.8191 (2) Å	μ = 5.45 mm^{-1}
c = 18.4454 (3) Å	*T* = 295 (2) K
V = 1555.46 (4) Å^3	Block, colourless
Z = 4	0.28 × 0.25 × 0.17 mm

Data collection

Bruker APEXII diffractometer	1844 independent reflections
Radiation source: medium-focus sealed tube	1625 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.042$
T = 295(2) K	$\theta_{max} = 27.5$º
φ and ω scans	$\theta_{min} = 2.2$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −8→8
$T_{min} = 0.397$, $T_{max} = 0.516$	*k* = −15→16
13530 measured reflections	*l* = −23→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.022$

$wR(F^2) = 0.055$

$S = 1.05$

1844 reflections

178 parameters

127 restraints

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0306P)^2 + 0.6341P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.58$ e Å^{-3}

$\Delta\rho_{min} = -0.60$ e Å^{-3}

Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Er1	0.10963 (3)	0.056040 (16)	0.2500	0.01744 (9)	
O1	0.0662 (5)	0.0340 (3)	0.12694 (17)	0.0470 (8)	
O2	0.1143 (5)	0.0745 (3)	0.0123 (2)	0.0657 (12)	
O3O	−0.2598 (19)	0.2009 (9)	−0.0529 (6)	0.193 (4)	0.67
O1W	0.467 (3)	0.0586 (11)	−0.0724 (9)	0.110 (5)	0.33
C1	0.1464 (6)	0.0880 (4)	0.0798 (2)	0.0353 (10)	
O3	0.4409 (6)	0.0109 (4)	0.2763 (3)	0.0257 (12)	0.50
O4	0.7699 (6)	0.0110 (3)	0.2591 (12)	0.023 (3)	0.50
N1	0.3667 (8)	0.1616 (5)	0.1747 (3)	0.0215 (12)	0.50
C2	0.296 (5)	0.178 (2)	0.1012 (6)	0.026 (6)	0.50
H2A	0.4104	0.1792	0.0681	0.031*	0.50
H2B	0.2265	0.2448	0.0979	0.031*	0.50
C3	0.429 (3)	0.2612 (12)	0.2061 (14)	0.018 (4)	0.50
H3A	0.3359	0.3158	0.1910	0.021*	0.50
H3B	0.5641	0.2794	0.1895	0.021*	0.50
C4	0.5488 (10)	0.0954 (6)	0.1695 (4)	0.0259 (16)	0.50
H4A	0.6652	0.1389	0.1581	0.031*	0.50
H4B	0.5310	0.0462	0.1300	0.031*	0.50
C5	0.5917 (7)	0.0360 (5)	0.2383 (5)	0.020 (2)	0.50
O3'	−0.0518 (7)	0.2097 (3)	0.2261 (3)	0.0277 (14)	0.50
O4'	−0.1176 (5)	0.3776 (3)	0.2392 (8)	0.023 (3)	0.50
N1'	0.2526 (8)	0.2089 (4)	0.3255 (3)	0.0220 (12)	0.50
C2'	0.279 (5)	0.171 (2)	0.3991 (6)	0.038 (9)	0.50
H2'1	0.4188	0.1480	0.4047	0.046*	0.50
H2'2	0.2592	0.2294	0.4322	0.046*	0.50
C3'	0.427 (3)	0.2520 (16)	0.2867 (15)	0.031 (6)	0.50
H3'1	0.5445	0.2101	0.3000	0.037*	0.50
H3'2	0.4510	0.3213	0.3060	0.037*	0.50
C4'	0.0935 (9)	0.2884 (6)	0.3296 (4)	0.0277 (16)	0.50
H4'1	0.1557	0.3558	0.3384	0.033*	0.50
H4'2	0.0051	0.2729	0.3703	0.033*	0.50
C5'	−0.0325 (8)	0.2940 (4)	0.2612 (6)	0.022 (2)	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Er1	0.01162 (11)	0.01093 (13)	0.02976 (15)	−0.00036 (8)	0.000	0.000
O1	0.0624 (19)	0.0457 (19)	0.0329 (17)	−0.0331 (16)	−0.0058 (15)	−0.0023 (14)
O2	0.093 (3)	0.071 (3)	0.0324 (19)	−0.039 (2)	−0.0147 (17)	0.0000 (18)
O3O	0.181 (7)	0.192 (8)	0.206 (8)	0.049 (7)	−0.044 (7)	0.036 (7)
O1W	0.122 (8)	0.108 (9)	0.099 (8)	0.043 (7)	0.022 (8)	0.007 (7)
C1	0.039 (2)	0.036 (2)	0.031 (2)	−0.0068 (18)	−0.0096 (18)	−0.0033 (19)
O3	0.017 (2)	0.020 (2)	0.041 (3)	0.0008 (19)	0.0019 (18)	0.006 (2)
O4	0.0124 (15)	0.0214 (19)	0.035 (9)	0.0022 (14)	−0.002 (3)	−0.002 (3)
N1	0.021 (3)	0.021 (3)	0.022 (3)	0.000 (2)	−0.004 (2)	−0.003 (3)
C2	0.032 (7)	0.022 (7)	0.024 (9)	−0.014 (5)	−0.006 (5)	−0.009 (5)
C3	0.024 (6)	0.016 (6)	0.013 (5)	−0.005 (5)	−0.005 (4)	0.008 (5)
C4	0.022 (3)	0.025 (4)	0.030 (4)	0.000 (3)	0.006 (3)	−0.003 (3)
C5	0.015 (2)	0.011 (3)	0.033 (7)	−0.0030 (18)	0.001 (3)	−0.005 (3)
O3'	0.0187 (17)	0.016 (2)	0.048 (4)	0.0036 (18)	−0.0081 (18)	−0.006 (2)
O4'	0.0220 (17)	0.0112 (18)	0.037 (8)	0.0022 (14)	−0.004 (3)	0.003 (3)
N1'	0.022 (2)	0.017 (3)	0.027 (3)	−0.008 (3)	0.000 (2)	0.001 (3)
C2'	0.040 (10)	0.043 (12)	0.032 (10)	−0.008 (7)	0.004 (6)	−0.008 (7)
C3'	0.031 (7)	0.022 (7)	0.040 (10)	−0.016 (5)	−0.005 (5)	−0.006 (6)
C4'	0.028 (3)	0.019 (4)	0.036 (4)	0.003 (3)	0.007 (3)	−0.003 (3)
C5'	0.0131 (19)	0.016 (3)	0.036 (7)	−0.001 (2)	0.003 (3)	0.001 (4)

Geometric parameters (Å, °)

Er1—O1	2.305 (3)	C3—C3'	1.491 (8)
Er1—O1^{i}	2.305 (3)	C3—H3A	0.9700
Er1—O3	2.307 (4)	C3—H3B	0.9700
Er1—O4^{ii}	2.314 (4)	C4—C5	1.508 (8)
Er1—O3'	2.281 (4)	C4—H4A	0.9700
Er1—O4'^{iii}	2.297 (5)	C4—H4B	0.9700
Er1—N1	2.574 (6)	O3'—C5'	1.266 (7)
Er1—N1'	2.582 (6)	O4'—C5'	1.274 (7)
O1—C1	1.231 (5)	O4'—Er1^{v}	2.297 (5)
O2—C1	1.273 (6)	N1'—C2'	1.452 (10)
C1—C2^{i}	1.44 (3)	N1'—C4'	1.462 (7)
C1—C2	1.57 (3)	N1'—C3'	1.464 (10)
O3—C5	1.256 (7)	C2'—C1^{i}	1.44 (3)
O4—C5	1.274 (7)	C2'—H2'1	0.9700
O4—Er1^{iv}	2.314 (4)	C2'—H2'2	0.9700
N1—C3	1.461 (9)	C3'—H3'1	0.9700
N1—C2	1.449 (10)	C3'—H3'2	0.9700
N1—C4	1.471 (7)	C4'—C5'	1.512 (8)
C2—H2A	0.9700	C4'—H4'1	0.9700
C2—H2B	0.9700	C4'—H4'2	0.9700

O3'^{i}—Er1—O3'	22.3 (2)	N1^{i}—Er1—N1	65.4 (2)
O3'^{i}—Er1—O4'^{iii}	152.57 (17)	C1—O1—Er1	125.0 (3)
O3'—Er1—O4'^{iii}	148.6 (2)	O1—C1—O2	122.9 (4)
O3'^{i}—Er1—O4'^{vi}	148.6 (2)	O1—C1—C2'^{i}	119.3 (8)
O3'—Er1—O4'^{vi}	152.57 (17)	O2—C1—C2'^{i}	117.8 (8)
O4'^{iii}—Er1—O4'^{vi}	10.0 (8)	O1—C1—C2	120.4 (7)
O3'^{i}—Er1—O1^{i}	81.84 (15)	O2—C1—C2	116.7 (7)
O3'—Er1—O1^{i}	103.82 (15)	C5—O3—Er1	124.3 (4)
O4'^{iii}—Er1—O1^{i}	88.1 (4)	C5—O4—Er1^{iv}	143.5 (9)
O4'^{vi}—Er1—O1^{i}	78.2 (4)	C3—N1—C2	109.5 (15)
O3'^{i}—Er1—O1	103.82 (15)	C3—N1—C4	107.6 (9)
O3'—Er1—O1	81.84 (15)	C2—N1—C4	106.6 (10)
O4'^{iii}—Er1—O1	78.2 (4)	C3—N1—Er1	115.4 (12)
O4'^{vi}—Er1—O1	88.1 (4)	C2—N1—Er1	111.7 (15)
O1^{i}—Er1—O1	159.90 (15)	C4—N1—Er1	105.5 (4)
O3'^{i}—Er1—O4^{vii}	77.28 (19)	N1—C2—C1	109.2 (19)
O3'—Er1—O4^{vii}	75.62 (19)	N1—C2—H2A	109.8
O4'^{iii}—Er1—O4^{vii}	76.55 (14)	C1—C2—H2A	109.8
O4'^{vi}—Er1—O4^{vii}	77.29 (16)	N1—C2—H2B	109.8
O1^{i}—Er1—O4^{vii}	85.5 (5)	C1—C2—H2B	109.8
O1—Er1—O4^{vii}	77.2 (5)	H2A—C2—H2B	108.3
O3'^{i}—Er1—O4^{ii}	75.62 (19)	N1—C3—C3'	109 (2)
O3'—Er1—O4^{ii}	77.28 (19)	N1—C3—H3A	109.9
O4'^{iii}—Er1—O4^{ii}	77.29 (16)	C3'—C3—H3A	109.9
O4'^{vi}—Er1—O4^{ii}	76.55 (14)	N1—C3—H3B	109.9
O1^{i}—Er1—O4^{ii}	77.2 (5)	C3'—C3—H3B	109.9
O1—Er1—O4^{ii}	85.5 (5)	H3A—C3—H3B	108.3
O4^{vii}—Er1—O4^{ii}	8.3 (11)	N1—C4—C5	112.9 (5)
O3'^{i}—Er1—O3	128.02 (17)	N1—C4—H4A	109.0
O3'—Er1—O3	134.21 (16)	C5—C4—H4A	109.0
O4'^{iii}—Er1—O3	75.33 (18)	N1—C4—H4B	109.0
O4'^{vi}—Er1—O3	73.15 (17)	C5—C4—H4B	109.0
O1^{i}—Er1—O3	83.05 (14)	H4A—C4—H4B	107.8
O1—Er1—O3	107.07 (15)	O4—C5—O3	119.6 (10)
O4^{vii}—Er1—O3	149.9 (2)	O4—C5—C4	123.6 (9)
O4^{ii}—Er1—O3	146.6 (3)	O3—C5—C4	116.8 (5)
O3'^{i}—Er1—O3^{i}	134.21 (16)	C5'—O3'—Er1	126.3 (4)
O3'—Er1—O3^{i}	128.02 (17)	C5'—O4'—Er1^{v}	143.0 (7)
O4'^{iii}—Er1—O3^{i}	73.15 (17)	C2'—N1'—C4'	105.6 (11)
O4'^{vi}—Er1—O3^{i}	75.33 (18)	C2'—N1'—C3'	119.2 (19)
O1^{i}—Er1—O3^{i}	107.07 (15)	C4'—N1'—C3'	109.0 (11)

O1—Er1—O3^{i}	83.05 (14)	C2'—N1'—Er1	107.3 (14)
O4^{vii}—Er1—O3^{i}	146.6 (3)	C4'—N1'—Er1	107.2 (4)
O4^{ii}—Er1—O3^{i}	149.9 (2)	C3'—N1'—Er1	108.0 (11)
O3—Er1—O3^{i}	24.3 (2)	C1^{i}—C2'—N1'	115 (2)
O3'^{i}—Er1—N1^{i}	75.35 (18)	C1^{i}—C2'—H2'1	108.5
O3'—Er1—N1^{i}	87.47 (17)	N1'—C2'—H2'1	108.5
O4'^{iii}—Er1—N1^{i}	123.8 (3)	C1^{i}—C2'—H2'2	108.5
O4'^{vi}—Er1—N1^{i}	117.5 (3)	N1'—C2'—H2'2	108.5
O1^{i}—Er1—N1^{i}	67.31 (14)	H2'1—C2'—H2'2	107.5
O1—Er1—N1^{i}	132.67 (14)	N1'—C3'—C3	122 (2)
O4^{vii}—Er1—N1^{i}	143.6 (4)	N1'—C3'—H3'1	107.0
O4^{ii}—Er1—N1^{i}	136.6 (5)	C3—C3'—H3'1	107.0
O3—Er1—N1^{i}	52.96 (18)	N1'—C3'—H3'2	107.0
O3^{i}—Er1—N1^{i}	67.97 (16)	C3—C3'—H3'2	107.0
O3'^{i}—Er1—N1	87.47 (17)	H3'1—C3'—H3'2	106.7
O3'—Er1—N1	75.35 (18)	N1'—C4'—C5'	112.5 (5)
O4'^{iii}—Er1—N1	117.5 (3)	N1'—C4'—H4'1	109.1
O4'^{vi}—Er1—N1	123.8 (3)	C5'—C4'—H4'1	109.1
O1^{i}—Er1—N1	132.67 (14)	N1'—C4'—H4'2	109.1
O1—Er1—N1	67.31 (14)	C5'—C4'—H4'2	109.1
O4^{vii}—Er1—N1	136.6 (5)	H4'1—C4'—H4'2	107.8
O4^{ii}—Er1—N1	143.6 (4)	O4'—C5'—O3'	120.7 (8)
O3—Er1—N1	67.97 (16)	O4'—C5'—C4'	123.2 (8)
O3^{i}—Er1—N1	52.96 (18)	O3'—C5'—C4'	116.1 (5)
O3'^{i}—Er1—O1—C1	68.8 (4)	Er1^{iv}—O4—C5—O3	−155.3 (15)
O3'—Er1—O1—C1	65.0 (4)	Er1^{iv}—O4—C5—C4	25 (2)
O4'^{iii}—Er1—O1—C1	−139.2 (4)	Er1—O3—C5—O4	177.0 (7)
O4'^{vi}—Er1—O1—C1	−140.5 (4)	Er1—O3—C5—C4	−2.8 (9)
O1^{i}—Er1—O1—C1	173.1 (3)	N1—C4—C5—O4	−149.2 (9)
O4^{vii}—Er1—O1—C1	142.1 (4)	N1—C4—C5—O3	30.6 (9)
O4^{ii}—Er1—O1—C1	142.8 (4)	O3'^{i}—Er1—O3'—C5'	37.7 (6)
O3—Er1—O1—C1	−68.8 (4)	O4'^{iii}—Er1—O3'—C5'	157.3 (9)
O3^{i}—Er1—O1—C1	−65.1 (4)	O4'^{vi}—Er1—O3'—C5'	138.5 (9)
N1^{i}—Er1—O1—C1	−13.8 (5)	O1^{i}—Er1—O3'—C5'	47.6 (6)
N1—Er1—O1—C1	−12.4 (4)	O1—Er1—O3'—C5'	−152.0 (6)
Er1—O1—C1—O2	−178.3 (3)	O4^{vii}—Er1—O3'—C5'	129.2 (8)
Er1—O1—C1—C2'^{i}	0.6 (13)	O4^{ii}—Er1—O3'—C5'	120.8 (8)
Er1—O1—C1—C2	1.8 (11)	O3—Er1—O3'—C5'	−46.1 (7)
O3'^{i}—Er1—O3—C5	−81.7 (6)	O3^{i}—Er1—O3'—C5'	−77.5 (6)
O3'—Er1—O3—C5	−53.1 (6)	N1^{i}—Er1—O3'—C5'	−18.3 (6)
O4'^{iii}—Er1—O3—C5	114.5 (7)	N1—Er1—O3'—C5'	−83.5 (6)

O4'^{vi}—Er1—O3—C5	124.6 (7)	O3'^{i}—Er1—N1'—C2'	116.0 (12)
O1^{i}—Er1—O3—C5	−155.7 (6)	O3'—Er1—N1'—C2'	136.3 (12)
O1—Er1—O3—C5	42.1 (6)	O4'^{iii}—Er1—N1'—C2'	−32.6 (13)
O4^{vii}—Er1—O3—C5	135.9 (11)	O4'^{vi}—Er1—N1'—C2'	−23.9 (13)
O4^{ii}—Er1—O3—C5	150.5 (10)	O1^{i}—Er1—N1'—C2'	19.0 (12)
O3^{i}—Er1—O3—C5	33.1 (6)	O1—Er1—N1'—C2'	−169.1 (12)
N1^{i}—Er1—O3—C5	−88.9 (6)	O4^{vii}—Er1—N1'—C2'	84.9 (13)
N1—Er1—O3—C5	−13.9 (6)	O4^{ii}—Er1—N1'—C2'	77.2 (13)
O3'^{i}—Er1—N1—C3	40.9 (8)	O3—Er1—N1'—C2'	−69.9 (12)
O3'—Er1—N1—C3	59.8 (8)	O3^{i}—Er1—N1'—C2'	−90.6 (12)
O4'^{iii}—Er1—N1—C3	−151.0 (9)	N1^{i}—Er1—N1'—C2'	−67.5 (13)
O4'^{vi}—Er1—N1—C3	−141.9 (9)	N1—Er1—N1'—C2'	−141.7 (12)
O1^{i}—Er1—N1—C3	−35.6 (9)	O3'^{i}—Er1—N1'—C4'	2.9 (4)
O1—Er1—N1—C3	147.0 (8)	O3'—Er1—N1'—C4'	23.2 (4)
O4^{vii}—Er1—N1—C3	109.3 (9)	O4'^{iii}—Er1—N1'—C4'	−145.7 (5)
O4^{ii}—Er1—N1—C3	102.3 (10)	O4'^{vi}—Er1—N1'—C4'	−137.0 (5)
O3—Er1—N1—C3	−92.2 (8)	O1^{i}—Er1—N1'—C4'	−94.1 (4)
O3^{i}—Er1—N1—C3	−114.3 (9)	O1—Er1—N1'—C4'	77.8 (5)
N1^{i}—Er1—N1—C3	−34.2 (8)	O4^{vii}—Er1—N1'—C4'	−28.2 (7)
O3'^{i}—Er1—N1—C2	−85.1 (9)	O4^{ii}—Er1—N1'—C4'	−35.8 (6)
O3'—Er1—N1—C2	−66.1 (9)	O3—Er1—N1'—C4'	177.0 (4)
O4'^{iii}—Er1—N1—C2	83.1 (10)	O3^{i}—Er1—N1'—C4'	156.3 (4)
O4'^{vi}—Er1—N1—C2	92.1 (10)	N1^{i}—Er1—N1'—C4'	179.4 (8)
O1^{i}—Er1—N1—C2	−161.6 (9)	N1—Er1—N1'—C4'	105.2 (4)
O1—Er1—N1—C2	21.0 (9)	O3'^{i}—Er1—N1'—C3'	−114.4 (12)
O4^{vii}—Er1—N1—C2	−16.7 (10)	O3'—Er1—N1'—C3'	−94.1 (11)
O4^{ii}—Er1—N1—C2	−23.7 (11)	O4'^{iii}—Er1—N1'—C3'	97.0 (12)
O3—Er1—N1—C2	141.8 (9)	O4'^{vi}—Er1—N1'—C3'	105.7 (12)
O3^{i}—Er1—N1—C2	119.7 (9)	O1^{i}—Er1—N1'—C3'	148.6 (11)
N1^{i}—Er1—N1—C2	−160.1 (9)	O1—Er1—N1'—C3'	−39.5 (12)
O3'^{i}—Er1—N1—C4	159.4 (4)	O4^{vii}—Er1—N1'—C3'	−145.5 (12)
O3'—Er1—N1—C4	178.4 (4)	O4^{ii}—Er1—N1'—C3'	−153.1 (12)
O4'^{iii}—Er1—N1—C4	−32.4 (6)	O3—Er1—N1'—C3'	59.7 (11)
O4'^{vi}—Er1—N1—C4	−23.3 (6)	O3^{i}—Er1—N1'—C3'	39.0 (11)
O1^{i}—Er1—N1—C4	83.0 (5)	N1^{i}—Er1—N1'—C3'	62.1 (12)
O1—Er1—N1—C4	−94.5 (4)	N1—Er1—N1'—C3'	−12.1 (11)
O4^{vii}—Er1—N1—C4	−132.1 (5)	C4'—N1'—C2'—C1^{i}	86.9 (16)
O4^{ii}—Er1—N1—C4	−139.2 (7)	C3'—N1'—C2'—C1^{i}	−150.2 (16)
O3—Er1—N1—C4	26.4 (4)	Er1—N1'—C2'—C1^{i}	−27.2 (18)
O3^{i}—Er1—N1—C4	4.2 (4)	C2'—N1'—C3'—C3	161 (2)
N1^{i}—Er1—N1—C4	84.4 (4)	C4'—N1'—C3'—C3	−78 (2)

C3—N1—C2—C1	−155.5 (14)	Er1—N1'—C3'—C3	38 (3)
C4—N1—C2—C1	88.4 (15)	N1—C3—C3'—N1'	−49 (3)
Er1—N1—C2—C1	−26.4 (15)	C2'—N1'—C4'—C5'	−148.8 (16)
O1—C1—C2—N1	18.6 (18)	C3'—N1'—C4'—C5'	82.1 (14)
O2—C1—C2—N1	−161.3 (9)	Er1—N1'—C4'—C5'	−34.6 (6)
C2—N1—C3—C3'	159 (2)	Er1^{v}—O4'—C5'—O3'	−161.0 (10)
C4—N1—C3—C3'	−85 (2)	Er1^{v}—O4'—C5'—C4'	19.5 (18)
Er1—N1—C3—C3'	32 (2)	Er1—O3'—C5'—O4'	174.1 (6)
C3—N1—C4—C5	85.9 (13)	Er1—O3'—C5'—C4'	−6.5 (9)
C2—N1—C4—C5	−156.7 (15)	N1'—C4'—C5'—O4'	−150.5 (8)
Er1—N1—C4—C5	−37.8 (6)	N1'—C4'—C5'—O3'	30.0 (9)

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

Fig. 1

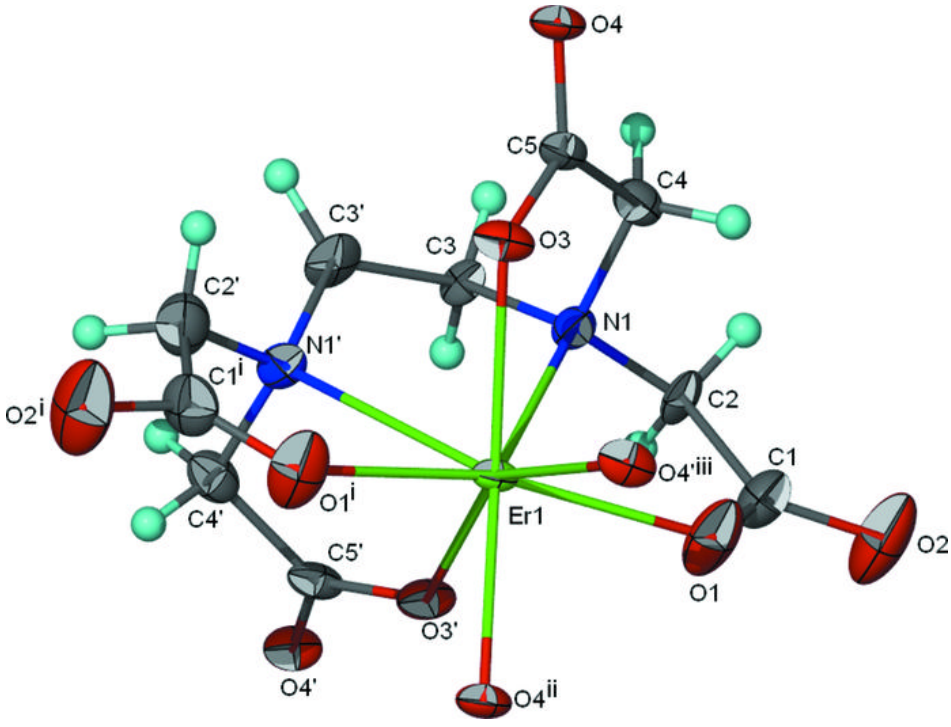
O4
C5
C4
C3'
C3
O3
C2'
N1
N1'
C1i
C2
O2i
O4'iii
C1
O1i
Er1
C4'
C5'
O2
O1
O3'
O4'
O4ii

Fig. 2