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Poly[[aqua-μ_3-picolinato-μ_2-picolinato-dipicolinatopotassium(I)terbium(III)] 2.5-hydrate]

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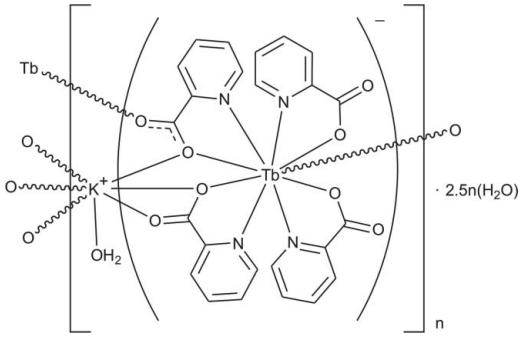
Key indicators: single-crystal X-ray study; T = 180 K; mean σ(C–C) = 0.007 Å; R factor = 0.033; wR factor = 0.095; data-to-parameter ratio = 13.3.

In the title compound, $[KTb(C_6H_4NO_2)_4(H_2O)]\cdot 2.5H_2O$, each Tb^{3+} centre is coordinated by four N and five O atoms from five distinct picolinate ligands in a geometry resembling a highly distorted tricapped trigonal prism. One of the ligands establishes a skew bridge between neighbouring Tb^{3+} centres, leading to the formation of one-dimensional anionic polymeric chains, $\{[(C_6H_4NO_2)_4Tb]^-\}_n$, running along the direction [010]. Each K^+ cation is seven-coordinated by six O atoms from one anionic polymeric chain and one water molecule [K···O 2.676 (3)–3.208 (4) Å]. The uncoordinated water molecules are involved in O—H···O hydrogen bonding.

Related literature

For recent research on metal–organic frameworks (MOFs) or coordination polymers from our research group, see: Shi *et al.* (2008); Cunha-Silva *et al.* (2007); Paz & Klinowski (2007); Soares-Santos *et al.* (2006); Paz *et al.* (2005). For relevant examples of discrete complexes or MOFs incorporating lanthanide centres and pyridine–carboxylic acid derivative ligands, see: Sendor *et al.* (2003); Jian-Fang *et al.* (1996); Starynowicz (1993).



Experimental

Crystal data

$[KTb(C_6H_4NO_2)_4(H_2O)]\cdot 2.5H_2O$
M_r = 749.49
Hexagonal, $P6_522$
a = 12.7187 (2) Å
c = 62.2321 (9) Å
V = 8718.3 (2) Å^3
Z = 12
Mo $K\alpha$ radiation
μ = 2.64 mm^{-1}
T = 180 (2) K
0.39 × 0.28 × 0.23 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.426, T_{max} = 0.582
(expected range = 0.398–0.545)
31023 measured reflections
5031 independent reflections
4488 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.094
S = 1.14
5031 reflections
377 parameters
14 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.00 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}
Absolute structure: Flack (1983), 1938 Friedel pairs
Flack parameter: −0.020 (15)

Table 1
Selected bond lengths (Å).

Tb1—O1	2.380 (2)	Tb1—N4	2.626 (3)
Tb1—O3	2.354 (2)	K1—O1	2.676 (3)
Tb1—O5	2.333 (2)	K1—O2	3.208 (4)
Tb1—O7^{i}	2.352 (3)	K1—O3	2.972 (2)
Tb1—O8	2.385 (3)	K1—O5^{i}	2.725 (3)
Tb1—N1	2.640 (3)	K1—O6^{i}	2.985 (4)
Tb1—N2	2.575 (3)	K1—O8^{i}	2.959 (2)
Tb1—N3	2.736 (4)	K1—O3*W*	2.661 (5)

Symmetry code: (i) $x-y, -y+1, -z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O4	0.84	2.09	2.858 (4)	152
O2*W*—H2*W*···O6^{ii}	0.85	2.48	3.219 (5)	146
O3*W*—H3*WA*···O6^{iii}	0.86	2.09	2.647 (5)	121
O4*W*—H4*WB*···O2^{iv}	0.86	1.92	2.711 (6)	152
O5*W*—H5*W*···O4*W*	0.85	2.34	3.080 (13)	145

Symmetry codes: (ii) $x-y+1, -y+1, -z$; (iii) $y-1, -x+y, z+\frac{1}{6}$; (iv) $x+1, y, z$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2369).

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supporting information

Acta Cryst. (2008). E**64**, m529–m530 [doi:10.1107/S1600536808005758]

Poly[[aqua-μ_3-picolinato-μ_2-picolinato-dipicolinatopotassium(I)terbium(III)] 2.5-hydrate]

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S1. Comment

In the last years research on multidimensional Metal-Organic Frameworks (MOFs), or coordination polymers, has received a remarkable interest as consequence of the their fascinating structural architectures which, in many cases, are also associated with interesting potential applications (*e.g.*, gas storage, separation, catalysis, guest exchange, magnetic or optical sensors). Following our ongoing research focused on the preparation and structural characterization of these interesting compounds (for recent examples see: Shi *et al.*, 2008; Cunha-Silva *et al.*, 2007; Paz & Klinowski, 2007; Soares-Santos *et al.*, 2006; Paz *et al.*, 2005), we report in this short communication the crystalline structure of the title compound, $K_2[Tb_2(pic)_6(\mu\text{-pic})_2].7(H_2O)$ [where pic^- stands for the picolinate anion, $C_6H_4NO_2^-$].

The crystalline structure of the title compound contains a single crystallographically independent Tb^{3+}site, Tb1, which is coordinated to four *N* and five *O*-donor atoms belonging to five distinct picolinate anionic (pic^-) ligands, with a nine-coordination sphere $\{TbN_4O_5\}$ resembling a highly distorted tricapped trigonal prism (Figure 1). The Tb—O and Tb—N bond distances are found in the 2.333 (2)–2.385 (3) Å and 2.575 (3)–2.736 (4) Å, respectively. The O—Tb—O, O—Tb—N and N—Tb—N angles are ranging from 68.75 (9) to 142.62 (9)°, 62.59 (10) to 142.63 (9)° and 69.62 (10) to 150.65 (10)°, respectively (see Figure 1 and Table 1).

As usually found in related compounds (see for example: Soares-Santos *et al.*, 2006; Sendor *et al.*, 2003; Starynowicz, 1993; Jian-Fang *et al.*, 1996), all pic^- ligands are coordinated to the Tb^{3+} metal centre *via* the typical *N*,*O*-chelation mode (Figure 1). Furthermore, one pic^- establishes a *skew*-bridge (through the O7 atom; Figure 1) with a neighbouring Tb^{3+}, thus completing the nine-coordination environment of the lanthanide centre and leading to the formation of the one-dimensional (one-dimensional) anionic coordination polymer (chain), $[Tb_2(pic)_6(\mu\text{-pic})_2]_n^{2n-}$, running along the [010] direction (Figure 2). The *skew*-bridge is also responsible for the zigzag distribution of the Tb^{3+}centres along the aforementioned crystallographic direction, imposing an intermetallic Tb1···$Tb1^i$ distance of 6.4375 (4) Å [symmetry code: (i) *1 + x*-*y*, *1 - y*, -*z*]. Adjacent polymers close pack along the [001] direction of the unit cell with an arrangement resembling a layered-like structure. The water molecules of crystallization and the potassion cations are housed in the interchain empty spaces (Figure 2c with the K^+ cations being omitted for clarity).

S2. Experimental

Starting materials were purchased from commercial sources and were used as received without further purification. The title compound has been prepared by adding an aqueous solution (5 ml) of $TbCl_3.6H_2O$ (1 mmol, 373 mg) to a solution of picolinic acid (Hpic, 4 mmol, 492 mg) and KOH (4 mmol, 220 mg) in distilled water (20 ml, pH = 6.8). After stirring the mixture for 1 h, an aqueous solution (5 ml) of tetrabutylammonium chloride hydrate ($^nBu_4NCl.nH_2O$, 4 mmol, 1.12 g)

was added drop wise. The resulting mixture was heated and the formed white precipitate was collected by vacuum filtering. Colourless crystals suitable for single-crystal X-ray analysis were obtained from the mother solution after three days.

S3. Refinement

Hydrogen atoms attached to carbon were located at their idealized positions and were included in the refinement in riding-motion approximation with isotropic displacement parameters fixed at 1.2 times U_{eq} of the carbon atom to which they are attached. The five crystallographically unique water molecules of crystallization were directly located from difference Fourier maps and refined successfully using anisotropic displacement parameters. All H atoms associated with the water molecules were geometrically positioned (and not refined) with O—H distances in the range 0.85–0.89 Å and U_{iso} fixed at 1.5 times U_{eq} of the oxygen atom to which they are attached.

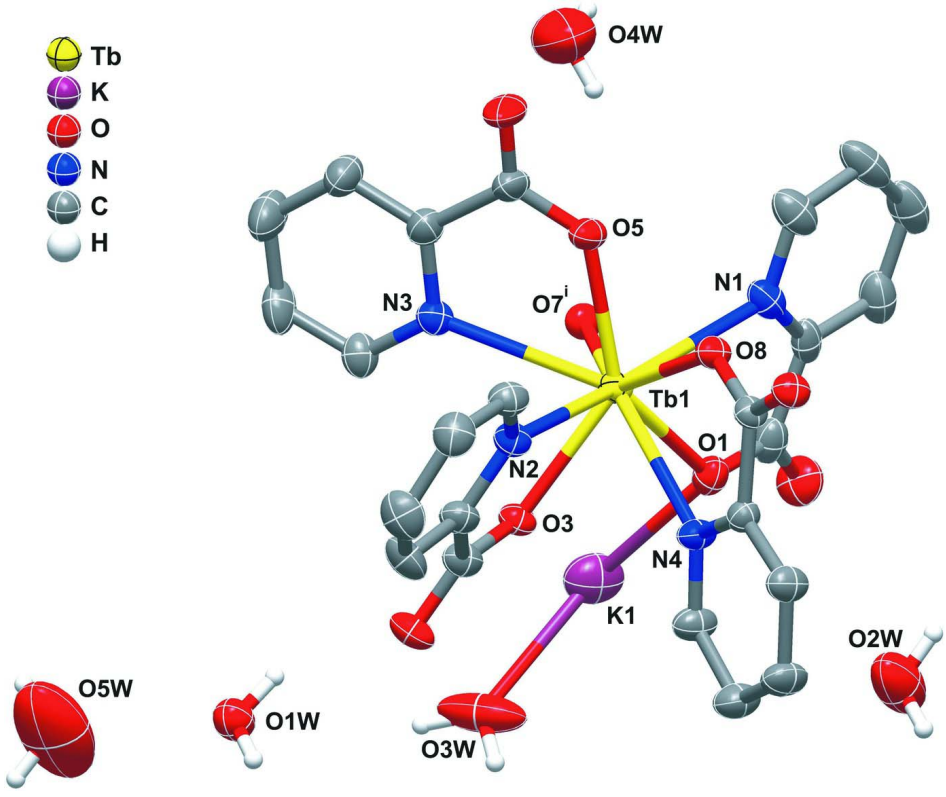

Figure 1

Schematic representation of a fragment of the title compound, emphasizing the coordination environment of the crystallographically unique Tb centre, showing the labelling scheme for all atoms composing the first coordination sphere. Displacement ellipsoids are drawn at the 30% probability level and H atoms associated with the water molecules are represented as spheres with arbitrary radii. All H-atoms bound to carbon were omitted for clarity. Symmetry code used to generate equivalent atoms (represented in the ball-and-stick mode): (i) *x*, *1 + y*, *z*.

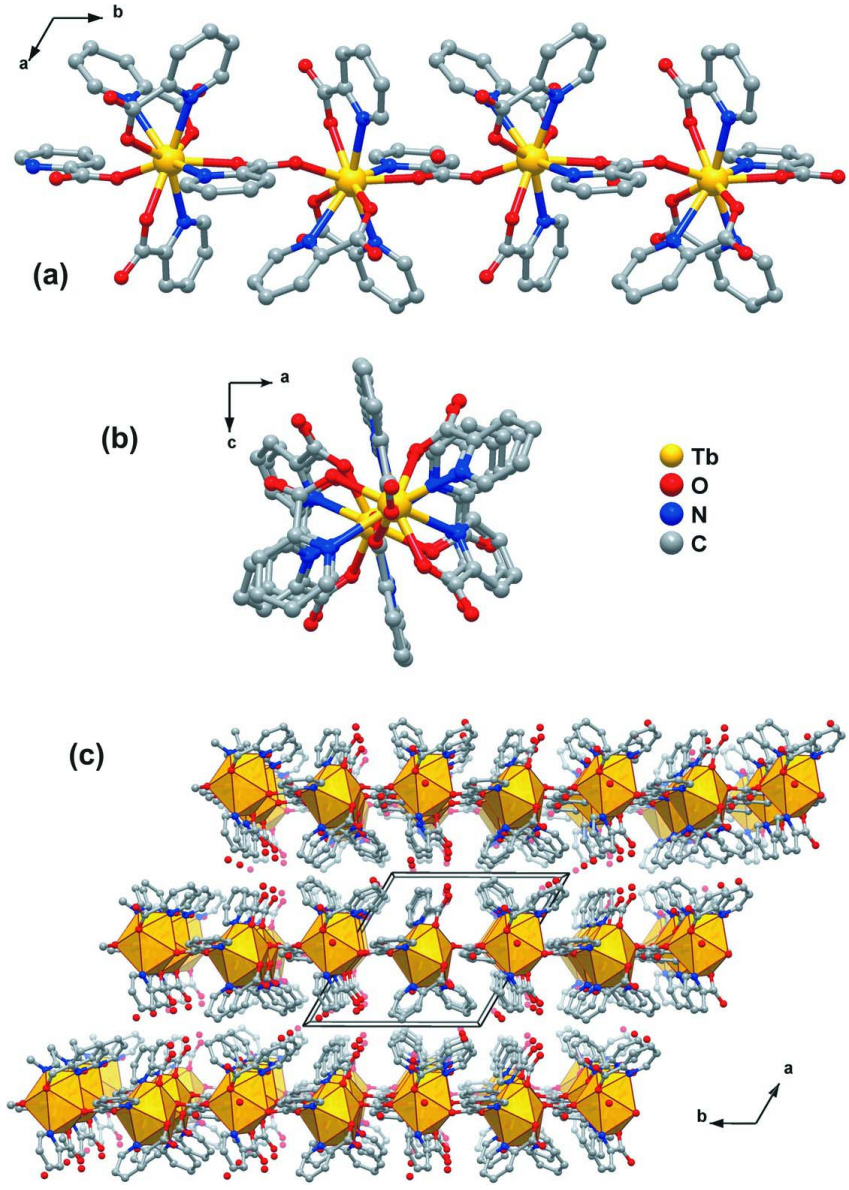

Figure 2

Perspective views of the one-dimensional anionic $[Tb_2(pic)_6(\mu\text{-pic})_2]_n^{2n-}$ coordination polymer viewed along the ***(a)*** [010] and ***(b)*** [001] directions of the unit cell. ***(c)*** Crystal packing of the title compound viewed in perspective along the [010] direction of the unit cell (K^+ cations and H-atoms were omitted for clarity).

Poly[[aqua-μ_3-picolinato-μ_2-picolinato- dipicolinatopotassium(I)terbium(III)] 2.5-hydrate]

Crystal data

$[KTb(C_6H_4NO_2)_4(H_2O)]\cdot 2.5H_2O$
M_r = 1498.97
Hexagonal, $P6_522$
Hall symbol: P 65 2 (0 0 1)
a = 12.7187 (2) Å
c = 62.2321 (9) Å
V = 8718.3 (2) Å^3
Z = 12
$F(000)$ = 4452
D_x = 1.713 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 28400 reflections
θ = 1.0–25.0°
μ = 2.64 mm^{-1}

T = 180 K
Block, colourless

0.39 × 0.28 × 0.23 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Thin slice ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.426, T_{max} = 0.582
31023 measured reflections

5031 independent reflections
4488 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 25.0°, θ_{min} = 3.6°
h = −14→15
k = −15→14
l = −67→73

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.094
S = 1.14
5031 reflections
377 parameters
14 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
$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 2.1846P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 1.00 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}
Absolute structure: Flack (1983)
Absolute structure parameter: −0.020 (15)

Special details

Experimental. Please see the details in the main paper

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}
Tb1	0.078634 (13)	0.533458 (14)	0.005432 (2)	0.03612 (4)
K1	−0.23692 (8)	0.38564 (10)	0.040543 (15)	0.0593 (3)
O1	−0.0725 (2)	0.3470 (2)	0.02072 (4)	0.0505 (7)
O2	−0.2334 (3)	0.1630 (3)	0.01703 (6)	0.0757 (11)
O3	0.00810 (19)	0.6012 (2)	0.03429 (4)	0.0404 (6)
O4	0.0360 (2)	0.7288 (3)	0.06104 (4)	0.0560 (8)
O5	0.1777 (2)	0.6215 (2)	−0.02676 (4)	0.0507 (7)
O6	0.2602 (3)	0.7599 (3)	−0.05195 (5)	0.0925 (10)
O7	0.4239 (2)	0.5234 (2)	0.01432 (4)	0.0454 (7)
O8	0.2598 (2)	0.5230 (2)	0.00168 (4)	0.0413 (6)
N1	0.0152 (3)	0.3362 (3)	−0.01757 (5)	0.0512 (9)
N2	0.2430 (2)	0.7330 (3)	0.02245 (5)	0.0428 (8)

N3	0.0606 (3)	0.7255 (3)	−0.00984 (5)	0.0445 (8)
N4	0.1596 (2)	0.4834 (3)	0.04055 (5)	0.0423 (8)
C1	−0.1366 (4)	0.2477 (4)	0.01065 (7)	0.0565 (12)
C2	−0.0837 (3)	0.2389 (3)	−0.01096 (7)	0.0514 (10)
C3	−0.1393 (4)	0.1320 (4)	−0.02296 (9)	0.0729 (14)
H3	−0.2113	0.0629	−0.0180	0.087*
C4	−0.0875 (4)	0.1287 (5)	−0.04229 (8)	0.0797 (15)
H4	−0.1221	0.0570	−0.0507	0.096*
C5	0.0153 (4)	0.2318 (5)	−0.04897 (8)	0.0765 (15)
H5	0.0527	0.2326	−0.0622	0.092*
C6	0.0631 (4)	0.3330 (4)	−0.03634 (7)	0.0663 (13)
H6	0.1336	0.4042	−0.0412	0.080*
C7	0.0742 (3)	0.6955 (4)	0.04553 (6)	0.0476 (10)
C8	0.2077 (3)	0.7708 (4)	0.03953 (6)	0.0472 (10)
C9	0.2864 (4)	0.8706 (4)	0.05138 (7)	0.0605 (13)
H9	0.2593	0.8927	0.0639	0.073*
C10	0.4059 (4)	0.9384 (4)	0.04475 (8)	0.0684 (15)
H10	0.4620	1.0087	0.0525	0.082*
C11	0.4415 (4)	0.9027 (4)	0.02702 (8)	0.0592 (13)
H11	0.5228	0.9482	0.0220	0.071*
C12	0.3585 (3)	0.7999 (4)	0.01633 (7)	0.0489 (11)
H12	0.3847	0.7752	0.0040	0.059*
C13	0.1919 (4)	0.7149 (4)	−0.03693 (6)	0.0528 (11)
C14	0.1186 (3)	0.7695 (3)	−0.02886 (7)	0.0500 (11)
C15	0.1069 (4)	0.8548 (4)	−0.04020 (8)	0.0673 (13)
H15	0.1495	0.8849	−0.0533	0.081*
C16	0.0336 (4)	0.8974 (5)	−0.03266 (9)	0.0832 (16)
H16	0.0237	0.9560	−0.0405	0.100*
C17	−0.0243 (4)	0.8527 (4)	−0.01355 (10)	0.0710 (15)
H17	−0.0758	0.8802	−0.0079	0.085*
C18	−0.0092 (3)	0.7700 (4)	−0.00260 (8)	0.0546 (12)
H18	−0.0495	0.7418	0.0108	0.066*
C19	0.3216 (3)	0.5129 (3)	0.01674 (6)	0.0361 (9)
C20	0.2693 (3)	0.4904 (3)	0.03900 (6)	0.0379 (9)
C21	0.3275 (3)	0.4709 (4)	0.05577 (6)	0.0529 (10)
H21	0.4045	0.4771	0.0538	0.063*
C22	0.2705 (4)	0.4417 (5)	0.07585 (7)	0.0629 (13)
H22	0.3083	0.4275	0.0878	0.075*
C23	0.1574 (4)	0.4335 (4)	0.07812 (7)	0.0610 (13)
H23	0.1165	0.4145	0.0916	0.073*
C24	0.1061 (3)	0.4547 (4)	0.05951 (6)	0.0539 (11)
H24	0.0285	0.4478	0.0608	0.065*
O1W	0.06278 (19)	0.93722 (19)	0.0833	0.0632 (11)
H1W	0.0617	0.8930	0.0732	0.095*
O2W	0.5413 (3)	0.4587 (3)	0.0833	0.134 (2)
H2W	0.5540	0.4285	0.0722	0.200*
O3W	−0.1780 (4)	0.5373 (5)	0.07365 (6)	0.145 (3)
H3WA	−0.1443	0.5384	0.0857	0.218*

H3WB	−0.2010	0.5906	0.0761	0.218*
O4W	0.7402 (6)	0.1052 (5)	0.05936 (7)	0.188 (4)
H4WA	0.7373	0.1610	0.0670	0.282*
H4WB	0.7729	0.1408	0.0475	0.282*
O5W	0.9314 (6)	0.0686 (6)	0.0833	0.262 (6)
H5W	0.9021	0.0847	0.0723	0.393*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Tb1	0.03522 (7)	0.04700 (8)	0.03202 (8)	0.02495 (6)	0.00027 (6)	−0.00075 (7)
K1	0.0491 (4)	0.0827 (5)	0.0514 (5)	0.0369 (4)	−0.0055 (4)	0.0029 (5)
O1	0.0550 (13)	0.0407 (12)	0.0521 (15)	0.0211 (10)	−0.0067 (13)	0.0005 (11)
O2	0.0649 (18)	0.0485 (16)	0.088 (2)	0.0088 (14)	−0.0043 (18)	−0.0049 (16)
O3	0.0358 (10)	0.0519 (12)	0.0356 (12)	0.0235 (9)	0.0025 (10)	−0.0050 (10)
O4	0.0474 (13)	0.0689 (15)	0.0482 (15)	0.0264 (11)	0.0052 (12)	−0.0175 (12)
O5	0.0628 (12)	0.0699 (13)	0.0379 (13)	0.0471 (10)	0.0083 (11)	0.0070 (11)
O6	0.154 (2)	0.1116 (19)	0.0538 (17)	0.0975 (16)	0.0544 (17)	0.0407 (14)
O7	0.0386 (10)	0.0549 (13)	0.0459 (14)	0.0257 (9)	0.0029 (10)	−0.0006 (11)
O8	0.0426 (9)	0.0566 (12)	0.0356 (12)	0.0330 (9)	0.0007 (10)	0.0010 (10)
N1	0.0494 (14)	0.0641 (16)	0.0513 (18)	0.0368 (12)	−0.0120 (14)	−0.0162 (15)
N2	0.0384 (13)	0.0492 (15)	0.0416 (16)	0.0226 (11)	0.0020 (13)	−0.0011 (13)
N3	0.0409 (13)	0.0536 (14)	0.0439 (16)	0.0271 (12)	0.0000 (13)	−0.0008 (13)
N4	0.0395 (12)	0.0607 (16)	0.0319 (14)	0.0290 (11)	0.0025 (12)	0.0060 (13)
C1	0.0606 (19)	0.0488 (18)	0.066 (3)	0.0320 (16)	−0.021 (2)	−0.0019 (19)
C2	0.0586 (17)	0.0459 (16)	0.063 (2)	0.0366 (13)	−0.0211 (18)	−0.0112 (16)
C3	0.082 (2)	0.058 (2)	0.088 (3)	0.0421 (18)	−0.028 (2)	−0.021 (2)
C4	0.090 (3)	0.085 (3)	0.082 (3)	0.057 (2)	−0.039 (2)	−0.043 (2)
C5	0.069 (2)	0.111 (3)	0.067 (3)	0.058 (2)	−0.023 (2)	−0.045 (2)
C6	0.0546 (19)	0.084 (2)	0.071 (3)	0.0421 (18)	−0.011 (2)	−0.025 (2)
C7	0.0425 (16)	0.066 (2)	0.042 (2)	0.0323 (14)	−0.0012 (16)	−0.0020 (17)
C8	0.0493 (18)	0.0567 (19)	0.0365 (19)	0.0271 (15)	−0.0025 (16)	−0.0033 (16)
C9	0.058 (2)	0.062 (2)	0.062 (3)	0.0294 (17)	−0.006 (2)	−0.0259 (19)
C10	0.050 (2)	0.058 (2)	0.085 (3)	0.0187 (19)	−0.011 (2)	−0.019 (2)
C11	0.0401 (18)	0.055 (2)	0.074 (3)	0.0179 (16)	0.006 (2)	0.005 (2)
C12	0.0437 (17)	0.060 (2)	0.044 (2)	0.0267 (15)	0.0059 (17)	0.0056 (18)
C13	0.069 (2)	0.067 (2)	0.037 (2)	0.0454 (16)	0.0036 (17)	0.0095 (17)
C14	0.0554 (19)	0.053 (2)	0.046 (2)	0.0308 (15)	−0.0032 (17)	0.0009 (17)
C15	0.083 (2)	0.068 (2)	0.066 (3)	0.0491 (18)	0.013 (2)	0.019 (2)
C16	0.093 (2)	0.087 (2)	0.099 (4)	0.067 (2)	0.026 (3)	0.032 (3)
C17	0.061 (2)	0.056 (2)	0.110 (4)	0.0400 (16)	0.015 (2)	0.005 (2)
C18	0.0450 (17)	0.0511 (19)	0.071 (3)	0.0263 (15)	−0.001 (2)	−0.0019 (19)
C19	0.0285 (14)	0.0402 (16)	0.0403 (19)	0.0178 (12)	0.0058 (14)	0.0015 (14)
C20	0.0377 (15)	0.0406 (16)	0.0370 (18)	0.0209 (12)	0.0009 (14)	0.0014 (14)
C21	0.0492 (16)	0.077 (2)	0.045 (2)	0.0410 (15)	0.0004 (16)	0.0020 (19)
C22	0.070 (2)	0.093 (3)	0.038 (2)	0.0504 (19)	−0.0038 (18)	0.008 (2)
C23	0.059 (2)	0.082 (3)	0.044 (2)	0.0368 (19)	0.0064 (18)	0.0116 (19)
C24	0.0479 (17)	0.078 (2)	0.043 (2)	0.0369 (16)	0.0033 (16)	0.0074 (18)

O1W	0.0694 (12)	0.0694 (12)	0.059 (2)	0.0408 (16)	−0.008 (2)	−0.008 (2)
O2W	0.171 (2)	0.171 (2)	0.121 (5)	0.133 (3)	−0.048 (4)	−0.048 (4)
O3W	0.102 (3)	0.166 (5)	0.055 (2)	−0.018 (3)	0.010 (2)	−0.023 (3)
O4W	0.199 (6)	0.164 (6)	0.119 (4)	0.029 (5)	−0.018 (5)	0.028 (4)
O5W	0.281 (6)	0.281 (6)	0.282 (12)	0.184 (8)	−0.151 (8)	−0.151 (8)

Geometric parameters (Å, º)

Tb1—O1	2.380 (2)	C3—H3	0.9500
Tb1—O3	2.354 (2)	C4—C5	1.373 (7)
Tb1—O5	2.333 (2)	C4—H4	0.9500
Tb1—O7^{i}	2.352 (3)	C5—C6	1.365 (7)
Tb1—O8	2.385 (3)	C5—H5	0.9500
Tb1—N1	2.640 (3)	C6—H6	0.9500
Tb1—N2	2.575 (3)	C7—C8	1.520 (5)
Tb1—N3	2.736 (4)	C8—C9	1.374 (5)
Tb1—N4	2.626 (3)	C9—C10	1.383 (6)
K1—O1	2.676 (3)	C9—H9	0.9500
K1—O2	3.208 (4)	C10—C11	1.354 (7)
K1—O3	2.972 (2)	C10—H10	0.9500
K1—O5^{i}	2.725 (3)	C11—C12	1.373 (6)
K1—O6^{i}	2.985 (4)	C11—H11	0.9500
K1—O8^{i}	2.959 (2)	C12—H12	0.9500
K1—O3W	2.661 (5)	C13—C14	1.501 (7)
Tb1—K1	4.1075 (9)	C13—K1^{ii}	3.204 (5)
Tb1—K1^{ii}	4.4471 (10)	C14—C15	1.364 (6)
K1—Tb1^{i}	4.4471 (10)	C15—C16	1.374 (8)
O1—C1	1.274 (5)	C15—H15	0.9500
O2—C1	1.228 (5)	C16—C17	1.364 (8)
O3—C7	1.276 (4)	C16—H16	0.9500
O4—C7	1.246 (5)	C17—C18	1.345 (7)
O5—C13	1.276 (5)	C17—H17	0.9500
O5—K1^{ii}	2.725 (3)	C18—H18	0.9500
O6—C13	1.207 (5)	C19—C20	1.501 (5)
O6—K1^{ii}	2.985 (4)	C20—C21	1.372 (6)
O7—C19	1.248 (4)	C21—C22	1.398 (6)
O7—Tb1^{ii}	2.352 (3)	C21—H21	0.9500
O8—C19	1.271 (4)	C22—C23	1.397 (7)
O8—K1^{ii}	2.959 (2)	C22—H22	0.9500
N1—C2	1.314 (5)	C23—C24	1.420 (6)
N1—C6	1.327 (5)	C23—H23	0.9500
N2—C12	1.333 (5)	C24—H24	0.9500
N2—C8	1.334 (5)	O1W—H1W	0.8423
N3—C18	1.347 (6)	O2W—H2W	0.8472
N3—C14	1.358 (5)	O3W—H3WA	0.8616
N4—C24	1.319 (5)	O3W—H3WB	0.8749
N4—C20	1.356 (5)	O4W—H4WA	0.8712
C1—C2	1.532 (6)	O4W—H4WB	0.8598

C2—C3	1.394 (6)	O5W—H5W	0.8517
C3—C4	1.383 (7)		

O5—Tb1—O7^{i}	84.54 (9)	C1—O1—Tb1	126.1 (3)
O5—Tb1—O3	133.84 (9)	C1—O1—K1	103.8 (3)
O7^{i}—Tb1—O3	91.51 (8)	Tb1—O1—K1	108.51 (11)
O5—Tb1—O1	142.62 (9)	C1—O2—K1	79.9 (3)
O7^{i}—Tb1—O1	74.24 (9)	C7—O3—Tb1	124.7 (2)
O3—Tb1—O1	78.10 (9)	C7—O3—K1	133.6 (2)
O5—Tb1—O8	68.75 (9)	Tb1—O3—K1	100.26 (8)
O7^{i}—Tb1—O8	137.81 (8)	C13—O5—Tb1	131.6 (3)
O3—Tb1—O8	130.58 (8)	C13—O5—K1^{ii}	100.0 (2)
O1—Tb1—O8	107.77 (9)	Tb1—O5—K1^{ii}	122.89 (12)
O5—Tb1—N2	84.42 (9)	C13—O6—K1^{ii}	89.2 (3)
O7^{i}—Tb1—N2	134.49 (10)	C19—O7—Tb1^{ii}	147.0 (2)
O3—Tb1—N2	66.16 (8)	C19—O8—Tb1	126.7 (2)
O1—Tb1—N2	132.14 (9)	C19—O8—K1^{ii}	118.6 (2)
O8—Tb1—N2	76.37 (9)	Tb1—O8—K1^{ii}	112.22 (9)
O5—Tb1—N4	130.37 (9)	C2—N1—C6	119.0 (4)
O7^{i}—Tb1—N4	142.63 (9)	C2—N1—Tb1	114.8 (3)
O3—Tb1—N4	73.81 (10)	C6—N1—Tb1	125.4 (3)
O1—Tb1—N4	69.22 (9)	C12—N2—C8	117.4 (3)
O8—Tb1—N4	63.97 (9)	C12—N2—Tb1	127.1 (3)
N2—Tb1—N4	70.92 (10)	C8—N2—Tb1	115.4 (2)
O5—Tb1—N1	79.95 (10)	C18—N3—C14	117.1 (4)
O7^{i}—Tb1—N1	68.57 (9)	C18—N3—Tb1	128.8 (3)
O3—Tb1—N1	140.33 (8)	C14—N3—Tb1	113.5 (3)
O1—Tb1—N1	63.84 (10)	C24—N4—C20	116.9 (3)
O8—Tb1—N1	74.85 (9)	C24—N4—Tb1	126.9 (3)
N2—Tb1—N1	150.65 (10)	C20—N4—Tb1	116.1 (2)
N4—Tb1—N1	101.03 (11)	O2—C1—O1	125.0 (4)
O5—Tb1—N3	62.59 (10)	O2—C1—C2	120.2 (4)
O7^{i}—Tb1—N3	66.11 (8)	O1—C1—C2	114.7 (3)
O3—Tb1—N3	73.80 (9)	O2—C1—K1	78.1 (3)
O1—Tb1—N3	129.94 (10)	O1—C1—K1	53.7 (2)
O8—Tb1—N3	122.04 (8)	C2—C1—K1	148.5 (3)
N2—Tb1—N3	69.62 (10)	N1—C2—C3	122.1 (4)
N4—Tb1—N3	136.35 (9)	N1—C2—C1	117.0 (3)
N1—Tb1—N3	122.56 (10)	C3—C2—C1	120.9 (4)
O5—Tb1—K1	147.78 (7)	C4—C3—C2	118.6 (4)
O7^{i}—Tb1—K1	64.31 (7)	C4—C3—H3	120.7
O3—Tb1—K1	45.40 (5)	C2—C3—H3	120.7
O1—Tb1—K1	38.16 (8)	C5—C4—C3	118.4 (4)
O8—Tb1—K1	140.97 (6)	C5—C4—H4	120.8
N2—Tb1—K1	111.00 (7)	C3—C4—H4	120.8
N4—Tb1—K1	81.85 (6)	C6—C5—C4	119.2 (5)
N1—Tb1—K1	95.11 (7)	C6—C5—H5	120.4
N3—Tb1—K1	95.42 (6)	C4—C5—H5	120.4

O5—Tb1—K1^{ii}	30.97 (7)	N1—C6—C5	122.7 (4)
O7^{i}—Tb1—K1^{ii}	108.39 (7)	N1—C6—H6	118.6
O3—Tb1—K1^{ii}	147.55 (5)	C5—C6—H6	118.6
O1—Tb1—K1^{ii}	131.21 (7)	O4—C7—O3	123.9 (3)
O8—Tb1—K1^{ii}	38.02 (6)	O4—C7—C8	118.6 (3)
N2—Tb1—K1^{ii}	81.83 (7)	O3—C7—C8	117.5 (3)
N4—Tb1—K1^{ii}	101.43 (6)	N2—C8—C9	122.7 (4)
N1—Tb1—K1^{ii}	71.99 (7)	N2—C8—C7	116.1 (3)
N3—Tb1—K1^{ii}	90.77 (6)	C9—C8—C7	121.3 (4)
K1—Tb1—K1^{ii}	167.044 (5)	C8—C9—C10	118.8 (4)
O3W—K1—O1	121.80 (14)	C8—C9—H9	120.6
O3W—K1—O5^{i}	100.66 (15)	C10—C9—H9	120.6
O1—K1—O5^{i}	132.75 (8)	C11—C10—C9	118.8 (4)
O3W—K1—O8^{i}	116.68 (14)	C11—C10—H10	120.6
O1—K1—O8^{i}	85.12 (8)	C9—C10—H10	120.6
O5^{i}—K1—O8^{i}	55.72 (8)	C10—C11—C12	119.2 (4)
O3W—K1—O3	69.35 (11)	C10—C11—H11	120.4
O1—K1—O3	63.49 (7)	C12—C11—H11	120.4
O5^{i}—K1—O3	122.62 (9)	N2—C12—C11	123.1 (4)
O8^{i}—K1—O3	78.10 (8)	N2—C12—H12	118.5
O3W—K1—O6^{i}	95.03 (12)	C11—C12—H12	118.5
O1—K1—O6^{i}	136.98 (9)	O6—C13—O5	124.0 (5)
O5^{i}—K1—O6^{i}	44.88 (8)	O6—C13—C14	120.4 (4)
O8^{i}—K1—O6^{i}	98.24 (8)	O5—C13—C14	115.6 (3)
O3—K1—O6^{i}	159.29 (9)	O6—C13—K1^{ii}	68.7 (3)
O3W—K1—C13^{i}	101.29 (14)	O5—C13—K1^{ii}	56.9 (2)
O1—K1—C13^{i}	136.87 (9)	C14—C13—K1^{ii}	163.7 (3)
O5^{i}—K1—C13^{i}	23.10 (9)	N3—C14—C15	121.7 (4)
O8^{i}—K1—C13^{i}	76.45 (9)	N3—C14—C13	115.9 (4)
O3—K1—C13^{i}	144.73 (10)	C15—C14—C13	122.4 (4)
O6^{i}—K1—C13^{i}	22.14 (9)	C14—C15—C16	120.2 (5)
O3W—K1—O2	150.45 (16)	C14—C15—H15	119.9
O1—K1—O2	43.17 (8)	C16—C15—H15	119.9
O5^{i}—K1—O2	105.46 (9)	C17—C16—C15	117.7 (5)
O8^{i}—K1—O2	89.76 (8)	C17—C16—H16	121.2
O3—K1—O2	106.46 (8)	C15—C16—H16	121.2
O6^{i}—K1—O2	93.82 (9)	C18—C17—C16	120.6 (5)
C13^{i}—K1—O2	97.47 (10)	C18—C17—H17	119.7
O3W—K1—C1	142.75 (15)	C16—C17—H17	119.7
O1—K1—C1	22.56 (8)	C17—C18—N3	122.7 (4)
O5^{i}—K1—C1	116.01 (9)	C17—C18—H18	118.6
O8^{i}—K1—C1	81.64 (9)	N3—C18—H18	118.6
O3—K1—C1	84.75 (9)	O7—C19—O8	124.3 (3)
O6^{i}—K1—C1	115.13 (10)	O7—C19—C20	118.1 (3)
C13^{i}—K1—C1	114.93 (10)	O8—C19—C20	117.6 (3)
O2—K1—C1	22.01 (9)	N4—C20—C21	124.4 (3)
O3W—K1—Tb1	102.90 (10)	N4—C20—C19	114.9 (3)
O1—K1—Tb1	33.33 (5)	C21—C20—C19	120.6 (3)

O5^{i}—K1—Tb1	123.64 (6)	C20—C21—C22	118.3 (4)
O8^{i}—K1—Tb1	67.93 (5)	C20—C21—H21	120.9
O3—K1—Tb1	34.34 (5)	C22—C21—H21	120.9
O6^{i}—K1—Tb1	160.91 (7)	C23—C22—C21	119.2 (4)
C13^{i}—K1—Tb1	143.12 (7)	C23—C22—H22	120.4
O2—K1—Tb1	73.72 (6)	C21—C22—H22	120.4
C1—K1—Tb1	51.71 (7)	C22—C23—C24	117.2 (4)
O3W—K1—Tb1^{i}	108.22 (14)	C22—C23—H23	121.4
O1—K1—Tb1^{i}	112.36 (6)	C24—C23—H23	121.4
O5^{i}—K1—Tb1^{i}	26.14 (6)	N4—C24—C23	124.1 (4)
O8^{i}—K1—Tb1^{i}	29.77 (5)	N4—C24—H24	118.0
O3—K1—Tb1^{i}	100.94 (6)	C23—C24—H24	118.0
O6^{i}—K1—Tb1^{i}	70.27 (6)	K1—O3W—H3WA	130.1
C13^{i}—K1—Tb1^{i}	48.14 (7)	K1—O3W—H3WB	127.8
O2—K1—Tb1^{i}	101.31 (7)	H3WA—O3W—H3WB	101.2
C1—K1—Tb1^{i}	102.51 (8)	H4WA—O4W—H4WB	104.4
Tb1—K1—Tb1^{i}	97.539 (19)		

O5—Tb1—K1—O3W	−117.41 (19)	K1—Tb1—O8—C19	−39.4 (3)
O7^{i}—Tb1—K1—O3W	−133.39 (16)	K1^{ii}—Tb1—O8—C19	161.4 (3)
O3—Tb1—K1—O3W	−12.35 (17)	O5—Tb1—O8—K1^{ii}	−4.91 (9)
O1—Tb1—K1—O3W	129.46 (18)	O7^{i}—Tb1—O8—K1^{ii}	49.58 (15)
O8—Tb1—K1—O3W	91.20 (17)	O3—Tb1—O8—K1^{ii}	−135.11 (9)
N2—Tb1—K1—O3W	−2.97 (16)	O1—Tb1—O8—K1^{ii}	135.50 (9)
N4—Tb1—K1—O3W	62.91 (16)	N2—Tb1—O8—K1^{ii}	−94.16 (10)
N1—Tb1—K1—O3W	163.36 (16)	N4—Tb1—O8—K1^{ii}	−169.33 (13)
N3—Tb1—K1—O3W	−73.19 (15)	N1—Tb1—O8—K1^{ii}	80.00 (10)
K1^{ii}—Tb1—K1—O3W	168.59 (15)	N3—Tb1—O8—K1^{ii}	−39.22 (13)
O5—Tb1—K1—O1	113.13 (17)	K1—Tb1—O8—K1^{ii}	159.19 (3)
O7^{i}—Tb1—K1—O1	97.15 (12)	O5—Tb1—N1—C2	−157.6 (3)
O3—Tb1—K1—O1	−141.81 (14)	O7^{i}—Tb1—N1—C2	−69.6 (3)
O8—Tb1—K1—O1	−38.26 (14)	O3—Tb1—N1—C2	−5.0 (4)
N2—Tb1—K1—O1	−132.43 (13)	O1—Tb1—N1—C2	12.8 (3)
N4—Tb1—K1—O1	−66.55 (12)	O8—Tb1—N1—C2	131.9 (3)
N1—Tb1—K1—O1	33.90 (13)	N2—Tb1—N1—C2	143.5 (3)
N3—Tb1—K1—O1	157.35 (12)	N4—Tb1—N1—C2	72.9 (3)
K1^{ii}—Tb1—K1—O1	39.13 (14)	N3—Tb1—N1—C2	−109.5 (3)
O5—Tb1—K1—O5^{i}	−5.0 (2)	K1—Tb1—N1—C2	−9.8 (3)
O7^{i}—Tb1—K1—O5^{i}	−21.03 (9)	K1^{ii}—Tb1—N1—C2	171.5 (3)
O3—Tb1—K1—O5^{i}	100.01 (12)	O5—Tb1—N1—C6	11.7 (3)
O1—Tb1—K1—O5^{i}	−118.18 (13)	O7^{i}—Tb1—N1—C6	99.7 (4)
O8—Tb1—K1—O5^{i}	−156.44 (11)	O3—Tb1—N1—C6	164.4 (3)
N2—Tb1—K1—O5^{i}	109.39 (11)	O1—Tb1—N1—C6	−177.9 (4)
N4—Tb1—K1—O5^{i}	175.27 (11)	O8—Tb1—N1—C6	−58.8 (4)
N1—Tb1—K1—O5^{i}	−84.28 (11)	N2—Tb1—N1—C6	−47.2 (5)
N3—Tb1—K1—O5^{i}	39.17 (10)	N4—Tb1—N1—C6	−117.8 (4)
K1^{ii}—Tb1—K1—O5^{i}	−79.04 (12)	N3—Tb1—N1—C6	59.8 (4)
O5—Tb1—K1—O8^{i}	−3.57 (15)	K1—Tb1—N1—C6	159.6 (3)

O7^{i}—Tb1—K1—O8^{i}	−19.55 (8)	K1^{ii}—Tb1—N1—C6	−19.2 (3)
O3—Tb1—K1—O8^{i}	101.48 (11)	O5—Tb1—N2—C12	−34.9 (3)
O1—Tb1—K1—O8^{i}	−116.70 (11)	O7^{i}—Tb1—N2—C12	−111.6 (3)
O8—Tb1—K1—O8^{i}	−154.96 (5)	O3—Tb1—N2—C12	−178.4 (4)
N2—Tb1—K1—O8^{i}	110.87 (10)	O1—Tb1—N2—C12	136.4 (3)
N4—Tb1—K1—O8^{i}	176.75 (9)	O8—Tb1—N2—C12	34.6 (3)
N1—Tb1—K1—O8^{i}	−82.81 (9)	N4—Tb1—N2—C12	101.4 (4)
N3—Tb1—K1—O8^{i}	40.64 (8)	N1—Tb1—N2—C12	23.0 (5)
K1^{ii}—Tb1—K1—O8^{i}	−77.57 (10)	N3—Tb1—N2—C12	−97.7 (4)
O5—Tb1—K1—O3	−105.06 (16)	K1—Tb1—N2—C12	174.3 (3)
O7^{i}—Tb1—K1—O3	−121.03 (11)	K1^{ii}—Tb1—N2—C12	−3.8 (3)
O1—Tb1—K1—O3	141.81 (14)	O5—Tb1—N2—C8	146.8 (3)
O8—Tb1—K1—O3	103.56 (13)	O7^{i}—Tb1—N2—C8	70.0 (3)
N2—Tb1—K1—O3	9.39 (12)	O3—Tb1—N2—C8	3.2 (3)
N4—Tb1—K1—O3	75.26 (12)	O1—Tb1—N2—C8	−42.0 (3)
N1—Tb1—K1—O3	175.71 (12)	O8—Tb1—N2—C8	−143.8 (3)
N3—Tb1—K1—O3	−60.84 (11)	N4—Tb1—N2—C8	−77.0 (3)
O5—Tb1—K1—O6^{i}	42.1 (3)	N1—Tb1—N2—C8	−155.3 (3)
O7^{i}—Tb1—K1—O6^{i}	26.1 (2)	N3—Tb1—N2—C8	84.0 (3)
O3—Tb1—K1—O6^{i}	147.2 (2)	K1—Tb1—N2—C8	−4.1 (3)
O1—Tb1—K1—O6^{i}	−71.0 (2)	K1^{ii}—Tb1—N2—C8	177.8 (3)
O8—Tb1—K1—O6^{i}	−109.3 (2)	O5—Tb1—N3—C18	171.9 (3)
N2—Tb1—K1—O6^{i}	156.6 (2)	O7^{i}—Tb1—N3—C18	75.5 (3)
N4—Tb1—K1—O6^{i}	−137.6 (2)	O3—Tb1—N3—C18	−23.6 (3)
N1—Tb1—K1—O6^{i}	−37.1 (2)	O1—Tb1—N3—C18	34.8 (3)
N3—Tb1—K1—O6^{i}	86.3 (2)	O8—Tb1—N3—C18	−151.8 (3)
K1^{ii}—Tb1—K1—O6^{i}	−31.9 (3)	N2—Tb1—N3—C18	−93.7 (3)
O5—Tb1—K1—C13^{i}	12.37 (19)	N4—Tb1—N3—C18	−67.2 (3)
O7^{i}—Tb1—K1—C13^{i}	−3.61 (14)	N1—Tb1—N3—C18	116.3 (3)
O3—Tb1—K1—C13^{i}	117.43 (16)	K1—Tb1—N3—C18	16.7 (3)
O1—Tb1—K1—C13^{i}	−100.76 (17)	K1^{ii}—Tb1—N3—C18	−174.7 (3)
O8—Tb1—K1—C13^{i}	−139.01 (15)	O5—Tb1—N3—C14	1.4 (2)
N2—Tb1—K1—C13^{i}	126.81 (15)	O7^{i}—Tb1—N3—C14	−95.1 (2)
N4—Tb1—K1—C13^{i}	−167.31 (15)	O3—Tb1—N3—C14	165.8 (2)
N1—Tb1—K1—C13^{i}	−66.86 (15)	O1—Tb1—N3—C14	−135.8 (2)
N3—Tb1—K1—C13^{i}	56.59 (14)	O8—Tb1—N3—C14	37.7 (3)
K1^{ii}—Tb1—K1—C13^{i}	−61.62 (17)	N2—Tb1—N3—C14	95.7 (2)
O5—Tb1—K1—O2	92.95 (15)	N4—Tb1—N3—C14	122.3 (2)
O7^{i}—Tb1—K1—O2	76.97 (9)	N1—Tb1—N3—C14	−54.3 (3)
O3—Tb1—K1—O2	−161.99 (12)	K1—Tb1—N3—C14	−153.9 (2)
O1—Tb1—K1—O2	−20.18 (13)	K1^{ii}—Tb1—N3—C14	14.7 (2)
O8—Tb1—K1—O2	−58.43 (11)	O5—Tb1—N4—C24	166.3 (3)
N2—Tb1—K1—O2	−152.61 (11)	O7^{i}—Tb1—N4—C24	−38.5 (4)
N4—Tb1—K1—O2	−86.73 (10)	O3—Tb1—N4—C24	31.9 (3)
N1—Tb1—K1—O2	13.72 (11)	O1—Tb1—N4—C24	−51.2 (3)
N3—Tb1—K1—O2	137.17 (9)	O8—Tb1—N4—C24	−174.5 (4)
K1^{ii}—Tb1—K1—O2	18.96 (12)	N2—Tb1—N4—C24	101.7 (3)
O5—Tb1—K1—C1	93.33 (16)	N1—Tb1—N4—C24	−107.5 (3)

O7^{i}—Tb1—K1—C1	77.35 (12)	N3—Tb1—N4—C24	75.4 (3)
O3—Tb1—K1—C1	−161.61 (13)	K1—Tb1—N4—C24	−13.9 (3)
O1—Tb1—K1—C1	−19.80 (14)	K1^{ii}—Tb1—N4—C24	178.8 (3)
O8—Tb1—K1—C1	−58.05 (13)	O5—Tb1—N4—C20	−12.3 (3)
N2—Tb1—K1—C1	−152.23 (13)	O7^{i}—Tb1—N4—C20	142.9 (2)
N4—Tb1—K1—C1	−86.35 (12)	O3—Tb1—N4—C20	−146.7 (3)
N1—Tb1—K1—C1	14.10 (12)	O1—Tb1—N4—C20	130.2 (3)
N3—Tb1—K1—C1	137.55 (11)	O8—Tb1—N4—C20	6.9 (2)
K1^{ii}—Tb1—K1—C1	19.34 (13)	N2—Tb1—N4—C20	−76.9 (3)
O5—Tb1—K1—Tb1^{i}	−6.69 (14)	N1—Tb1—N4—C20	73.8 (3)
O7^{i}—Tb1—K1—Tb1^{i}	−22.67 (6)	N3—Tb1—N4—C20	−103.2 (3)
O3—Tb1—K1—Tb1^{i}	98.37 (9)	K1—Tb1—N4—C20	167.5 (3)
O1—Tb1—K1—Tb1^{i}	−119.82 (10)	K1^{ii}—Tb1—N4—C20	0.2 (3)
O8—Tb1—K1—Tb1^{i}	−158.07 (9)	K1—O2—C1—O1	27.6 (4)
N2—Tb1—K1—Tb1^{i}	107.75 (8)	K1—O2—C1—C2	−152.4 (4)
N4—Tb1—K1—Tb1^{i}	173.63 (7)	Tb1—O1—C1—O2	−159.8 (4)
N1—Tb1—K1—Tb1^{i}	−85.92 (8)	K1—O1—C1—O2	−34.2 (5)
N3—Tb1—K1—Tb1^{i}	37.53 (6)	Tb1—O1—C1—C2	20.2 (5)
K1^{ii}—Tb1—K1—Tb1^{i}	−80.68 (9)	K1—O1—C1—C2	145.8 (3)
O5—Tb1—O1—C1	−2.5 (4)	Tb1—O1—C1—K1	−125.6 (3)
O7^{i}—Tb1—O1—C1	55.4 (3)	O3W—K1—C1—O2	125.6 (3)
O3—Tb1—O1—C1	150.4 (4)	O1—K1—C1—O2	152.0 (4)
O8—Tb1—O1—C1	−80.5 (4)	O5^{i}—K1—C1—O2	−65.4 (3)
N2—Tb1—O1—C1	−168.0 (3)	O8^{i}—K1—C1—O2	−110.6 (3)
N4—Tb1—O1—C1	−132.6 (4)	O3—K1—C1—O2	170.7 (3)
N1—Tb1—O1—C1	−18.1 (3)	O6^{i}—K1—C1—O2	−15.4 (3)
N3—Tb1—O1—C1	93.6 (4)	C13^{i}—K1—C1—O2	−39.8 (3)
K1—Tb1—O1—C1	123.6 (4)	Tb1—K1—C1—O2	−179.0 (3)
K1^{ii}—Tb1—O1—C1	−45.5 (4)	Tb1^{i}—K1—C1—O2	−89.3 (3)
O5—Tb1—O1—K1	−126.14 (15)	O3W—K1—C1—O1	−26.4 (4)
O7^{i}—Tb1—O1—K1	−68.28 (10)	O5^{i}—K1—C1—O1	142.6 (2)
O3—Tb1—O1—K1	26.73 (9)	O8^{i}—K1—C1—O1	97.4 (2)
O8—Tb1—O1—K1	155.83 (9)	O3—K1—C1—O1	18.7 (2)
N2—Tb1—O1—K1	68.33 (16)	O6^{i}—K1—C1—O1	−167.3 (2)
N4—Tb1—O1—K1	103.74 (12)	C13^{i}—K1—C1—O1	168.2 (2)
N1—Tb1—O1—K1	−141.77 (14)	O2—K1—C1—O1	−152.0 (4)
N3—Tb1—O1—K1	−30.01 (15)	Tb1—K1—C1—O1	29.0 (2)
K1^{ii}—Tb1—O1—K1	−169.16 (4)	Tb1^{i}—K1—C1—O1	118.8 (2)
O3W—K1—O1—C1	161.6 (3)	O3W—K1—C1—C2	−104.4 (5)
O5^{i}—K1—O1—C1	−48.0 (3)	O1—K1—C1—C2	−78.0 (5)
O8^{i}—K1—O1—C1	−79.9 (2)	O5^{i}—K1—C1—C2	64.6 (5)
O3—K1—O1—C1	−159.1 (3)	O8^{i}—K1—C1—C2	19.4 (5)
O6^{i}—K1—O1—C1	16.9 (3)	O3—K1—C1—C2	−59.3 (5)
C13^{i}—K1—O1—C1	−15.7 (3)	O6^{i}—K1—C1—C2	114.6 (5)
O2—K1—O1—C1	14.9 (2)	C13^{i}—K1—C1—C2	90.2 (5)
Tb1—K1—O1—C1	−136.1 (3)	O2—K1—C1—C2	130.0 (6)
Tb1^{i}—K1—O1—C1	−67.7 (3)	Tb1—K1—C1—C2	−49.0 (4)
O3W—K1—O1—Tb1	−62.31 (18)	Tb1^{i}—K1—C1—C2	40.8 (5)

O5^{i}—K1—O1—Tb1	88.12 (13)	C6—N1—C2—C3	0.6 (7)
O8^{i}—K1—O1—Tb1	56.19 (10)	Tb1—N1—C2—C3	170.7 (4)
O3—K1—O1—Tb1	−22.93 (8)	C6—N1—C2—C1	−179.1 (4)
O6^{i}—K1—O1—Tb1	153.05 (10)	Tb1—N1—C2—C1	−9.1 (5)
C13^{i}—K1—O1—Tb1	120.40 (13)	O2—C1—C2—N1	174.9 (4)
O2—K1—O1—Tb1	151.06 (18)	O1—C1—C2—N1	−5.1 (6)
C1—K1—O1—Tb1	136.1 (3)	K1—C1—C2—N1	55.1 (7)
Tb1^{i}—K1—O1—Tb1	68.45 (10)	O2—C1—C2—C3	−4.9 (7)
O3W—K1—O2—C1	−86.7 (3)	O1—C1—C2—C3	175.1 (4)
O1—K1—O2—C1	−15.3 (2)	K1—C1—C2—C3	−124.7 (5)
O5^{i}—K1—O2—C1	122.0 (3)	N1—C2—C3—C4	0.6 (7)
O8^{i}—K1—O2—C1	67.8 (3)	C1—C2—C3—C4	−179.6 (5)
O3—K1—O2—C1	−9.7 (3)	C2—C3—C4—C5	−1.2 (8)
O6^{i}—K1—O2—C1	166.1 (3)	C3—C4—C5—C6	0.5 (8)
C13^{i}—K1—O2—C1	144.1 (3)	C2—N1—C6—C5	−1.4 (7)
Tb1—K1—O2—C1	0.8 (3)	Tb1—N1—C6—C5	−170.3 (4)
Tb1^{i}—K1—O2—C1	95.4 (3)	C4—C5—C6—N1	0.8 (8)
O5—Tb1—O3—C7	−57.5 (3)	Tb1—O3—C7—O4	−178.5 (3)
O7^{i}—Tb1—O3—C7	−141.4 (3)	K1—O3—C7—O4	−14.8 (6)
O1—Tb1—O3—C7	145.1 (3)	Tb1—O3—C7—C8	1.3 (5)
O8—Tb1—O3—C7	41.8 (3)	K1—O3—C7—C8	165.0 (3)
N2—Tb1—O3—C7	−2.3 (3)	C12—N2—C8—C9	−3.4 (7)
N4—Tb1—O3—C7	73.5 (3)	Tb1—N2—C8—C9	175.2 (4)
N1—Tb1—O3—C7	161.4 (3)	C12—N2—C8—C7	177.6 (4)
N3—Tb1—O3—C7	−76.8 (3)	Tb1—N2—C8—C7	−3.9 (5)
K1—Tb1—O3—C7	168.1 (3)	O4—C7—C8—N2	−178.2 (4)
K1^{ii}—Tb1—O3—C7	−12.3 (4)	O3—C7—C8—N2	2.0 (6)
O5—Tb1—O3—K1	134.46 (10)	O4—C7—C8—C9	2.7 (7)
O7^{i}—Tb1—O3—K1	50.57 (9)	O3—C7—C8—C9	−177.0 (4)
O1—Tb1—O3—K1	−22.98 (9)	N2—C8—C9—C10	3.3 (8)
O8—Tb1—O3—K1	−126.28 (9)	C7—C8—C9—C10	−177.7 (5)
N2—Tb1—O3—K1	−170.42 (12)	C8—C9—C10—C11	−1.1 (8)
N4—Tb1—O3—K1	−94.53 (9)	C9—C10—C11—C12	−0.7 (8)
N1—Tb1—O3—K1	−6.70 (19)	C8—N2—C12—C11	1.4 (7)
N3—Tb1—O3—K1	115.13 (10)	Tb1—N2—C12—C11	−177.0 (3)
K1^{ii}—Tb1—O3—K1	179.60 (5)	C10—C11—C12—N2	0.6 (8)
O3W—K1—O3—C7	0.7 (4)	K1^{ii}—O6—C13—O5	−14.1 (4)
O1—K1—O3—C7	−144.1 (4)	K1^{ii}—O6—C13—C14	165.0 (3)
O5^{i}—K1—O3—C7	90.3 (4)	Tb1—O5—C13—O6	169.0 (3)
O8^{i}—K1—O3—C7	125.4 (4)	K1^{ii}—O5—C13—O6	15.7 (4)
O6^{i}—K1—O3—C7	43.6 (5)	Tb1—O5—C13—C14	−10.1 (5)
C13^{i}—K1—O3—C7	80.9 (4)	K1^{ii}—O5—C13—C14	−163.4 (3)
O2—K1—O3—C7	−148.4 (4)	Tb1—O5—C13—K1^{ii}	153.3 (3)
C1—K1—O3—C7	−152.0 (4)	C18—N3—C14—C15	0.0 (5)
Tb1—K1—O3—C7	−166.4 (4)	Tb1—N3—C14—C15	171.7 (3)
Tb1^{i}—K1—O3—C7	106.2 (4)	C18—N3—C14—C13	−177.8 (3)
O3W—K1—O3—Tb1	167.12 (17)	Tb1—N3—C14—C13	−6.0 (4)
O1—K1—O3—Tb1	22.31 (8)	O6—C13—C14—N3	−169.3 (4)

O5^{i}—K1—O3—Tb1	−103.24 (11)	O5—C13—C14—N3	9.9 (5)
O8^{i}—K1—O3—Tb1	−68.14 (8)	K1^{ii}—C13—C14—N3	−48.9 (10)
O6^{i}—K1—O3—Tb1	−149.9 (2)	O6—C13—C14—C15	13.0 (6)
C13^{i}—K1—O3—Tb1	−112.70 (15)	O5—C13—C14—C15	−167.9 (4)
O2—K1—O3—Tb1	18.03 (11)	K1^{ii}—C13—C14—C15	133.4 (8)
C1—K1—O3—Tb1	14.40 (11)	N3—C14—C15—C16	−1.0 (6)
Tb1^{i}—K1—O3—Tb1	−87.37 (8)	C13—C14—C15—C16	176.6 (4)
O7^{i}—Tb1—O5—C13	70.9 (3)	C14—C15—C16—C17	0.9 (7)
O3—Tb1—O5—C13	−15.9 (4)	C15—C16—C17—C18	0.2 (7)
O1—Tb1—O5—C13	125.9 (3)	C16—C17—C18—N3	−1.3 (7)
O8—Tb1—O5—C13	−142.4 (3)	C14—N3—C18—C17	1.2 (5)
N2—Tb1—O5—C13	−64.8 (3)	Tb1—N3—C18—C17	−169.1 (3)
N4—Tb1—O5—C13	−123.9 (3)	Tb1^{ii}—O7—C19—O8	−49.3 (6)
N1—Tb1—O5—C13	140.1 (3)	Tb1^{ii}—O7—C19—C20	132.6 (4)
N3—Tb1—O5—C13	5.1 (3)	Tb1—O8—C19—O7	−170.3 (2)
K1—Tb1—O5—C13	56.5 (4)	K1^{ii}—O8—C19—O7	−9.9 (4)
K1^{ii}—Tb1—O5—C13	−148.2 (4)	Tb1—O8—C19—C20	7.8 (4)
O7^{i}—Tb1—O5—K1^{ii}	−140.81 (13)	K1^{ii}—O8—C19—C20	168.2 (2)
O3—Tb1—O5—K1^{ii}	132.34 (12)	C24—N4—C20—C21	−0.7 (6)
O1—Tb1—O5—K1^{ii}	−85.86 (18)	Tb1—N4—C20—C21	178.0 (3)
O8—Tb1—O5—K1^{ii}	5.88 (10)	C24—N4—C20—C19	175.1 (3)
N2—Tb1—O5—K1^{ii}	83.41 (13)	Tb1—N4—C20—C19	−6.2 (4)
N4—Tb1—O5—K1^{ii}	24.35 (19)	O7—C19—C20—N4	178.1 (3)
N1—Tb1—O5—K1^{ii}	−71.65 (13)	O8—C19—C20—N4	−0.1 (5)
N3—Tb1—O5—K1^{ii}	153.31 (15)	O7—C19—C20—C21	−5.9 (5)
K1—Tb1—O5—K1^{ii}	−155.24 (5)	O8—C19—C20—C21	175.9 (3)
O5—Tb1—O8—C19	156.5 (3)	N4—C20—C21—C22	0.2 (6)
O7^{i}—Tb1—O8—C19	−149.0 (2)	C19—C20—C21—C22	−175.4 (4)
O3—Tb1—O8—C19	26.3 (3)	C20—C21—C22—C23	−0.1 (7)
O1—Tb1—O8—C19	−63.1 (3)	C21—C22—C23—C24	0.6 (7)
N2—Tb1—O8—C19	67.3 (3)	C20—N4—C24—C23	1.3 (6)
N4—Tb1—O8—C19	−7.9 (2)	Tb1—N4—C24—C23	−177.3 (3)
N1—Tb1—O8—C19	−118.6 (3)	C22—C23—C24—N4	−1.2 (7)
N3—Tb1—O8—C19	122.2 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O4	0.84	2.09	2.858 (4)	152
O2*W*—H2*W*···O6^{ii}	0.85	2.48	3.219 (5)	146
O3*W*—H3*WA*···O6^{iii}	0.86	2.09	2.647 (5)	121
O4*W*—H4*WB*···O2^{iv}	0.86	1.92	2.711 (6)	152
O5*W*—H5*W*···O4*W*	0.85	2.34	3.080 (13)	145

Symmetry codes: (ii) *x*−*y*+1, −*y*+1, −*z*; (iii) *y*−1, −*x*+*y*, *z*+1/6; (iv) *x*+1, *y*, *z*.