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catena-Poly[[[diaqua(3-nitrobenzoato-κ^2O,O')erbium(III)]-di-μ-3-nitrobenzoato-$\kappa^4O:O'$] 2,2′-diamino-4,4′-bi-1,3-thiazole]

Bing-Xin Liu,[a]* Guang-Hua Chen[a] and Liang-Jun Zhang[b]

[a]Department of Chemistry, Shanghai University, People's Republic of China, and [b]Department of Petroleum and Chemical Industry, Guangxi Vocational and Technical Institute of Industry, People's Republic of China
Correspondence e-mail: r5744011@yahoo.com.cn

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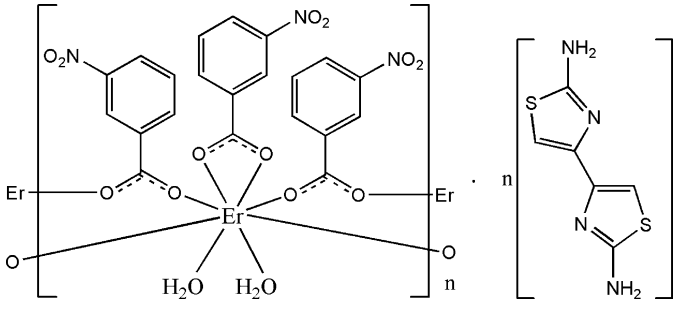
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.008 Å; R factor = 0.032; wR factor = 0.066; data-to-parameter ratio = 12.5.

In the title compound, $\{[Er(C_7H_4NO_4)_3(H_2O)_2]\cdot C_6H_6N_4S_2\}_n$, the Er^{III} ion displays a distorted tetragonal-antiprismatic coordination geometry, formed by five 3-nitrobenzoate anions and two water molecules. Among the three crystallographically independent nitrobenzoate anions, one chelates an Er^{III} ion and two bridge adjacent Er^{III} ions to form a one-dimensional polymeric chain extending along the *a* axis. The uncoordinated diaminobithiazole molecules are centrosymmetric and link with the Er^{III} complex *via* hydrogen bonding.

Related literature

For general background, see: Wu *et al.* (2003); Luo *et al.* (2004); Liu & Xu (2004). For related structures, see: Liu *et al.* (2003, 2005).



Experimental

Crystal data

$[Er(C_7H_4NO_4)_3(H_2O)_2]\cdot C_6H_6N_4S_2$
M_r = 899.90
Triclinic, $P\overline{1}$
a = 9.6739 (7) Å
b = 12.993 (1) Å
c = 14.5927 (11) Å
α = 68.148 (1)°
β = 86.352 (1)°
γ = 75.553 (1)°
V = 1647.7 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.75 mm^{-1}
T = 295 (2) K
0.20 × 0.17 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.560, T_{max} = 0.680
8623 measured reflections
5731 independent reflections
5127 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.066
S = 1.04
5731 reflections
460 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}

Table 1
Selected bond lengths (Å).

Er—O1	2.378 (3)	Er—O21	2.293 (3)
Er—O2	2.419 (3)	Er—O22^{i}	2.254 (3)
Er—O11	2.417 (3)	Er—O31	2.262 (3)
Er—O12	2.455 (3)	Er—O32^{ii}	2.280 (3)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O12^{i}	0.81	2.07	2.857 (4)	163
O1—H1B···N41	0.80	1.94	2.737 (5)	173
O2—H2A···O11^{ii}	0.82	2.19	2.903 (4)	146
O2—H2B···O14^{iii}	0.82	2.23	2.864 (5)	135
N42—H42A···O22^{i}	0.87	2.35	3.208 (6)	170
N42—H42B···N51^{iv}	0.84	2.15	2.973 (6)	169
N52—H52A···O24	0.87	2.47	3.239 (7)	148

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2305).

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supplementary materials

Acta Cryst. (2007). E**63**, m2263-m2264 [**doi:10.1107/S1600536807037087**]

catena-Poly[[[diaqua(3-nitrobenzoato-κ^2O,O')erbium(III)]-di-μ-3-nitrobenzoato-$\kappa^4O:O'$] 2,2'-diamino-4,4'-bi-1,3-thiazole]

B.-X. Liu, G.-H. Chen and L.-J. Zhang

Comment

As part of our ongoing investigation on metal complexes with diaminobithiazole (DABT) ligand (Wu *et al.*, 2003; Luo *et al.*, 2004; Liu & Xu, 2004), the title Er^{III} complex was recently prepared and its X-ray structure is presented here.

The molecular structure of the title compound is shown in Fig. 1. The Er^{III} has a distorted tetragonal antiprism coordination geometry (Table 1), formed by five 3-nitrobenzoate anions and two water molecules. One 3-nitrobenzoate anion chelates to Er^{III} ion by the carboxyl group, another four 3-nitrobenzoate anions bridge Er^{III} ions to form the polymeric complex chain. The C17-carboxyl group makes a dihedral angle of 28.2 (3)° with the benzene ring. The C2-carboxylate group and C37-carboxyl group make different dihedral angles with the benzene rings, 2.4 (4) and 17.5 (6)°, respectively. The average bond length 2.272 (3) Å of Er—$O_{bridging}$ is shorter than average Er—$O_{chelating}$ bond length of 2.436 (3) Å.

The DABT molecules located on individual inversion centers display a *trans* configuration, which agrees with that found in a uncoordinated DABT (Liu *et al.*, 2003). The DABT molecules linked two neighboring complex to form the supra-molecular chains by N—H···O and O—H···N hydrogen bonding (Fig. 1., Table 2). This bridging feature of DABT molecule agrees with that found in $(C_6H_8N_4S_2)^{2+}\cdot 2(C_6H_7N_4S_2)^{+}\cdot 4(C_7H_4NO_4)^{-}$ reported previously (Liu *et al.*, 2005).

Experimental

An ethanol solution (20 ml) containing diaminobithiazole (DABT) (0.23 g, 1.14 mmol) and $ErCl_3\cdot 6H_2O$ (0.22 g, 0.57 mmol) was mixed with an aqueous solution (10 ml) of 3-nitrobenzoic acid (0.19 g, 1.14 mmol) and NaOH (0.05 g, 1.14 mmol). The mixture was refluxed for 6 h. After cooling to room temperature the solution was filtered. Single crystals of the title compound were obtained from the filtrate after 7 d.

Refinement

Aromatic H atoms were placed in calculated positions with C—H = 0.93 Å and were included in the final cycles of refinement in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms of amino groups and water molecules were located in a difference Fourier map and refined as riding in their as-found relative positions with $U_{iso}(H) = 1.2U_{eq}(N,O)$.

Figures

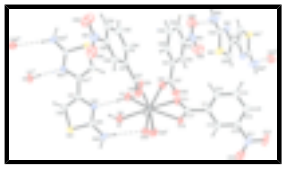

Fig. 1. The molecular structure of the title compound with 30% probability displacement ellipsoids (arbitrary spheres for H atoms), dashed lines showing the hydrogen bonding [symmetry codes: (i) −*x*,1 − *y*,1 − *z*; (ii) 1 − *x*, 1 − *y*, 1 − *z*; (iii) −*x*, 2 − *y*, 1 − *z*; (iv) *x*, 1 + *y*, *z*; (v) −2 − *x*, 1 − *y*, −*z*].

catena-Poly[[[diaqua(3-nitrobenzoato-κ^2*O*,*O*')erbium(III)]-di-μ-3-\ nitrobenzoato-κ^4*O*:*O*'] 2,2'-diamino-4,4'-bi-1,3-thiazole]

Crystal data

$[Er(C_7H_4NO_4)_3(H_2O)_2]\cdot C_6H_6N_4S_2$	$Z = 2$
$M_r = 899.90$	$F_{000} = 890$
Triclinic, $P\overline{1}$	$D_x = 1.814$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
$a = 9.6739$ (7) Å	Cell parameters from 5670 reflections
$b = 12.993$ (1) Å	θ = 2.0–25.0º
$c = 14.5927$ (11) Å	μ = 2.75 mm^{-1}
α = 68.148 (1)º	$T = 295$ (2) K
β = 86.352 (1)º	Prism, red
γ = 75.553 (1)º	0.20 × 0.17 × 0.14 mm
$V = 1647.7$ (2) Å^3	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	5731 independent reflections
Radiation source: fine-focus sealed tube	5127 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 25.0$º
$T = 295$(2) K	$\theta_{min} = 2.1$º
ω scans	$h = -9\rightarrow11$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -12\rightarrow15$
$T_{min} = 0.560$, $T_{max} = 0.680$	$l = -16\rightarrow17$
8623 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H-atom parameters constrained
$wR(F^2) = 0.066$	$w = 1/[\sigma^2(F_o^2) + (0.0253P)^2 + 0.8606P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
5731 reflections	$\Delta\rho_{max} = 0.56$ e Å^{-3}
460 parameters	$\Delta\rho_{min} = -0.73$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Er	0.23836 (2)	0.534282 (16)	0.488335 (14)	0.02794 (7)
O1	0.0653 (3)	0.7073 (2)	0.4698 (2)	0.0404 (8)
H1A	−0.0140	0.6984	0.4654	0.048*
H1B	0.0630	0.7445	0.5034	0.048*
O2	0.3274 (3)	0.6254 (3)	0.5816 (2)	0.0411 (8)
H2A	0.4053	0.5942	0.6099	0.049*
H2B	0.3058	0.6920	0.5776	0.049*
O11	0.3646 (3)	0.4181 (3)	0.3984 (2)	0.0411 (8)
O12	0.2065 (3)	0.3474 (2)	0.5022 (2)	0.0378 (7)
O13	0.3152 (4)	−0.0827 (3)	0.5920 (3)	0.0612 (10)
O14	0.3511 (4)	−0.1456 (3)	0.4731 (3)	0.0708 (12)
O21	0.0899 (3)	0.5813 (3)	0.3549 (2)	0.0439 (8)
O22	−0.1017 (3)	0.5123 (3)	0.3786 (2)	0.0446 (8)
O23	−0.4305 (5)	0.6104 (5)	0.1072 (4)	0.1089 (19)
O24	−0.4168 (5)	0.7462 (4)	−0.0301 (3)	0.1030 (17)
O31	0.3488 (3)	0.6566 (3)	0.3733 (2)	0.0420 (8)
O32	0.5808 (3)	0.5949 (3)	0.4063 (2)	0.0453 (8)
O33	0.7828 (6)	1.0268 (5)	0.1239 (4)	0.124 (2)
O34	0.8555 (5)	0.8901 (5)	0.2628 (4)	0.0907 (15)
N11	0.3339 (4)	−0.0681 (4)	0.5054 (4)	0.0508 (11)
N21	−0.3713 (6)	0.6810 (5)	0.0532 (4)	0.0677 (15)
N31	0.7672 (6)	0.9441 (5)	0.1964 (4)	0.0699 (14)
N41	0.0331 (4)	0.8453 (3)	0.5768 (3)	0.0332 (8)
N42	0.0566 (5)	0.6783 (3)	0.7180 (3)	0.0520 (11)
H42A	0.0793	0.6283	0.6901	0.062*
H42B	0.0619	0.6540	0.7798	0.062*

N51	−0.8833 (4)	0.5964 (3)	−0.0659 (3)	0.0472 (10)
N52	−0.6912 (5)	0.6844 (4)	−0.0938 (4)	0.0840 (17)
H52A	−0.6039	0.6718	−0.0733	0.101*
H52B	−0.7197	0.7411	−0.1494	0.101*
S41	−0.00548 (15)	0.88246 (11)	0.73874 (9)	0.0470 (3)
S51	−0.70468 (15)	0.51627 (13)	0.08145 (11)	0.0623 (4)
C11	0.3284 (5)	0.2406 (4)	0.4055 (3)	0.0366 (11)
C12	0.3083 (4)	0.1363 (4)	0.4694 (4)	0.0368 (11)
H12	0.2738	0.1269	0.5322	0.044*
C13	0.3416 (5)	0.0458 (4)	0.4361 (4)	0.0421 (12)
C14	0.3832 (6)	0.0586 (5)	0.3419 (4)	0.0569 (15)
H14	0.3995	−0.0025	0.3207	0.068*
C15	0.4004 (6)	0.1631 (5)	0.2796 (4)	0.0625 (16)
H15	0.4283	0.1737	0.2152	0.075*
C16	0.3765 (5)	0.2529 (4)	0.3121 (4)	0.0468 (12)
H16	0.3931	0.3225	0.2704	0.056*
C17	0.2972 (5)	0.3413 (4)	0.4373 (3)	0.0359 (11)
C21	−0.0676 (5)	0.6362 (4)	0.2196 (3)	0.0325 (10)
C22	−0.1923 (5)	0.6271 (4)	0.1846 (3)	0.0378 (11)
H22	−0.2463	0.5795	0.2261	0.045*
C23	−0.2346 (6)	0.6900 (4)	0.0871 (4)	0.0494 (13)
C24	−0.1618 (7)	0.7615 (5)	0.0232 (4)	0.0625 (16)
H24	−0.1947	0.8034	−0.0418	0.075*
C25	−0.0383 (7)	0.7705 (5)	0.0570 (4)	0.0637 (16)
H25	0.0150	0.8177	0.0141	0.076*
C26	0.0088 (6)	0.7088 (4)	0.1561 (4)	0.0506 (13)
H26	0.0916	0.7169	0.1788	0.061*
C27	−0.0222 (4)	0.5716 (4)	0.3263 (3)	0.0309 (10)
C31	0.4937 (5)	0.7748 (4)	0.2790 (3)	0.0324 (10)
C32	0.6194 (5)	0.8086 (4)	0.2749 (3)	0.0384 (11)
H32	0.6927	0.7653	0.3219	0.046*
C33	0.6337 (6)	0.9073 (4)	0.2003 (4)	0.0456 (12)
C34	0.5288 (7)	0.9735 (5)	0.1300 (4)	0.0635 (16)
H34	0.5415	1.0401	0.0802	0.076*
C35	0.4040 (7)	0.9397 (5)	0.1343 (4)	0.0663 (17)
H35	0.3314	0.9835	0.0869	0.080*
C36	0.3857 (5)	0.8404 (4)	0.2091 (4)	0.0502 (13)
H36	0.3008	0.8182	0.2121	0.060*
C37	0.4740 (5)	0.6664 (3)	0.3589 (3)	0.0297 (9)
C41	0.0016 (4)	0.9632 (3)	0.5521 (3)	0.0314 (10)
C42	−0.0232 (5)	0.9975 (4)	0.6293 (3)	0.0407 (11)
H42	−0.0468	1.0734	0.6240	0.049*
C43	0.0330 (5)	0.7925 (4)	0.6719 (3)	0.0365 (11)
C51	−0.9334 (5)	0.5121 (4)	0.0086 (3)	0.0415 (11)
C52	−0.8513 (5)	0.4608 (5)	0.0911 (4)	0.0544 (14)
H52	−0.8710	0.4025	0.1468	0.065*
C53	−0.7648 (6)	0.6076 (4)	−0.0381 (4)	0.0516 (13)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Er	0.02554 (11)	0.02397 (11)	0.03386 (12)	−0.00788 (8)	−0.00287 (8)	−0.00838 (8)
O1	0.0322 (17)	0.0376 (18)	0.056 (2)	−0.0026 (14)	−0.0047 (15)	−0.0251 (16)
O2	0.0345 (17)	0.0352 (18)	0.058 (2)	−0.0059 (14)	−0.0066 (15)	−0.0228 (16)
O11	0.0404 (18)	0.0341 (18)	0.054 (2)	−0.0135 (15)	0.0042 (15)	−0.0201 (16)
O12	0.0384 (18)	0.0296 (17)	0.0514 (19)	−0.0152 (14)	0.0035 (15)	−0.0176 (15)
O13	0.051 (2)	0.043 (2)	0.080 (3)	−0.0158 (18)	−0.005 (2)	−0.008 (2)
O14	0.063 (2)	0.034 (2)	0.124 (4)	−0.0105 (18)	−0.001 (2)	−0.039 (2)
O21	0.0432 (19)	0.042 (2)	0.0489 (19)	−0.0117 (15)	−0.0143 (16)	−0.0164 (16)
O22	0.0453 (19)	0.049 (2)	0.0373 (18)	−0.0163 (16)	0.0048 (15)	−0.0105 (16)
O23	0.084 (4)	0.136 (5)	0.108 (4)	−0.049 (3)	−0.039 (3)	−0.025 (4)
O24	0.115 (4)	0.098 (4)	0.077 (3)	0.009 (3)	−0.060 (3)	−0.024 (3)
O31	0.0346 (18)	0.0390 (19)	0.0487 (19)	−0.0168 (15)	0.0032 (15)	−0.0073 (16)
O32	0.0420 (19)	0.0265 (17)	0.056 (2)	−0.0037 (15)	−0.0204 (16)	−0.0017 (15)
O33	0.148 (5)	0.100 (4)	0.128 (4)	−0.095 (4)	0.034 (4)	−0.011 (4)
O34	0.085 (3)	0.102 (4)	0.113 (4)	−0.063 (3)	0.011 (3)	−0.047 (3)
N11	0.030 (2)	0.037 (3)	0.084 (4)	−0.0081 (19)	−0.007 (2)	−0.020 (3)
N21	0.069 (4)	0.068 (4)	0.068 (4)	0.005 (3)	−0.032 (3)	−0.035 (3)
N31	0.087 (4)	0.063 (4)	0.080 (4)	−0.051 (3)	0.023 (3)	−0.032 (3)
N41	0.036 (2)	0.031 (2)	0.033 (2)	−0.0119 (16)	0.0000 (16)	−0.0103 (17)
N42	0.081 (3)	0.031 (2)	0.037 (2)	−0.012 (2)	0.004 (2)	−0.0067 (19)
N51	0.048 (3)	0.043 (2)	0.047 (2)	−0.015 (2)	−0.006 (2)	−0.009 (2)
N52	0.062 (3)	0.083 (4)	0.084 (4)	−0.035 (3)	−0.013 (3)	0.009 (3)
S41	0.0646 (8)	0.0419 (7)	0.0350 (6)	−0.0115 (6)	0.0013 (6)	−0.0157 (6)
S51	0.0514 (8)	0.0658 (10)	0.0603 (9)	−0.0205 (7)	−0.0158 (7)	−0.0058 (7)
C11	0.035 (3)	0.026 (2)	0.046 (3)	−0.0019 (19)	−0.011 (2)	−0.012 (2)
C12	0.030 (2)	0.031 (3)	0.052 (3)	−0.0052 (19)	−0.004 (2)	−0.019 (2)
C13	0.034 (3)	0.028 (3)	0.062 (3)	−0.006 (2)	−0.010 (2)	−0.013 (2)
C14	0.061 (4)	0.048 (3)	0.073 (4)	−0.007 (3)	−0.011 (3)	−0.037 (3)
C15	0.086 (4)	0.056 (4)	0.049 (3)	−0.010 (3)	−0.005 (3)	−0.026 (3)
C16	0.058 (3)	0.034 (3)	0.045 (3)	−0.009 (2)	−0.013 (2)	−0.010 (2)
C17	0.031 (2)	0.029 (2)	0.047 (3)	−0.004 (2)	−0.011 (2)	−0.013 (2)
C21	0.037 (2)	0.028 (2)	0.033 (2)	−0.0051 (19)	0.0001 (19)	−0.013 (2)
C22	0.039 (3)	0.035 (3)	0.039 (3)	−0.005 (2)	−0.004 (2)	−0.016 (2)
C23	0.057 (3)	0.043 (3)	0.045 (3)	−0.001 (3)	−0.018 (3)	−0.016 (3)
C24	0.096 (5)	0.046 (3)	0.035 (3)	−0.007 (3)	−0.012 (3)	−0.008 (3)
C25	0.089 (5)	0.048 (3)	0.046 (3)	−0.025 (3)	0.015 (3)	−0.005 (3)
C26	0.057 (3)	0.043 (3)	0.055 (3)	−0.020 (3)	0.003 (3)	−0.017 (3)
C27	0.029 (2)	0.027 (2)	0.036 (2)	−0.0031 (19)	−0.001 (2)	−0.014 (2)
C31	0.036 (2)	0.025 (2)	0.034 (2)	−0.0071 (19)	−0.0001 (19)	−0.0084 (19)
C32	0.043 (3)	0.030 (3)	0.044 (3)	−0.010 (2)	0.003 (2)	−0.015 (2)
C33	0.061 (3)	0.039 (3)	0.048 (3)	−0.027 (3)	0.016 (3)	−0.020 (2)
C34	0.099 (5)	0.038 (3)	0.047 (3)	−0.027 (3)	0.011 (3)	−0.002 (3)
C35	0.080 (4)	0.049 (3)	0.051 (3)	−0.012 (3)	−0.019 (3)	0.004 (3)
C36	0.046 (3)	0.045 (3)	0.049 (3)	−0.010 (2)	−0.008 (2)	−0.004 (3)

C37	0.035 (3)	0.026 (2)	0.033 (2)	−0.0092 (19)	−0.001 (2)	−0.0144 (19)
C41	0.029 (2)	0.028 (2)	0.038 (2)	−0.0084 (19)	0.0013 (19)	−0.012 (2)
C42	0.050 (3)	0.030 (3)	0.041 (3)	−0.009 (2)	−0.004 (2)	−0.012 (2)
C43	0.040 (3)	0.034 (3)	0.040 (3)	−0.012 (2)	0.001 (2)	−0.017 (2)
C51	0.040 (3)	0.039 (3)	0.041 (3)	−0.008 (2)	−0.002 (2)	−0.009 (2)
C52	0.050 (3)	0.054 (3)	0.052 (3)	−0.018 (3)	−0.004 (3)	−0.008 (3)
C53	0.048 (3)	0.045 (3)	0.054 (3)	−0.014 (3)	−0.003 (3)	−0.008 (3)

Geometric parameters (Å, °)

Er—O1	2.378 (3)	S51—C52	1.721 (5)
Er—O2	2.419 (3)	S51—C53	1.742 (5)
Er—O11	2.417 (3)	C11—C16	1.376 (6)
Er—O12	2.455 (3)	C11—C12	1.382 (6)
Er—O21	2.293 (3)	C11—C17	1.502 (6)
Er—O22^{i}	2.254 (3)	C12—C13	1.392 (6)
Er—O31	2.262 (3)	C12—H12	0.9300
Er—O32^{ii}	2.280 (3)	C13—C14	1.368 (7)
Er—C17	2.791 (4)	C14—C15	1.369 (8)
O1—H1A	0.8137	C14—H14	0.9300
O1—H1B	0.8020	C15—C16	1.378 (7)
O2—H2A	0.8155	C15—H15	0.9300
O2—H2B	0.8188	C16—H16	0.9300
O11—C17	1.265 (5)	C21—C26	1.379 (6)
O12—C17	1.261 (5)	C21—C22	1.387 (6)
O13—N11	1.214 (5)	C21—C27	1.500 (6)
O14—N11	1.235 (5)	C22—C23	1.379 (6)
O21—C27	1.238 (5)	C22—H22	0.9300
O22—C27	1.245 (5)	C23—C24	1.351 (8)
O22—Er^{i}	2.254 (3)	C24—C25	1.368 (8)
O23—N21	1.207 (7)	C24—H24	0.9300
O24—N21	1.227 (6)	C25—C26	1.407 (7)
O31—C37	1.246 (5)	C25—H25	0.9300
O32—C37	1.242 (5)	C26—H26	0.9300
O32—Er^{ii}	2.280 (3)	C31—C36	1.379 (6)
O33—N31	1.229 (6)	C31—C32	1.383 (6)
O34—N31	1.209 (6)	C31—C37	1.504 (6)
N11—C13	1.467 (6)	C32—C33	1.371 (6)
N21—C23	1.487 (7)	C32—H32	0.9300
N31—C33	1.476 (7)	C33—C34	1.364 (7)
N41—C43	1.299 (5)	C34—C35	1.375 (8)
N41—C41	1.392 (5)	C34—H34	0.9300
N42—C43	1.347 (5)	C35—C36	1.387 (7)
N42—H42A	0.8667	C35—H35	0.9300
N42—H42B	0.8371	C36—H36	0.9300
N51—C53	1.299 (6)	C41—C42	1.346 (6)
N51—C51	1.388 (6)	C41—C41^{iii}	1.461 (8)
N52—C53	1.357 (7)	C42—H42	0.9300

N52—H52A	0.8698	C51—C52	1.336 (6)
N52—H52B	0.8715	C51—C51^{iv}	1.457 (9)
S41—C42	1.716 (5)	C52—H52	0.9300
S41—C43	1.744 (4)		
O22^{i}—Er—O31	152.41 (12)	C13—C14—C15	118.6 (5)
O22^{i}—Er—O32^{ii}	84.35 (12)	C13—C14—H14	120.7
O31—Er—O32^{ii}	104.12 (11)	C15—C14—H14	120.7
O22^{i}—Er—O21	105.35 (11)	C14—C15—C16	120.2 (5)
O31—Er—O21	81.29 (11)	C14—C15—H15	119.9
O32^{ii}—Er—O21	148.41 (11)	C16—C15—H15	119.9
O22^{i}—Er—O1	75.53 (11)	C11—C16—C15	120.8 (5)
O31—Er—O1	81.78 (11)	C11—C16—H16	119.6
O32^{ii}—Er—O1	140.33 (11)	C15—C16—H16	119.6
O21—Er—O1	70.92 (10)	O12—C17—O11	121.3 (4)
O22^{i}—Er—O11	129.54 (11)	O12—C17—C11	120.1 (4)
O31—Er—O11	77.98 (11)	O11—C17—C11	118.6 (4)
O32^{ii}—Er—O11	75.16 (11)	O12—C17—Er	61.6 (2)
O21—Er—O11	75.68 (11)	O11—C17—Er	59.8 (2)
O1—Er—O11	143.06 (10)	C11—C17—Er	177.6 (3)
O22^{i}—Er—O2	81.49 (11)	C26—C21—C22	118.9 (4)
O31—Er—O2	76.92 (11)	C26—C21—C27	121.4 (4)
O32^{ii}—Er—O2	70.61 (10)	C22—C21—C27	119.6 (4)
O21—Er—O2	139.80 (11)	C23—C22—C21	118.7 (5)
O1—Er—O2	72.82 (10)	C23—C22—H22	120.6
O11—Er—O2	130.44 (10)	C21—C22—H22	120.6
O22^{i}—Er—O12	76.80 (11)	C24—C23—C22	123.6 (5)
O31—Er—O12	130.58 (11)	C24—C23—N21	119.2 (5)
O32^{ii}—Er—O12	75.58 (10)	C22—C23—N21	117.1 (5)
O21—Er—O12	77.55 (10)	C23—C24—C25	118.0 (5)
O1—Er—O12	130.06 (10)	C23—C24—H24	121.0
O11—Er—O12	53.73 (10)	C25—C24—H24	121.0
O2—Er—O12	141.23 (10)	C24—C25—C26	120.5 (5)
O22^{i}—Er—C17	103.32 (13)	C24—C25—H25	119.7
O31—Er—C17	104.25 (13)	C26—C25—H25	119.7
O32^{ii}—Er—C17	74.21 (12)	C21—C26—C25	120.2 (5)
O21—Er—C17	74.30 (11)	C21—C26—H26	119.9
O1—Er—C17	143.33 (11)	C25—C26—H26	119.9
O11—Er—C17	26.90 (12)	O21—C27—O22	125.5 (4)
O2—Er—C17	143.84 (11)	O21—C27—C21	117.9 (4)
O12—Er—C17	26.84 (11)	O22—C27—C21	116.6 (4)
Er—O1—H1A	109.2	C36—C31—C32	119.9 (4)
Er—O1—H1B	124.7	C36—C31—C37	119.6 (4)
H1A—O1—H1B	109.5	C32—C31—C37	120.5 (4)
Er—O2—H2A	118.2	C33—C32—C31	118.7 (4)
Er—O2—H2B	130.3	C33—C32—H32	120.7

H2A—O2—H2B	108.8	C31—C32—H32	120.7
C17—O11—Er	93.3 (3)	C34—C33—C32	122.6 (5)
C17—O12—Er	91.6 (3)	C34—C33—N31	118.7 (5)
C27—O21—Er	145.7 (3)	C32—C33—N31	118.7 (5)
C27—O22—Er^{i}	150.7 (3)	C33—C34—C35	118.6 (5)
C37—O31—Er	135.7 (3)	C33—C34—H34	120.7
C37—O32—Er^{ii}	172.3 (3)	C35—C34—H34	120.7
O13—N11—O14	123.1 (5)	C34—C35—C36	120.3 (5)
O13—N11—C13	118.8 (4)	C34—C35—H35	119.8
O14—N11—C13	118.0 (5)	C36—C35—H35	119.8
O23—N21—O24	123.5 (6)	C31—C36—C35	119.9 (5)
O23—N21—C23	119.4 (5)	C31—C36—H36	120.0
O24—N21—C23	117.1 (6)	C35—C36—H36	120.0
O34—N31—O33	124.0 (6)	O32—C37—O31	124.9 (4)
O34—N31—C33	118.6 (5)	O32—C37—C31	118.8 (4)
O33—N31—C33	117.4 (6)	O31—C37—C31	116.3 (4)
C43—N41—C41	110.9 (4)	C42—C41—N41	114.9 (4)
C43—N42—H42A	126.1	C42—C41—C41^{iii}	126.5 (5)
C43—N42—H42B	115.7	N41—C41—C41^{iii}	118.6 (5)
H42A—N42—H42B	117.5	C41—C42—S41	111.0 (3)
C53—N51—C51	110.9 (4)	C41—C42—H42	124.5
C53—N52—H52A	115.5	S41—C42—H42	124.5
C53—N52—H52B	127.2	N41—C43—N42	124.7 (4)
H52A—N52—H52B	117.2	N41—C43—S41	114.4 (3)
C42—S41—C43	88.8 (2)	N42—C43—S41	120.9 (3)
C52—S51—C53	88.2 (2)	C52—C51—N51	114.7 (4)
C16—C11—C12	120.1 (4)	C52—C51—C51^{iv}	126.3 (6)
C16—C11—C17	119.6 (4)	N51—C51—C51^{iv}	119.0 (5)
C12—C11—C17	120.3 (4)	C51—C52—S51	111.5 (4)
C11—C12—C13	117.5 (4)	C51—C52—H52	124.2
C11—C12—H12	121.3	S51—C52—H52	124.2
C13—C12—H12	121.3	N51—C53—N52	124.9 (5)
C14—C13—C12	122.7 (5)	N51—C53—S51	114.6 (4)
C14—C13—N11	118.8 (5)	N52—C53—S51	120.4 (4)
C12—C13—N11	118.5 (5)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···O12^{i}	0.81	2.07	2.857 (4)	163
O1—H1B···N41	0.80	1.94	2.737 (5)	173
O2—H2A···O11^{ii}	0.82	2.19	2.903 (4)	146
O2—H2B···O14^{v}	0.82	2.23	2.864 (5)	135
N42—H42A···O22^{i}	0.87	2.35	3.208 (6)	170
N42—H42B···N51^{vi}	0.84	2.15	2.973 (6)	169
N52—H52A···O24	0.87	2.47	3.239 (7)	148

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

Fig. 1