

### Electronic Supplementary Information

#### Complex three-dimensional lanthanide metal-organic frameworks with variable coordination spheres based on pyrazine-2,3,5,6-tetracarboxylate

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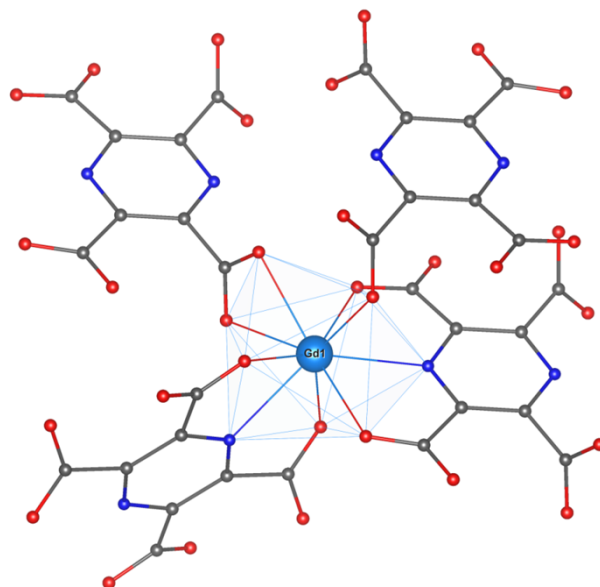


Fig. S1a.

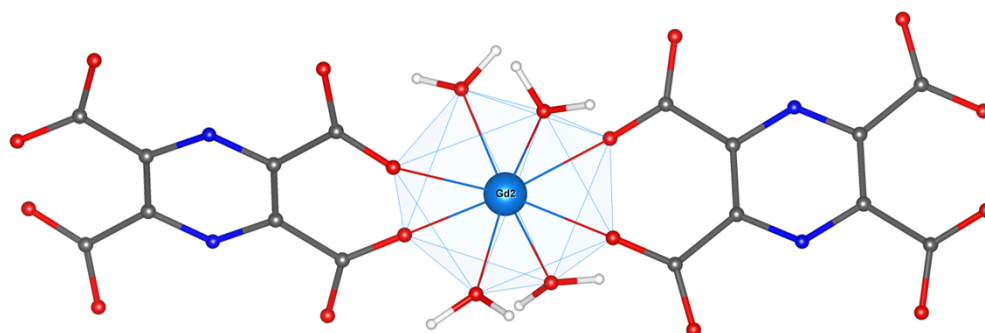


Fig. S1b.

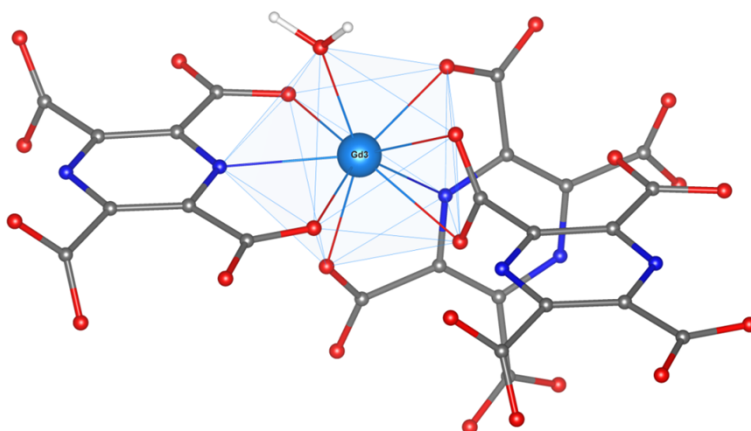


Fig. S1c.

Fig S1. Coordination environment of Gd1 (a), Gd2 (b), and Gd3 (c).  
(red = O, grey = C, blue = N)

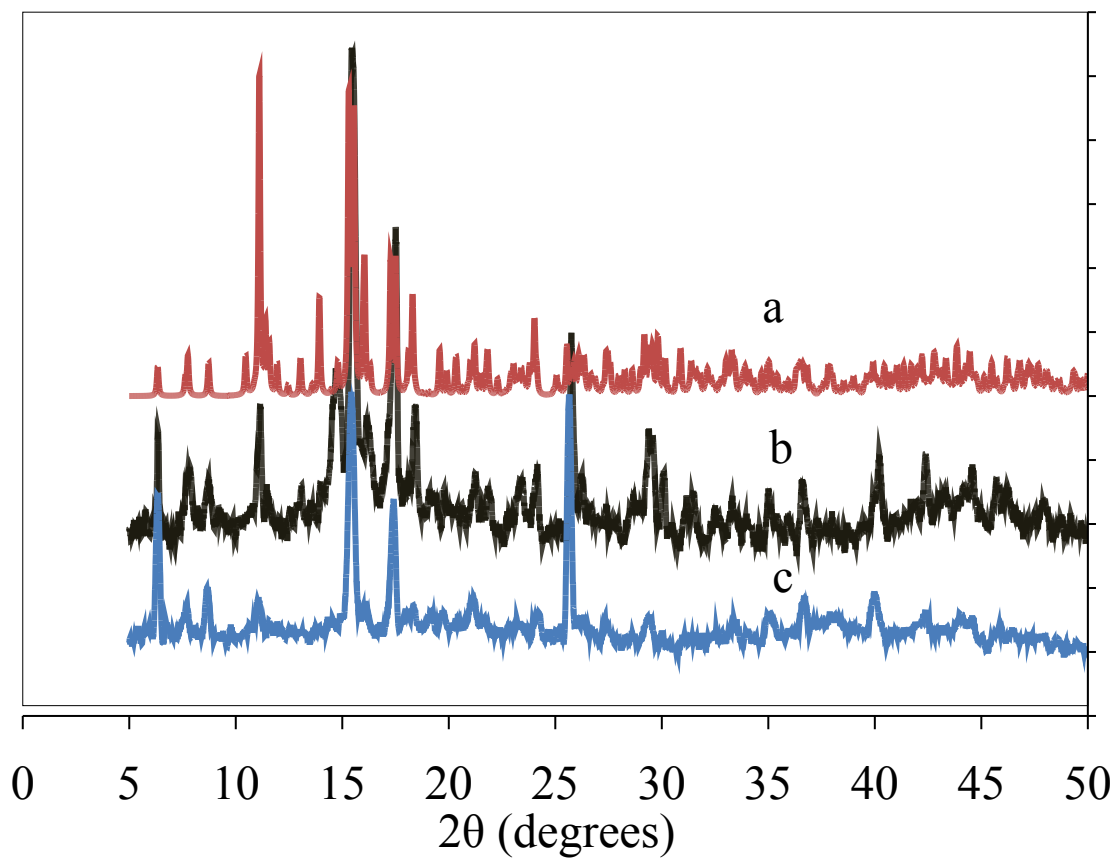


Fig. S2. Simulated (a) and measured powdered X-Ray diffraction pattern of “as synthesized” **1** (b) and **2** (c).

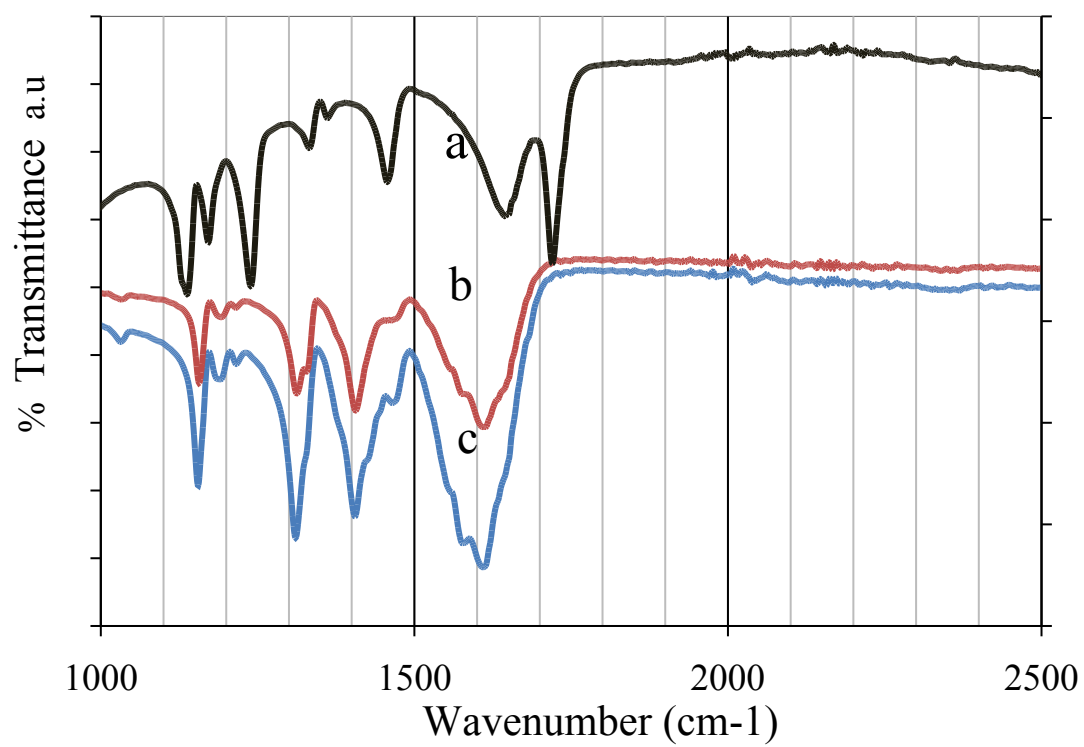


Fig. S3. FTIR spectra of H<sub>4</sub>pztc (a), **1** (b) and **2** (c).

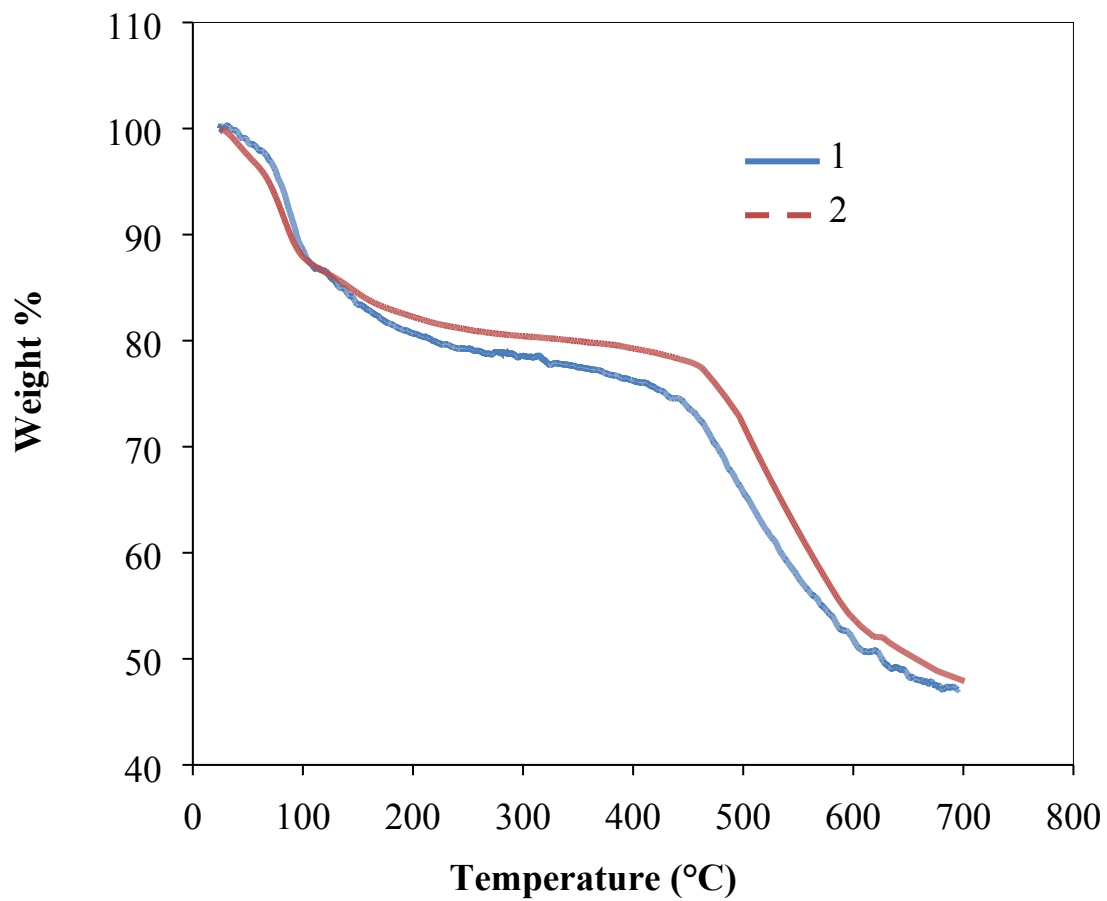


Fig. S4. Thermogravimetric curves of **1** and **2**.

Table S1. Crystal data and structure refinement for **1**.

Identification code	<b>1</b>	
Empirical formula	C <sub>24</sub> H <sub>42</sub> Gd <sub>4</sub> N <sub>6</sub> O <sub>45</sub>	
Formula weight	1763.63	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.5607(10) Å	α = 88.5392(17)°.
	b = 14.1023(17) Å	β = 86.4998(15)°.
	c = 20.294(2) Å	γ = 81.2519(16)°.
Volume	2416.6(5) Å <sup>3</sup>	
Z	2	
Density (calculated)	2.424 Mg/m <sup>3</sup>	
Absorption coefficient	5.552 mm <sup>-1</sup>	
F(000)	1688	
Crystal size	0.394 x 0.146 x 0.108 mm <sup>3</sup>	
Theta range for data collection	2.011 to 33.346°.	
Index ranges	-11 ≤ h ≤ 13, -21 ≤ k ≤ 21, -31 ≤ l ≤ 29	
Reflections collected	24173	
Independent reflections	17134 [R(int) = 0.0571]	
Completeness to theta = 26.000°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1 and 0.4305	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	17134 / 238 / 814	
Goodness-of-fit on F <sup>2</sup>	1.056	
Final R indices [I > 2σ(I)]	R1 = 0.0570, wR2 = 0.1455	
R indices (all data)	R1 = 0.0690, wR2 = 0.1516	
Extinction coefficient	n/a	
Largest diff. peak and hole	4.712 and -5.877 e.Å <sup>-3</sup>	

Table S2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **1**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	$U(\text{eq})$
C(1)	12525(5)	5883(3)	923(2)	9(1)
C(2)	13873(4)	5362(3)	473(2)	7(1)
C(3)	14905(4)	4508(3)	587(2)	8(1)
C(4)	15043(5)	3876(3)	1218(2)	11(1)
C(5)	11271(5)	9327(3)	901(2)	11(1)
C(6)	9776(4)	9105(3)	619(2)	9(1)
C(7)	8216(5)	9566(3)	776(2)	9(1)
C(8)	7238(5)	8484(3)	159(2)	9(1)
C(9)	8754(5)	8038(3)	-21(2)	9(1)
C(10)	9190(5)	7211(3)	-498(2)	13(1)
C(11)	7823(5)	10455(3)	1189(2)	11(1)
C(12)	5756(4)	8125(3)	-28(2)	8(1)
C(13)	12063(5)	5822(3)	4034(2)	10(1)
C(14)	10915(4)	5353(3)	4506(2)	8(1)
C(15)	9825(4)	5452(3)	5590(2)	8(1)
C(16)	9899(5)	5999(3)	6219(2)	11(1)
C(17)	14927(5)	10215(3)	3521(2)	12(1)
C(18)	14813(5)	9452(3)	4064(2)	11(1)
C(19)	13450(5)	9054(3)	4270(2)	9(1)
C(20)	14957(5)	7991(3)	4964(2)	10(1)
C(21)	16310(4)	8406(3)	4743(2)	7(1)
C(22)	17952(5)	8044(3)	4970(2)	11(1)
C(23)	14965(5)	7173(3)	5447(2)	9(1)
C(24)	11776(5)	9331(3)	4056(2)	10(1)
N(2)	10714(4)	5777(2)	5094(2)	8(1)
N(3)	13565(4)	8335(2)	4718(2)	7(1)
N(5)	10006(4)	8358(2)	221(2)	10(1)
N(6)	6964(4)	9236(2)	556(2)	10(1)
N(4)	16216(4)	9137(3)	4316(2)	12(1)
O(1)	12156(4)	6757(2)	792(2)	13(1)
O(1W)	10233(4)	6153(2)	2634(2)	20(1)

O(2)	11857(4)	5426(2)	1363(1)	12(1)
O(2W)	10935(4)	3794(2)	1963(2)	24(1)
N(1)	14006(4)	5826(2)	-109(2)	9(1)
O(3W)	13948(4)	6062(2)	2322(2)	19(1)
O(3)	14383(4)	4198(2)	1746(2)	16(1)
O(4W)	13606(5)	3473(3)	3022(2)	25(1)
O(4)	15868(4)	3067(2)	1147(2)	14(1)
O(5W)	13451(4)	11496(2)	1742(2)	21(1)
O(5)	10650(3)	6882(2)	-573(2)	12(1)
O(6W)	10295(4)	11624(2)	1941(2)	22(1)
O(6)	8089(4)	6951(2)	-788(2)	17(1)
O(7W)	11954(4)	11726(2)	3095(1)	16(1)
O(7)	12549(3)	8912(2)	638(2)	13(1)
O(8W)	14387(4)	9450(2)	1710(2)	18(1)
O(8)	11098(4)	9893(2)	1378(2)	14(1)
O(9W)	11438(3)	8825(2)	5909(2)	14(1)
O(9)	5306(3)	7443(2)	304(2)	12(1)
O(10)	4975(4)	8557(2)	-485(2)	13(1)
O(11)	8301(4)	11210(2)	955(1)	11(1)
O(12)	7021(4)	10390(2)	1716(2)	17(1)
O(13)	12785(4)	5362(2)	3570(1)	12(1)
O(14)	12246(3)	6660(2)	4185(2)	12(1)
O(15)	10332(4)	6811(2)	6135(1)	13(1)
O(16)	9621(4)	5603(2)	6762(2)	18(1)
O(17)	14455(4)	10039(2)	2974(2)	16(1)
O(18)	15576(4)	10920(2)	3660(2)	17(1)
O(20)	11493(3)	10005(2)	3636(1)	12(1)
O(20W)	12232(4)	8605(2)	2572(2)	18(1)
O(19)	10767(4)	8865(2)	4328(2)	14(1)
O(21W)	9392(3)	10053(2)	2684(1)	19(1)
O(21)	13618(4)	6906(2)	5586(2)	13(1)
O(22)	16244(4)	6812(2)	5668(2)	14(1)
O(23)	18457(4)	8405(2)	5445(2)	14(1)
O(24)	18761(4)	7411(2)	4599(2)	14(1)
Gd(1)	12750(1)	7629(1)	-190(1)	7(1)
Gd(2)	12317(1)	4858(1)	2477(1)	9(1)



Gd(3)	11190(1)	7596(1)	5143(1)	7(1)
Gd(4)	12116(1)	10302(1)	2415(1)	10(1)
O(15W)	6252(4)	6352(3)	1397(2)	20(1)
O(10W)	14451(4)	7300(2)	3263(2)	17(1)
O(16W)	10307(4)	7698(2)	1839(2)	20(1)
O(13W)	8918(6)	8370(3)	3171(2)	35(1)
O(19W)	15935(5)	2141(3)	2606(2)	23(1)
O(17W)	8736(5)	5111(3)	913(2)	32(1)
O(18W)	8518(5)	3015(3)	2606(2)	27(1)
O(14W)	7073(5)	7911(3)	2084(2)	33(1)
O(12W)	7640(4)	6473(2)	3560(2)	19(1)
O(11W)	16144(5)	4975(3)	3886(3)	48(1)

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Table S3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **1**.

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C(1)-C(2)	1.534(5)
C(1)-O(1)	1.252(5)
C(1)-O(2)	1.249(5)
C(2)-C(3)	1.405(5)
C(2)-N(1)	1.342(5)
C(3)-C(4)	1.541(5)
C(3)-N(1)#1	1.346(5)
C(4)-O(3)	1.244(5)
C(4)-O(4)	1.254(5)
C(5)-C(6)	1.512(6)
C(5)-O(7)	1.255(5)
C(5)-O(8)	1.257(5)
C(6)-C(7)	1.415(5)
C(6)-N(5)	1.327(5)
C(7)-C(11)	1.509(5)
C(7)-N(6)	1.336(5)
C(8)-C(9)	1.385(5)
C(8)-C(12)	1.508(6)
C(8)-N(6)	1.331(5)
C(9)-C(10)	1.522(6)
C(9)-N(5)	1.348(5)
C(10)-O(5)	1.266(5)
C(10)-O(6)	1.247(5)
C(11)-O(11)	1.269(5)
C(11)-O(12)	1.244(5)
C(12)-O(9)	1.255(5)
C(12)-O(10)	1.265(5)
C(12)-Gd(1)#2	2.807(4)
C(13)-C(14)	1.540(5)
C(13)-O(13)	1.237(5)
C(13)-O(14)	1.262(5)
C(14)-C(15)#3	1.405(5)
C(14)-N(2)	1.337(5)
C(15)-C(14)#3	1.405(5)

C(15)-C(16)	1.518(5)
C(15)-N(2)	1.340(5)
C(16)-O(15)	1.260(5)
C(16)-O(16)	1.248(5)
C(17)-C(18)	1.529(6)
C(17)-O(17)	1.247(5)
C(17)-O(18)	1.256(5)
C(18)-C(19)	1.407(6)
C(18)-N(4)	1.342(5)
C(19)-C(24)	1.513(6)
C(19)-N(3)	1.342(5)
C(20)-C(21)	1.419(5)
C(20)-C(23)	1.495(6)
C(20)-N(3)	1.337(5)
C(21)-C(22)	1.516(5)
C(21)-N(4)	1.325(5)
C(22)-O(23)	1.233(5)
C(22)-O(24)	1.275(5)
C(22)-Gd(3)#4	2.789(4)
C(23)-O(21)	1.280(5)
C(23)-O(22)	1.241(5)
C(24)-O(20)	1.266(5)
C(24)-O(19)	1.257(5)
N(2)-Gd(3)	2.662(3)
N(3)-Gd(3)	2.520(3)
N(5)-Gd(1)	2.519(3)
O(1)-Gd(1)	2.385(3)
O(1W)-H(1WA)	1.007(7)
O(1W)-H(1WB)	0.985(7)
O(1W)-Gd(2)	2.364(3)
O(2)-Gd(2)	2.413(3)
O(2W)-H(2WA)	0.984(8)
O(2W)-H(2WB)	0.987(13)
O(2W)-Gd(2)	2.347(3)
N(1)-C(3)#1	1.346(5)
N(1)-Gd(1)	2.611(3)

O(3W)-H(3WA)	0.992(7)
O(3W)-H(3WB)	0.985(8)
O(3W)-Gd(2)	2.360(3)
O(3)-Gd(2)	2.332(3)
O(4W)-H(4WA)	0.981(7)
O(4W)-H(4WB)	0.986(7)
O(4W)-Gd(2)	2.375(3)
O(4)-Gd(1)#1	2.366(3)
O(5W)-H(5WA)	1.008(7)
O(5W)-H(5WB)	1.011(4)
O(5W)-Gd(4)	2.507(3)
O(5)-Gd(1)	2.395(3)
O(6W)-H(6WA)	0.996(7)
O(6W)-H(6WB)	0.984(7)
O(6W)-Gd(4)	2.458(3)
O(7W)-H(7WA)	1.013(7)
O(7W)-H(7WB)	1.003(6)
O(7W)-Gd(4)	2.447(3)
O(7)-Gd(1)	2.482(3)
O(8W)-H(8WA)	0.997(7)
O(8W)-H(8WB)	0.984(8)
O(8W)-Gd(4)	2.512(3)
O(8)-Gd(4)	2.441(3)
O(9W)-H(9WA)	0.986(8)
O(9W)-H(9WB)	0.990(4)
O(9W)-Gd(3)	2.400(3)
O(9)-Gd(1)#2	2.437(3)
O(10)-Gd(1)#2	2.506(3)
O(11)-Gd(1)#5	2.344(3)
O(13)-Gd(2)	2.421(3)
O(14)-Gd(3)	2.427(3)
O(15)-Gd(3)	2.403(3)
O(16)-Gd(2)#3	2.351(3)
O(17)-Gd(4)	2.339(3)
O(20)-Gd(4)	2.541(3)
O(20W)-H(20A)	0.8500

O(20W)-H(20B)	0.8520
O(20W)-Gd(4)	2.393(3)
O(19)-Gd(3)	2.407(3)
O(21W)-H(21A)	0.975(4)
O(21W)-H(21B)	0.975(4)
O(21W)-Gd(4)	2.437(3)
O(21)-Gd(3)	2.376(3)
O(23)-Gd(3)#4	2.490(3)
O(24)-Gd(3)#4	2.464(3)
Gd(1)-O(4)#1	2.366(3)
Gd(1)-O(9)#4	2.437(3)
Gd(1)-O(10)#4	2.506(3)
Gd(1)-O(11)#5	2.344(3)
Gd(2)-O(16)#3	2.351(3)
Gd(3)-O(23)#2	2.490(3)
Gd(3)-O(24)#2	2.464(3)
O(15W)-H(15A)	0.8484
O(15W)-H(15B)	0.8493
O(10W)-H(10A)	0.986(7)
O(10W)-H(10B)	1.005(7)
O(16W)-H(16A)	0.8456
O(16W)-H(16B)	0.8501
O(13W)-H(13A)	0.8643
O(13W)-H(13B)	0.9018
O(19W)-H(19A)	0.8494
O(19W)-H(19B)	0.8492
O(17W)-H(17A)	0.8474
O(17W)-H(17B)	0.8494
O(18W)-H(18A)	0.8489
O(18W)-H(18B)	0.8494
O(14W)-H(14A)	0.8500
O(14W)-H(14B)	0.8492
O(12W)-H(12A)	0.984(6)
O(12W)-H(12B)	0.985(8)
O(11W)-H(11A)	1.000(7)
O(11W)-H(11B)	0.983(7)

O(1)-C(1)-C(2)	114.7(3)
O(2)-C(1)-C(2)	120.1(3)
O(2)-C(1)-O(1)	125.2(4)
C(3)-C(2)-C(1)	129.5(3)
N(1)-C(2)-C(1)	111.4(3)
N(1)-C(2)-C(3)	119.1(3)
C(2)-C(3)-C(4)	129.0(3)
N(1)#1-C(3)-C(2)	119.1(3)
N(1)#1-C(3)-C(4)	111.9(3)
O(3)-C(4)-C(3)	119.3(3)
O(3)-C(4)-O(4)	125.5(4)
O(4)-C(4)-C(3)	115.2(3)
O(7)-C(5)-C(6)	116.1(3)
O(7)-C(5)-O(8)	127.2(4)
O(8)-C(5)-C(6)	116.7(3)
C(7)-C(6)-C(5)	126.4(3)
N(5)-C(6)-C(5)	113.9(3)
N(5)-C(6)-C(7)	119.5(4)
C(6)-C(7)-C(11)	124.0(4)
N(6)-C(7)-C(6)	121.2(3)
N(6)-C(7)-C(11)	114.9(3)
C(9)-C(8)-C(12)	123.7(3)
N(6)-C(8)-C(9)	122.4(4)
N(6)-C(8)-C(12)	113.8(3)
C(8)-C(9)-C(10)	126.3(4)
N(5)-C(9)-C(8)	119.4(3)
N(5)-C(9)-C(10)	114.3(3)
O(5)-C(10)-C(9)	116.0(4)
O(6)-C(10)-C(9)	117.0(3)
O(6)-C(10)-O(5)	126.9(4)
O(11)-C(11)-C(7)	116.7(3)
O(12)-C(11)-C(7)	117.3(4)
O(12)-C(11)-O(11)	126.0(4)
C(8)-C(12)-Gd(1)#2	170.3(3)
O(9)-C(12)-C(8)	118.1(3)

O(9)-C(12)-O(10)	122.9(4)
O(9)-C(12)-Gd(1)#2	60.1(2)
O(10)-C(12)-C(8)	118.8(3)
O(10)-C(12)-Gd(1)#2	63.2(2)
O(13)-C(13)-C(14)	120.0(4)
O(13)-C(13)-O(14)	124.9(4)
O(14)-C(13)-C(14)	115.0(3)
C(15)#3-C(14)-C(13)	129.3(3)
N(2)-C(14)-C(13)	111.5(3)
N(2)-C(14)-C(15)#3	119.1(3)
C(14)#3-C(15)-C(16)	129.0(3)
N(2)-C(15)-C(14)#3	119.4(3)
N(2)-C(15)-C(16)	111.4(3)
O(15)-C(16)-C(15)	114.9(3)
O(16)-C(16)-C(15)	118.9(4)
O(16)-C(16)-O(15)	126.1(4)
O(17)-C(17)-C(18)	116.3(4)
O(17)-C(17)-O(18)	126.9(4)
O(18)-C(17)-C(18)	116.7(4)
C(19)-C(18)-C(17)	126.1(4)
N(4)-C(18)-C(17)	112.5(4)
N(4)-C(18)-C(19)	121.3(4)
C(18)-C(19)-C(24)	128.7(4)
N(3)-C(19)-C(18)	119.1(3)
N(3)-C(19)-C(24)	112.2(3)
C(21)-C(20)-C(23)	124.9(3)
N(3)-C(20)-C(21)	118.7(3)
N(3)-C(20)-C(23)	116.5(3)
C(20)-C(21)-C(22)	122.8(3)
N(4)-C(21)-C(20)	121.7(3)
N(4)-C(21)-C(22)	115.5(3)
C(21)-C(22)-Gd(3)#4	167.4(3)
O(23)-C(22)-C(21)	120.7(3)
O(23)-C(22)-O(24)	124.8(4)
O(23)-C(22)-Gd(3)#4	63.2(2)
O(24)-C(22)-C(21)	114.3(4)

O(24)-C(22)-Gd(3)#4	62.0(2)
O(21)-C(23)-C(20)	115.4(3)
O(22)-C(23)-C(20)	118.4(4)
O(22)-C(23)-O(21)	126.2(4)
O(20)-C(24)-C(19)	119.0(4)
O(19)-C(24)-C(19)	115.6(3)
O(19)-C(24)-O(20)	125.4(4)
C(14)-N(2)-C(15)	121.5(3)
C(14)-N(2)-Gd(3)	117.8(3)
C(15)-N(2)-Gd(3)	117.1(2)
C(19)-N(3)-Gd(3)	121.9(3)
C(20)-N(3)-C(19)	120.7(3)
C(20)-N(3)-Gd(3)	117.4(3)
C(6)-N(5)-C(9)	119.8(3)
C(6)-N(5)-Gd(1)	121.2(3)
C(9)-N(5)-Gd(1)	118.7(2)
C(8)-N(6)-C(7)	117.7(3)
C(21)-N(4)-C(18)	118.4(4)
C(1)-O(1)-Gd(1)	129.0(2)
H(1WA)-O(1W)-H(1WB)	102.2(9)
Gd(2)-O(1W)-H(1WA)	134.6(8)
Gd(2)-O(1W)-H(1WB)	122.6(8)
C(1)-O(2)-Gd(2)	137.7(3)
H(2WA)-O(2W)-H(2WB)	103.6(13)
Gd(2)-O(2W)-H(2WA)	124.7(9)
Gd(2)-O(2W)-H(2WB)	131.7(12)
C(2)-N(1)-C(3)#1	121.9(3)
C(2)-N(1)-Gd(1)	118.4(2)
C(3)#1-N(1)-Gd(1)	117.3(2)
H(3WA)-O(3W)-H(3WB)	102.8(11)
Gd(2)-O(3W)-H(3WA)	120.0(8)
Gd(2)-O(3W)-H(3WB)	133.5(12)
C(4)-O(3)-Gd(2)	157.7(3)
H(4WA)-O(4W)-H(4WB)	104.1(10)
Gd(2)-O(4W)-H(4WA)	121.4(8)
Gd(2)-O(4W)-H(4WB)	123.8(14)



C(4)-O(4)-Gd(1)#1	129.5(3)
H(5WA)-O(5W)-H(5WB)	98.8(7)
Gd(4)-O(5W)-H(5WA)	120.1(8)
Gd(4)-O(5W)-H(5WB)	123.2(5)
C(10)-O(5)-Gd(1)	125.1(3)
H(6WA)-O(6W)-H(6WB)	102.9(9)
Gd(4)-O(6W)-H(6WA)	122.5(9)
Gd(4)-O(6W)-H(6WB)	116.7(6)
H(7WA)-O(7W)-H(7WB)	100.1(9)
Gd(4)-O(7W)-H(7WA)	135.2(7)
Gd(4)-O(7W)-H(7WB)	117.4(8)
C(5)-O(7)-Gd(1)	124.4(3)
H(8WA)-O(8W)-H(8WB)	102.9(9)
Gd(4)-O(8W)-H(8WA)	103.0(6)
Gd(4)-O(8W)-H(8WB)	120.2(7)
C(5)-O(8)-Gd(4)	146.2(3)
H(9WA)-O(9W)-H(9WB)	103.6(8)
Gd(3)-O(9W)-H(9WA)	131.9(8)
Gd(3)-O(9W)-H(9WB)	124.1(5)
C(12)-O(9)-Gd(1)#2	93.4(2)
C(12)-O(10)-Gd(1)#2	90.0(2)
C(11)-O(11)-Gd(1)#5	132.1(3)
C(13)-O(13)-Gd(2)	139.3(3)
C(13)-O(14)-Gd(3)	129.5(3)
C(16)-O(15)-Gd(3)	130.2(3)
C(16)-O(16)-Gd(2)#3	146.6(3)
C(17)-O(17)-Gd(4)	138.7(3)
C(24)-O(20)-Gd(4)	137.8(2)
H(20A)-O(20W)-H(20B)	109.4
Gd(4)-O(20W)-H(20A)	109.3
Gd(4)-O(20W)-H(20B)	109.3
C(24)-O(19)-Gd(3)	127.6(3)
H(21A)-O(21W)-H(21B)	105.7(5)
Gd(4)-O(21W)-H(21A)	122.3(4)
Gd(4)-O(21W)-H(21B)	109.6(6)
C(23)-O(21)-Gd(3)	125.5(3)

C(22)-O(23)-Gd(3)#4	90.5(2)
C(22)-O(24)-Gd(3)#4	90.8(2)
N(5)-Gd(1)-N(1)	126.89(11)
O(1)-Gd(1)-N(5)	73.86(11)
O(1)-Gd(1)-N(1)	62.33(10)
O(1)-Gd(1)-O(5)	81.40(11)
O(1)-Gd(1)-O(7)	79.51(10)
O(1)-Gd(1)-O(9)#4	79.98(11)
O(1)-Gd(1)-O(10)#4	130.63(11)
O(4)#1-Gd(1)-N(5)	140.63(11)
O(4)#1-Gd(1)-O(1)	124.57(10)
O(4)#1-Gd(1)-N(1)	62.69(10)
O(4)#1-Gd(1)-O(5)	82.69(11)
O(4)#1-Gd(1)-O(7)	146.29(11)
O(4)#1-Gd(1)-O(9)#4	86.80(11)
O(4)#1-Gd(1)-O(10)#4	72.71(11)
O(5)-Gd(1)-N(5)	64.83(10)
O(5)-Gd(1)-N(1)	79.72(10)
O(5)-Gd(1)-O(7)	127.60(10)
O(5)-Gd(1)-O(9)#4	148.05(10)
O(5)-Gd(1)-O(10)#4	147.11(10)
O(7)-Gd(1)-N(5)	63.08(10)
O(7)-Gd(1)-N(1)	129.71(10)
O(7)-Gd(1)-O(10)#4	73.59(10)
O(9)#4-Gd(1)-N(5)	132.48(11)
O(9)#4-Gd(1)-N(1)	68.67(10)
O(9)#4-Gd(1)-O(7)	73.71(10)
O(9)#4-Gd(1)-O(10)#4	53.20(10)
O(10)#4-Gd(1)-N(5)	124.78(11)
O(10)#4-Gd(1)-N(1)	106.68(10)
O(11)#5-Gd(1)-N(5)	70.71(11)
O(11)#5-Gd(1)-O(1)	144.26(10)
O(11)#5-Gd(1)-N(1)	141.29(10)
O(11)#5-Gd(1)-O(4)#1	82.49(10)
O(11)#5-Gd(1)-O(5)	79.55(11)
O(11)#5-Gd(1)-O(7)	88.62(10)

O(11)#5-Gd(1)-O(9)#4	128.86(11)
O(11)#5-Gd(1)-O(10)#4	75.93(10)
O(1W)-Gd(2)-O(2)	77.28(11)
O(1W)-Gd(2)-O(4W)	141.73(11)
O(1W)-Gd(2)-O(13)	79.05(11)
O(2)-Gd(2)-O(13)	143.53(10)
O(2W)-Gd(2)-O(1W)	98.89(13)
O(2W)-Gd(2)-O(2)	71.27(11)
O(2W)-Gd(2)-O(3W)	146.07(11)
O(2W)-Gd(2)-O(4W)	85.59(13)
O(2W)-Gd(2)-O(13)	140.15(11)
O(2W)-Gd(2)-O(16)#3	71.24(11)
O(3W)-Gd(2)-O(1W)	84.89(12)
O(3W)-Gd(2)-O(2)	76.84(11)
O(3W)-Gd(2)-O(4W)	112.14(13)
O(3W)-Gd(2)-O(13)	73.76(10)
O(3)-Gd(2)-O(1W)	144.07(11)
O(3)-Gd(2)-O(2)	69.26(10)
O(3)-Gd(2)-O(2W)	82.77(12)
O(3)-Gd(2)-O(3W)	75.29(11)
O(3)-Gd(2)-O(4W)	74.15(11)
O(3)-Gd(2)-O(13)	121.87(11)
O(3)-Gd(2)-O(16)#3	140.90(12)
O(4W)-Gd(2)-O(2)	138.52(10)
O(4W)-Gd(2)-O(13)	73.87(11)
O(16)#3-Gd(2)-O(1W)	70.59(12)
O(16)#3-Gd(2)-O(2)	125.10(11)
O(16)#3-Gd(2)-O(3W)	139.76(11)
O(16)#3-Gd(2)-O(4W)	75.16(12)
O(16)#3-Gd(2)-O(13)	70.65(11)
N(3)-Gd(3)-N(2)	128.89(10)
O(9W)-Gd(3)-N(2)	141.86(10)
O(9W)-Gd(3)-N(3)	74.11(10)
O(9W)-Gd(3)-O(14)	149.15(10)
O(9W)-Gd(3)-O(15)	81.74(10)
O(9W)-Gd(3)-O(19)	86.40(11)

O(9W)-Gd(3)-O(23)#2	73.31(10)
O(9W)-Gd(3)-O(24)#2	125.54(10)
O(14)-Gd(3)-N(2)	61.20(10)
O(14)-Gd(3)-N(3)	75.22(10)
O(14)-Gd(3)-O(23)#2	130.86(10)
O(14)-Gd(3)-O(24)#2	78.16(10)
O(15)-Gd(3)-N(2)	60.85(10)
O(15)-Gd(3)-N(3)	137.66(11)
O(15)-Gd(3)-O(14)	120.25(10)
O(15)-Gd(3)-O(19)	150.13(10)
O(15)-Gd(3)-O(23)#2	73.68(11)
O(15)-Gd(3)-O(24)#2	92.11(11)
O(19)-Gd(3)-N(2)	129.80(10)
O(19)-Gd(3)-N(3)	62.69(10)
O(19)-Gd(3)-O(14)	82.53(10)
O(19)-Gd(3)-O(23)#2	76.68(10)
O(19)-Gd(3)-O(24)#2	72.80(11)
O(21)-Gd(3)-N(2)	83.49(11)
O(21)-Gd(3)-N(3)	65.19(10)
O(21)-Gd(3)-O(9W)	81.13(10)
O(21)-Gd(3)-O(14)	83.17(10)
O(21)-Gd(3)-O(15)	77.24(11)
O(21)-Gd(3)-O(19)	127.86(10)
O(21)-Gd(3)-O(23)#2	143.48(10)
O(21)-Gd(3)-O(24)#2	149.99(11)
O(23)#2-Gd(3)-N(2)	100.78(11)
O(23)#2-Gd(3)-N(3)	128.67(10)
O(24)#2-Gd(3)-N(2)	66.98(10)
O(24)#2-Gd(3)-N(3)	130.23(10)
O(24)#2-Gd(3)-O(23)#2	53.32(10)
O(5W)-Gd(4)-O(8W)	69.91(10)
O(5W)-Gd(4)-O(20)	135.83(10)
O(6W)-Gd(4)-O(5W)	65.51(11)
O(6W)-Gd(4)-O(8W)	119.88(11)
O(6W)-Gd(4)-O(20)	113.22(9)
O(7W)-Gd(4)-O(5W)	73.43(10)

O(7W)-Gd(4)-O(6W)	70.47(11)
O(7W)-Gd(4)-O(8W)	130.29(11)
O(7W)-Gd(4)-O(20)	65.82(9)
O(8W)-Gd(4)-O(20)	126.84(9)
O(8)-Gd(4)-O(5W)	85.86(11)
O(8)-Gd(4)-O(6W)	66.81(11)
O(8)-Gd(4)-O(7W)	137.13(10)
O(8)-Gd(4)-O(8W)	71.85(10)
O(8)-Gd(4)-O(20)	136.35(10)
O(17)-Gd(4)-O(5W)	84.75(11)
O(17)-Gd(4)-O(6W)	140.16(12)
O(17)-Gd(4)-O(7W)	76.16(11)
O(17)-Gd(4)-O(8W)	68.22(11)
O(17)-Gd(4)-O(8)	139.81(10)
O(17)-Gd(4)-O(20)	69.97(9)
O(17)-Gd(4)-O(20W)	82.95(12)
O(17)-Gd(4)-O(21W)	134.63(10)
O(20W)-Gd(4)-O(5W)	140.49(11)
O(20W)-Gd(4)-O(6W)	136.82(12)
O(20W)-Gd(4)-O(7W)	138.13(11)
O(20W)-Gd(4)-O(8W)	70.64(11)
O(20W)-Gd(4)-O(8)	79.89(11)
O(20W)-Gd(4)-O(20)	73.05(10)
O(20W)-Gd(4)-O(21W)	74.62(11)
O(21W)-Gd(4)-O(5W)	135.96(10)
O(21W)-Gd(4)-O(6W)	70.55(11)
O(21W)-Gd(4)-O(7W)	94.99(10)
O(21W)-Gd(4)-O(8W)	134.72(10)
O(21W)-Gd(4)-O(8)	74.26(10)
O(21W)-Gd(4)-O(20)	65.97(8)
H(15A)-O(15W)-H(15B)	109.8
H(10A)-O(10W)-H(10B)	102.0(9)
H(16A)-O(16W)-H(16B)	109.6
H(13A)-O(13W)-H(13B)	129.8
H(19A)-O(19W)-H(19B)	109.5
H(17A)-O(17W)-H(17B)	109.6

H(18A)-O(18W)-H(18B)	109.4
H(14A)-O(14W)-H(14B)	109.4
H(12A)-O(12W)-H(12B)	103.5(9)
H(11A)-O(11W)-H(11B)	102.4(9)

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Symmetry transformations used to generate equivalent atoms:

#1  $-x+3, -y+1, -z$  #2  $x-1, y, z$  #3  $-x+2, -y+1, -z+1$

#4  $x+1, y, z$  #5  $-x+2, -y+2, -z$

Table S4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **1**. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
C(1)	9(2)	12(2)	6(1)	-5(1)	0(1)	1(1)
C(2)	8(1)	8(1)	5(1)	-3(1)	-1(1)	1(1)
C(3)	7(1)	10(1)	7(1)	-3(1)	1(1)	-2(1)
C(4)	12(1)	11(1)	8(1)	-2(1)	3(1)	2(1)
C(5)	11(2)	11(2)	10(2)	-4(1)	-1(1)	-1(1)
C(6)	6(1)	11(1)	8(1)	-3(1)	0(1)	0(1)
C(7)	8(1)	10(1)	6(1)	-2(1)	1(1)	0(1)
C(8)	7(1)	10(1)	7(1)	-2(1)	1(1)	0(1)
C(9)	9(1)	8(1)	10(1)	-3(1)	1(1)	-1(1)
C(10)	7(1)	14(1)	17(1)	-7(1)	4(1)	2(1)
C(11)	5(1)	13(1)	13(1)	-6(1)	-2(1)	3(1)
C(12)	6(1)	9(1)	9(1)	-4(1)	1(1)	1(1)
C(13)	11(2)	12(2)	6(1)	-2(1)	2(1)	-2(1)
C(14)	8(1)	9(1)	8(1)	-4(1)	1(1)	-1(1)
C(15)	8(1)	9(1)	5(1)	-2(1)	1(1)	0(1)
C(16)	7(1)	19(2)	7(1)	-6(1)	3(1)	-5(1)
C(17)	7(2)	17(2)	12(2)	1(1)	1(1)	-1(1)
C(18)	10(1)	11(1)	11(1)	-1(1)	-2(1)	-1(1)
C(19)	7(1)	10(1)	9(1)	0(1)	-1(1)	0(1)
C(20)	8(1)	12(1)	10(1)	-1(1)	-1(1)	1(1)
C(21)	4(1)	11(1)	4(1)	-3(1)	-1(1)	0(1)
C(22)	10(2)	12(2)	9(2)	2(1)	1(1)	1(1)
C(23)	7(1)	11(1)	10(1)	-1(1)	0(1)	-1(1)
C(24)	10(2)	10(2)	10(2)	-2(1)	-2(1)	2(1)
N(2)	8(1)	11(1)	6(1)	-2(1)	0(1)	1(1)
N(3)	6(1)	7(1)	6(1)	-3(1)	1(1)	3(1)
N(5)	11(1)	10(1)	9(1)	-4(1)	0(1)	-2(1)
N(6)	9(1)	12(1)	10(1)	-4(1)	0(1)	1(1)
N(4)	10(1)	16(1)	11(1)	1(1)	-1(1)	-2(1)
O(1)	14(1)	12(1)	10(1)	-3(1)	4(1)	4(1)
O(1W)	16(1)	18(1)	21(2)	3(1)	9(1)	8(1)

O(2)	14(1)	16(1)	6(1)	-1(1)	3(1)	0(1)
O(2W)	36(2)	27(2)	13(1)	-11(1)	4(1)	-21(1)
N(1)	8(1)	11(1)	7(1)	-2(1)	2(1)	0(1)
O(3W)	22(1)	23(1)	13(1)	-8(1)	11(1)	-13(1)
O(3)	24(2)	15(1)	6(1)	-2(1)	5(1)	8(1)
O(4W)	36(2)	24(2)	9(1)	0(1)	3(1)	10(2)
O(4)	16(1)	11(1)	12(1)	-1(1)	4(1)	4(1)
O(5W)	20(2)	21(2)	19(2)	2(1)	5(1)	0(1)
O(5)	6(1)	14(1)	15(1)	-8(1)	2(1)	0(1)
O(6W)	26(2)	16(1)	23(2)	-4(1)	-11(1)	2(1)
O(6)	11(1)	20(1)	20(1)	-14(1)	1(1)	0(1)
O(7W)	19(1)	16(1)	13(1)	-5(1)	2(1)	-4(1)
O(7)	7(1)	15(1)	17(1)	-9(1)	0(1)	1(1)
O(8W)	12(1)	26(2)	14(1)	-7(1)	2(1)	1(1)
O(8)	10(1)	19(1)	11(1)	-9(1)	-1(1)	4(1)
O(9W)	11(1)	14(1)	16(1)	-11(1)	1(1)	-1(1)
O(9)	8(1)	14(1)	13(1)	0(1)	-3(1)	-2(1)
O(10)	9(1)	16(1)	14(1)	1(1)	-2(1)	-1(1)
O(11)	13(1)	10(1)	11(1)	-1(1)	-4(1)	2(1)
O(12)	16(1)	21(1)	16(1)	-6(1)	6(1)	-5(1)
O(13)	14(1)	15(1)	7(1)	-4(1)	2(1)	-2(1)
O(14)	10(1)	13(1)	13(1)	-5(1)	5(1)	-2(1)
O(15)	19(1)	14(1)	8(1)	-5(1)	2(1)	-8(1)
O(16)	22(2)	24(2)	8(1)	-4(1)	4(1)	-10(1)
O(17)	19(1)	20(1)	10(1)	1(1)	-2(1)	-4(1)
O(18)	18(1)	14(1)	19(1)	0(1)	-8(1)	-5(1)
O(20)	13(1)	12(1)	10(1)	-1(1)	-3(1)	0(1)
O(20W)	20(2)	14(1)	21(2)	-2(1)	-2(1)	0(1)
O(19)	8(1)	19(1)	15(1)	0(1)	-1(1)	-4(1)
O(21W)	14(1)	29(2)	16(1)	-2(1)	-4(1)	-4(1)
O(21)	8(1)	15(1)	16(1)	4(1)	-1(1)	-1(1)
O(22)	11(1)	17(1)	13(1)	4(1)	0(1)	2(1)
O(23)	9(1)	20(1)	13(1)	-6(1)	1(1)	-1(1)
O(24)	12(1)	15(1)	13(1)	-6(1)	2(1)	1(1)
Gd(1)	5(1)	8(1)	6(1)	-2(1)	1(1)	2(1)
Gd(2)	12(1)	9(1)	6(1)	-2(1)	3(1)	0(1)



Gd(3)	5(1)	9(1)	7(1)	-2(1)	1(1)	0(1)
Gd(4)	10(1)	10(1)	9(1)	-3(1)	0(1)	0(1)
O(15W)	18(2)	24(2)	14(1)	1(1)	4(1)	2(1)
O(10W)	20(1)	17(1)	14(1)	-2(1)	3(1)	-3(1)
O(16W)	21(2)	20(2)	18(1)	-4(1)	6(1)	-2(1)
O(13W)	43(2)	38(2)	27(2)	-2(2)	8(2)	-19(2)
O(19W)	28(2)	20(2)	19(2)	-1(1)	0(1)	1(1)
O(17W)	23(2)	21(2)	51(2)	-16(2)	-10(2)	3(1)
O(18W)	28(2)	30(2)	24(2)	-7(2)	4(2)	-7(2)
O(14W)	25(2)	28(2)	45(2)	1(2)	-14(2)	2(2)
O(12W)	22(2)	19(1)	18(1)	-3(1)	1(1)	-6(1)
O(11W)	26(2)	31(2)	92(4)	24(2)	-24(2)	-12(2)

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Table S5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for **1**.

	x	y	z	U(eq)
H(3WA)	14070(20)	6487(8)	2692(3)	23(16)
H(9WA)	12370(7)	9069(12)	6063(10)	14(14)
H(9WB)	10534(4)	9276(4)	6101(5)	20
H(1WA)	9298(10)	6295(12)	2961(4)	30
H(1WB)	10221(19)	6771(5)	2395(5)	30
H(2WA)	9934(9)	3601(14)	2140(5)	35
H(2WB)	11167(15)	3437(19)	1547(4)	35
H(3WB)	14871(11)	6135(16)	2021(4)	28
H(4WA)	14571(12)	3094(10)	2826(5)	37
H(4WB)	13760(20)	3430(20)	3501(3)	37
H(5WA)	14351(10)	11269(9)	1413(5)	31
H(5WB)	12858(8)	12021(4)	1464(3)	31
H(6WA)	9563(12)	11523(10)	1595(4)	32
H(6WB)	9609(17)	12043(7)	2255(4)	32
H(7WA)	12472(13)	12326(5)	3072(7)	24
H(7WB)	11820(20)	11635(9)	3585(3)	24
H(8WA)	13875(10)	9304(9)	1304(4)	26
H(8WB)	15241(8)	9797(7)	1535(8)	26
H(20A)	13177	8355	2638	27
H(20B)	11936	8367	2227	27
H(21A)	8626(6)	10057(6)	2347(2)	29
H(21B)	8899(12)	10519(4)	3010(2)	29
H(15A)	6066	6663	1040	30
H(15B)	6885	5838	1317	30
H(10A)	13833(8)	7106(12)	3656(5)	25
H(10B)	15567(6)	7048(18)	3376(9)	25
H(16A)	10586	8155	1605	30
H(16B)	9425	7575	1720	30
H(13A)	8932	8919	2972	53
H(13B)	8140	8004	3215	53

H(19A)	15890	1725	2914	35
H(19B)	15766	1901	2242	35
H(17A)	8701	4525	842	47
H(17B)	9402	5154	1200	47
H(18A)	7846	3421	2418	41
H(18B)	8427	3103	3020	41
H(14A)	6325	8341	1971	50
H(14B)	6850	7361	2001	50
H(12A)	7678(14)	6817(5)	3973(3)	29
H(12B)	7306(18)	5861(5)	3710(8)	29
H(11A)	15036(8)	5146(9)	3744(9)	73
H(11B)	16222(18)	4282(5)	3976(10)	73

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Table S6. Torsion angles [°] for **1**.

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C(1)-C(2)-C(3)-C(4)	-4.0(7)
C(1)-C(2)-C(3)-N(1)#1	178.8(4)
C(1)-C(2)-N(1)-C(3)#1	-178.9(4)
C(1)-C(2)-N(1)-Gd(1)	19.5(4)
C(2)-C(1)-O(1)-Gd(1)	17.3(5)
C(2)-C(1)-O(2)-Gd(2)	82.6(5)
C(2)-C(3)-C(4)-O(3)	-13.8(7)
C(2)-C(3)-C(4)-O(4)	167.8(4)
C(3)-C(2)-N(1)-C(3)#1	0.4(6)
C(3)-C(2)-N(1)-Gd(1)	-161.2(3)
C(3)-C(4)-O(3)-Gd(2)	57.3(10)
C(3)-C(4)-O(4)-Gd(1)#1	0.2(6)
C(5)-C(6)-C(7)-C(11)	8.7(6)
C(5)-C(6)-C(7)-N(6)	-172.0(4)
C(5)-C(6)-N(5)-C(9)	174.7(3)
C(5)-C(6)-N(5)-Gd(1)	-11.8(5)
C(6)-C(5)-O(7)-Gd(1)	-8.2(5)
C(6)-C(5)-O(8)-Gd(4)	144.7(4)
C(6)-C(7)-C(11)-O(11)	63.9(5)
C(6)-C(7)-C(11)-O(12)	-118.3(4)
C(6)-C(7)-N(6)-C(8)	-2.9(6)
C(7)-C(6)-N(5)-C(9)	-1.0(6)
C(7)-C(6)-N(5)-Gd(1)	172.5(3)
C(7)-C(11)-O(11)-Gd(1)#5	82.8(4)
C(8)-C(9)-C(10)-O(5)	-177.1(4)
C(8)-C(9)-C(10)-O(6)	5.1(6)
C(8)-C(9)-N(5)-C(6)	-1.1(6)
C(8)-C(9)-N(5)-Gd(1)	-174.8(3)
C(8)-C(12)-O(9)-Gd(1)#2	169.1(3)
C(8)-C(12)-O(10)-Gd(1)#2	-169.3(3)
C(9)-C(8)-C(12)-O(9)	80.1(5)
C(9)-C(8)-C(12)-O(10)	-104.0(4)
C(9)-C(8)-N(6)-C(7)	0.8(6)

C(9)-C(10)-O(5)-Gd(1)	-11.9(5)
C(10)-C(9)-N(5)-C(6)	177.0(4)
C(10)-C(9)-N(5)-Gd(1)	3.3(4)
C(11)-C(7)-N(6)-C(8)	176.4(3)
C(12)-C(8)-C(9)-C(10)	8.3(6)
C(12)-C(8)-C(9)-N(5)	-173.8(4)
C(12)-C(8)-N(6)-C(7)	176.3(3)
C(13)-C(14)-N(2)-C(15)	-176.6(3)
C(13)-C(14)-N(2)-Gd(3)	25.3(4)
C(14)-C(13)-O(13)-Gd(2)	78.2(5)
C(14)-C(13)-O(14)-Gd(3)	4.4(5)
C(14)#3-C(15)-C(16)-O(15)	-164.9(4)
C(14)#3-C(15)-C(16)-O(16)	18.9(6)
C(14)#3-C(15)-N(2)-C(14)	0.0(6)
C(14)#3-C(15)-N(2)-Gd(3)	158.2(3)
C(15)#3-C(14)-N(2)-C(15)	0.0(6)
C(15)#3-C(14)-N(2)-Gd(3)	-158.1(3)
C(15)-C(16)-O(15)-Gd(3)	-3.6(5)
C(15)-C(16)-O(16)-Gd(2)#3	-76.9(6)
C(16)-C(15)-N(2)-C(14)	175.1(3)
C(16)-C(15)-N(2)-Gd(3)	-26.7(4)
C(17)-C(18)-C(19)-C(24)	-5.9(7)
C(17)-C(18)-C(19)-N(3)	174.8(4)
C(17)-C(18)-N(4)-C(21)	-173.2(3)
C(18)-C(17)-O(17)-Gd(4)	90.8(5)
C(18)-C(19)-C(24)-O(20)	0.2(6)
C(18)-C(19)-C(24)-O(19)	-178.8(4)
C(18)-C(19)-N(3)-C(20)	-0.7(5)
C(18)-C(19)-N(3)-Gd(3)	178.5(3)
C(19)-C(18)-N(4)-C(21)	3.1(6)
C(19)-C(24)-O(20)-Gd(4)	69.5(5)
C(19)-C(24)-O(19)-Gd(3)	0.1(5)
C(20)-C(21)-C(22)-O(23)	-93.5(5)
C(20)-C(21)-C(22)-O(24)	91.8(5)
C(20)-C(21)-C(22)-Gd(3)#4	161.8(11)
C(20)-C(21)-N(4)-C(18)	-3.5(6)

C(20)-C(23)-O(21)-Gd(3)	0.1(5)
C(21)-C(20)-C(23)-O(21)	179.6(4)
C(21)-C(20)-C(23)-O(22)	-1.2(6)
C(21)-C(20)-N(3)-C(19)	0.4(5)
C(21)-C(20)-N(3)-Gd(3)	-178.8(3)
C(21)-C(22)-O(23)-Gd(3)#4	-166.4(3)
C(21)-C(22)-O(24)-Gd(3)#4	166.6(3)
C(22)-C(21)-N(4)-C(18)	175.8(3)
C(23)-C(20)-C(21)-C(22)	1.2(6)
C(23)-C(20)-C(21)-N(4)	-179.5(4)
C(23)-C(20)-N(3)-C(19)	-178.4(3)
C(23)-C(20)-N(3)-Gd(3)	2.4(4)
C(24)-C(19)-N(3)-C(20)	179.8(3)
C(24)-C(19)-N(3)-Gd(3)	-1.0(4)
N(2)-C(15)-C(16)-O(15)	20.7(5)
N(2)-C(15)-C(16)-O(16)	-155.5(4)
N(3)-C(19)-C(24)-O(20)	179.6(3)
N(3)-C(19)-C(24)-O(19)	0.6(5)
N(3)-C(20)-C(21)-C(22)	-177.5(3)
N(3)-C(20)-C(21)-N(4)	1.8(6)
N(3)-C(20)-C(23)-O(21)	-1.7(5)
N(3)-C(20)-C(23)-O(22)	177.6(4)
N(5)-C(6)-C(7)-C(11)	-176.2(4)
N(5)-C(6)-C(7)-N(6)	3.1(6)
N(5)-C(9)-C(10)-O(5)	4.9(5)
N(5)-C(9)-C(10)-O(6)	-172.9(4)
N(6)-C(7)-C(11)-O(11)	-115.4(4)
N(6)-C(7)-C(11)-O(12)	62.4(5)
N(6)-C(8)-C(9)-C(10)	-176.6(4)
N(6)-C(8)-C(9)-N(5)	1.3(6)
N(6)-C(8)-C(12)-O(9)	-95.4(4)
N(6)-C(8)-C(12)-O(10)	80.5(4)
N(4)-C(18)-C(19)-C(24)	178.3(4)
N(4)-C(18)-C(19)-N(3)	-1.1(6)
N(4)-C(21)-C(22)-O(23)	87.2(5)
N(4)-C(21)-C(22)-O(24)	-87.4(4)

N(4)-C(21)-C(22)-Gd(3)#4	-17.5(15)
O(1)-C(1)-C(2)-C(3)	157.6(4)
O(1)-C(1)-C(2)-N(1)	-23.1(5)
O(1)-C(1)-O(2)-Gd(2)	-99.8(5)
O(2)-C(1)-C(2)-C(3)	-24.5(6)
O(2)-C(1)-C(2)-N(1)	154.7(4)
O(2)-C(1)-O(1)-Gd(1)	-160.4(3)
N(1)-C(2)-C(3)-C(4)	176.8(4)
N(1)-C(2)-C(3)-N(1)#1	-0.4(6)
N(1)#1-C(3)-C(4)-O(3)	163.6(4)
N(1)#1-C(3)-C(4)-O(4)	-14.8(5)
O(3)-C(4)-O(4)-Gd(1)#1	-178.1(3)
O(4)-C(4)-O(3)-Gd(2)	-124.5(7)
O(6)-C(10)-O(5)-Gd(1)	165.7(3)
O(7)-C(5)-C(6)-C(7)	-171.9(4)
O(7)-C(5)-C(6)-N(5)	12.8(5)
O(7)-C(5)-O(8)-Gd(4)	-34.1(8)
O(8)-C(5)-C(6)-C(7)	9.1(6)
O(8)-C(5)-C(6)-N(5)	-166.2(4)
O(8)-C(5)-O(7)-Gd(1)	170.7(3)
O(9)-C(12)-O(10)-Gd(1)#2	6.5(4)
O(10)-C(12)-O(9)-Gd(1)#2	-6.7(4)
O(12)-C(11)-O(11)-Gd(1)#5	-94.8(5)
O(13)-C(13)-C(14)-C(15)#3	-19.8(6)
O(13)-C(13)-C(14)-N(2)	156.4(4)
O(13)-C(13)-O(14)-Gd(3)	-171.9(3)
O(14)-C(13)-C(14)-C(15)#3	163.8(4)
O(14)-C(13)-C(14)-N(2)	-20.0(5)
O(14)-C(13)-O(13)-Gd(2)	-105.8(5)
O(15)-C(16)-O(16)-Gd(2)#3	107.3(6)
O(16)-C(16)-O(15)-Gd(3)	172.3(3)
O(17)-C(17)-C(18)-C(19)	-52.9(6)
O(17)-C(17)-C(18)-N(4)	123.3(4)
O(18)-C(17)-C(18)-C(19)	131.5(4)
O(18)-C(17)-C(18)-N(4)	-52.3(5)
O(18)-C(17)-O(17)-Gd(4)	-94.1(6)

O(20)-C(24)-O(19)-Gd(3)	-178.9(3)
O(19)-C(24)-O(20)-Gd(4)	-111.6(4)
O(22)-C(23)-O(21)-Gd(3)	-179.1(3)
O(23)-C(22)-O(24)-Gd(3)#4	-7.8(4)
O(24)-C(22)-O(23)-Gd(3)#4	7.7(4)

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Symmetry transformations used to generate equivalent atoms:

#1  $-x+3, -y+1, -z$  #2  $x-1, y, z$  #3  $-x+2, -y+1, -z+1$

#4  $x+1, y, z$  #5  $-x+2, -y+2, -z$



Table S7. Hydrogen bonds lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **1**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(9W)-H(9WA)...O(18)#6	0.986(8)	1.881(7)	2.828(4)	160.2(13)
O(1W)-H(1WA)...O(12W)	1.007(7)	1.804(7)	2.809(4)	176.6(14)
O(1W)-H(1WB)...O(16W)	0.985(7)	1.713(7)	2.684(5)	168.0(10)
O(2W)-H(2WA)...O(18W)	0.984(8)	1.781(11)	2.736(5)	162.7(13)
O(2W)-H(2WB)...O(6)#7	0.987(13)	1.702(8)	2.665(4)	164(2)
O(3W)-H(3WB)...O(15W)#4	0.985(8)	1.733(9)	2.709(5)	170.1(12)
O(4W)-H(4WA)...O(19W)	0.981(7)	1.691(9)	2.638(5)	160.7(14)
O(4W)-H(4WB)...O(22)#8	0.986(7)	1.713(8)	2.685(4)	168(3)
O(5W)-H(5WA)...O(10)#5	1.008(7)	1.957(10)	2.809(4)	140.5(8)
O(6W)-H(6WA)...O(11)	0.996(7)	1.842(8)	2.834(5)	174.3(13)
O(6W)-H(6WB)...O(18W)#9	0.984(7)	1.684(8)	2.638(5)	162.1(11)
O(8W)-H(8WB)...O(12)#4	0.984(8)	1.905(8)	2.784(5)	147.3(13)
O(20W)-H(20A)...O(10W)	0.85	2.14	2.846(5)	139.9
O(21W)-H(21A)...O(12)	0.975(4)	1.933(5)	2.890(4)	166.3(8)
O(15W)-H(15A)...O(9)	0.85	1.92	2.758(5)	170.4
O(15W)-H(15B)...O(17W)	0.85	1.90	2.693(5)	153.9
O(10W)-H(10A)...O(14)	0.986(7)	1.855(8)	2.807(4)	161.3(10)
O(10W)-H(10B)...O(12W)#4	1.005(7)	1.890(8)	2.893(5)	175(2)
O(16W)-H(16B)...O(14W)	0.85	2.09	2.755(6)	134.7
O(13W)-H(13A)...O(21W)	0.86	1.78	2.626(5)	165.2
O(19W)-H(19A)...O(18)#10	0.85	1.90	2.744(5)	172.2
O(17W)-H(17A)...O(5)#7	0.85	2.06	2.873(5)	161.8
O(18W)-H(18A)...O(19W)#2	0.85	2.62	2.690(6)	85.5
O(18W)-H(18B)...O(15)#3	0.85	2.09	2.823(5)	144.6
O(14W)-H(14B)...O(15W)	0.85	2.04	2.831(6)	153.9
O(12W)-H(12A)...O(24)#2	0.984(6)	1.900(7)	2.810(4)	152.5(10)
O(12W)-H(12B)...O(11W)#2	0.985(8)	1.729(11)	2.681(5)	161.4(14)
O(11W)-H(11B)...O(21)#8	0.983(7)	1.866(9)	2.818(5)	162.3(17)

Symmetry transformations used to generate equivalent atoms:

#1 -x+3,-y+1,-z #2 x-1,y,z #3 -x+2,-y+1,-z+1, #4 x+1,y,z #5 -x+2,-y+2,-z #6 -x+3,-y+2,-z+1  
#7 -x+2,-y+1,-z #8 -x+3,-y+1,-z+1 #9 x,y+1,z , #10 x,y-1,z



Table S8. Crystal data and structure refinement for **2**.

Identification code	<b>2</b>	
Empirical formula	C <sub>24</sub> H <sub>42</sub> N <sub>6</sub> O <sub>45</sub> Tb <sub>4</sub>	
Formula weight	1770.31	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.5627(15) Å	α = 88.568(3)°.
	b = 14.078(3) Å	β = 86.325(4)°.
	c = 20.297(4) Å	γ = 81.382(3)°.
Volume	2413.9(7) Å <sup>3</sup>	
Z	2	
Density (calculated)	2.436 Mg/m <sup>3</sup>	
Absorption coefficient	5.923 mm <sup>-1</sup>	
F(000)	1696	
Crystal size	0.833 x 0.106 x 0.032 mm <sup>3</sup>	
Theta range for data collection	1.463 to 26.732°.	
Index ranges	-10 ≤ h ≤ 10, -17 ≤ k ≤ 17, -25 ≤ l ≤ 25	
Reflections collected	19021	
Independent reflections	10146 [R(int) = 0.1810]	
Completeness to theta = 26.000°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	10146 / 874 / 787	
Goodness-of-fit on F <sup>2</sup>	0.971	
Final R indices [I > 2σ(I)]	R1 = 0.1347, wR2 = 0.2557	
R indices (all data)	R1 = 0.2457, wR2 = 0.2983	
Extinction coefficient	n/a	
Largest diff. peak and hole	4.694 and -4.535 e.Å <sup>-3</sup>	

Table S9. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **2**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	$U(\text{eq})$
Tb(1)	12736(1)	7627(1)	-190(1)	9(1)
Tb(2)	12352(1)	4856(1)	2480(1)	13(1)
Tb(3)	1178(1)	7603(1)	5143(1)	10(1)
Tb(4)	2113(1)	10298(1)	2411(1)	18(1)
O(1)	12127(12)	6751(8)	792(6)	9(1)
O(1W)	10180(5)	6144(3)	2640(2)	20(2)
O(2)	11900(13)	5422(8)	1358(6)	9(1)
O(2W)	11058(5)	3738(7)	1967(5)	30(3)
O(3)	14401(14)	4175(8)	1752(6)	14(1)
O(3W)	14023(5)	6017(3)	2343(2)	25(3)
O(4)	15895(13)	3113(8)	1140(6)	11(1)
O(4W)	13632(5)	3452(5)	3055(2)	47(3)
O(5)	10642(13)	6884(8)	-567(6)	15(1)
O(5W)	3417(5)	11520(3)	1720(2)	31(3)
O(6)	8079(12)	6998(6)	-799(3)	18(1)
O(6W)	233(6)	11622(5)	1925(2)	30(3)
O(7)	12552(12)	8911(8)	647(5)	11(1)
O(7W)	1990(7)	11754(3)	3102(2)	18(3)
O(8)	11114(13)	9897(8)	1364(6)	14(1)
O(8W)	4340(5)	9470(4)	1698(2)	22(3)
O(9)	5256(13)	7466(8)	292(6)	12(1)
O(9W)	1446(4)	8831(4)	5906(3)	21(3)
O(10)	5000(13)	8557(8)	-507(5)	12(1)
O(11)	8287(12)	11193(8)	947(5)	12(1)
O(12)	6984(11)	10365(8)	1743(6)	14(1)
O(13)	12739(13)	5362(8)	3557(6)	16(1)
O(14)	12240(11)	6641(8)	4177(5)	14(1)
O(15)	10281(13)	6816(8)	6137(6)	10(1)
O(16)	9553(13)	5623(8)	6752(6)	14(1)
O(17)	4573(15)	10075(9)	2913(7)	22(1)
O(18)	5598(11)	10918(9)	3667(6)	19(1)

O(19)	769(13)	8857(8)	4325(6)	13(1)
O(20)	1486(4)	9997(4)	3633(4)	14(1)
O(20W)	2184(14)	8613(9)	2567(7)	25(3)
O(21)	3649(13)	6933(8)	5571(6)	16(1)
O(21W)	-564(16)	10068(10)	2623(7)	35(3)
O(22)	6205(13)	6827(8)	5668(5)	15(1)
O(23)	8458(14)	8422(9)	5458(5)	19(1)
O(24)	8731(13)	7403(8)	4592(6)	16(1)
N(1)	14004(16)	5856(10)	-120(7)	10(1)
N(2)	10721(16)	5743(10)	5083(7)	11(1)
N(3)	3568(16)	8329(10)	4723(7)	11(1)
N(4)	6228(17)	9157(10)	4311(8)	16(1)
N(5)	9996(16)	8360(10)	229(8)	13(1)
N(6)	6946(16)	9241(10)	565(7)	12(1)
C(1)	12521(19)	5866(12)	915(9)	9(1)
C(2)	13900(20)	5374(12)	464(9)	12(1)
C(3)	14921(19)	4539(12)	608(9)	9(1)
C(4)	15070(20)	3886(12)	1216(9)	11(1)
C(5)	11300(20)	9327(12)	909(9)	12(1)
C(6)	9760(20)	9124(12)	629(9)	13(1)
C(7)	8220(20)	9547(12)	760(9)	12(1)
C(8)	7210(20)	8492(12)	163(9)	13(1)
C(9)	8650(20)	8025(13)	-31(9)	14(1)
C(10)	9210(20)	7191(13)	-480(10)	15(1)
O(10W)	4514(5)	7269(5)	3261(3)	34(3)
C(11)	7790(20)	10443(12)	1203(9)	13(1)
C(12)	5740(20)	8138(12)	-27(9)	13(1)
C(13)	12040(20)	5812(13)	4019(9)	14(1)
C(14)	10880(20)	5383(12)	4530(9)	11(1)
C(15)	9801(19)	5477(12)	5580(9)	10(1)
C(16)	9860(19)	6016(12)	6223(9)	9(1)
C(17)	4910(20)	10231(13)	3533(10)	17(1)
C(18)	4780(20)	9440(13)	4065(10)	16(1)
C(19)	3460(20)	9022(12)	4272(9)	12(1)
C(20)	4980(20)	8001(12)	4949(9)	12(1)
C(21)	6260(20)	8395(13)	4747(10)	14(1)

C(22)	7880(20)	8068(13)	4976(10)	16(1)
C(23)	4970(20)	7170(12)	5439(9)	12(1)
C(24)	1770(20)	9332(12)	4023(9)	13(1)
O(11W)	-3822(19)	14910(11)	3872(9)	55(3)
O(12W)	-2338(9)	16472(8)	3567(5)	21(3)
O(13W)	8873(19)	8387(12)	3180(9)	54(3)
O(14W)	7093(17)	7929(11)	2103(8)	45(3)
O(15W)	6229(14)	6356(10)	1395(7)	25(3)
O(16W)	10338(17)	7655(9)	1840(6)	42(3)
O(17W)	8770(20)	5079(12)	924(9)	64(3)
O(18W)	-1488(18)	13001(9)	2613(8)	60(3)
O(19W)	5981(14)	12166(8)	2587(7)	35(3)

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Table S10. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **2**.

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Tb(1)-O(1)	2.389(12)
Tb(1)-O(5)	2.382(11)
Tb(1)-O(7)	2.493(11)
Tb(1)-N(1)	2.570(14)
Tb(1)-N(5)	2.522(14)
Tb(1)-O(9)#1	2.404(11)
Tb(1)-O(10)#1	2.538(11)
Tb(1)-O(11)#2	2.344(11)
Tb(1)-O(4)#3	2.370(12)
Tb(2)-O(1W)	2.407(4)
Tb(2)-O(2)	2.429(12)
Tb(2)-O(2W)	2.354(8)
Tb(2)-O(3)	2.327(12)
Tb(2)-O(3W)	2.329(4)
Tb(2)-O(4W)	2.423(6)
Tb(2)-O(13)	2.375(12)
Tb(2)-O(16)#4	2.345(12)
Tb(3)-O(9W)	2.395(6)
Tb(3)-O(19)	2.396(12)
Tb(3)-O(21)	2.391(11)
Tb(3)-N(3)	2.513(14)
Tb(3)-O(14)#5	2.458(10)
Tb(3)-O(15)#5	2.415(12)
Tb(3)-O(23)#5	2.491(12)
Tb(3)-O(24)#5	2.493(11)
Tb(3)-N(2)#5	2.712(14)
Tb(4)-O(5W)	2.535(4)
Tb(4)-O(6W)	2.500(6)
Tb(4)-O(7W)	2.497(4)
Tb(4)-O(8W)	2.481(5)
Tb(4)-O(17)	2.373(13)
Tb(4)-O(20)	2.542(8)
Tb(4)-O(20W)	2.378(13)
Tb(4)-O(21W)	2.374(14)

Tb(4)-O(8)#5	2.451(12)
O(1)-C(1)	1.26(2)
O(2)-C(1)	1.22(2)
O(3)-C(4)	1.25(2)
O(4)-C(4)	1.21(2)
O(5)-C(10)	1.24(2)
O(6)-C(10)	1.27(2)
O(7)-C(5)	1.24(2)
O(8)-C(5)	1.23(2)
O(9)-C(12)	1.24(2)
O(10)-C(12)	1.28(2)
O(11)-C(11)	1.28(2)
O(12)-C(11)	1.27(2)
O(13)-C(13)	1.22(2)
O(14)-C(13)	1.26(2)
O(15)-C(16)	1.24(2)
O(16)-C(16)	1.23(2)
O(17)-C(17)	1.34(2)
O(18)-C(17)	1.25(2)
O(19)-C(24)	1.28(2)
O(20)-C(24)	1.217(19)
O(21)-C(23)	1.24(2)
O(22)-C(23)	1.21(2)
O(23)-C(22)	1.27(2)
O(24)-C(22)	1.33(2)
N(1)-C(2)	1.36(2)
N(1)-C(3)#3	1.38(2)
O(1W)-H(1WB)	0.974(6)
O(1W)-H(1WA)	0.979(6)
N(2)-C(15)	1.32(2)
N(2)-C(14)	1.23(2)
O(2W)-H(2WB)	0.959(13)
O(2W)-H(2WA)	0.976(7)
N(3)-C(20)	1.33(2)
N(3)-C(19)	1.32(2)
O(3W)-H(3WB)	0.975(6)



O(3W)-H(3WA)	0.975(6)
N(4)-C(21)	1.37(2)
N(4)-C(18)	1.37(2)
O(4W)-H(4WA)	0.975(8)
O(4W)-H(4WB)	0.975(6)
N(5)-C(9)	1.44(2)
N(5)-C(6)	1.35(2)
O(5W)-H(5WB)	0.987(6)
O(5W)-H(5WA)	0.976(7)
N(6)-C(8)	1.33(2)
N(6)-C(7)	1.32(2)
O(6W)-H(6WB)	0.975(8)
O(6W)-H(6WA)	0.978(7)
O(7W)-H(7WA)	0.981(7)
O(7W)-H(7WB)	0.979(6)
O(8W)-H(8WB)	0.975(7)
O(8W)-H(8WA)	0.976(6)
O(9W)-H(9WB)	0.988(7)
O(9W)-H(9WA)	0.986(8)
O(20W)-H(20A)	0.8500
O(20W)-H(20B)	0.8500
O(21W)-H(21B)	0.8500
O(21W)-H(21A)	0.8500
C(1)-C(2)	1.54(2)
C(2)-C(3)	1.39(2)
C(3)-C(4)	1.52(3)
C(5)-C(6)	1.54(2)
C(6)-C(7)	1.38(2)
C(7)-C(11)	1.55(2)
C(8)-C(12)	1.50(2)
C(8)-C(9)	1.35(2)
C(9)-C(10)	1.51(3)
C(13)-C(14)	1.56(3)
C(14)-C(15)#4	1.45(2)
C(15)-C(16)	1.53(3)
C(17)-C(18)	1.54(3)

C(18)-C(19)	1.39(2)
C(19)-C(24)	1.56(2)
C(20)-C(21)	1.34(2)
C(20)-C(23)	1.52(2)
C(21)-C(22)	1.49(3)
O(10W)-H(10A)	0.984(9)
O(10W)-H(10B)	0.988(10)
O(14W)-H(14W)	0.8500
O(15W)-H(15A)	0.8500
O(15W)-H(15B)	0.8500
O(16W)-H(16A)	0.8400
O(16W)-H(16B)	0.8500
O(17W)-H(17A)	0.8400
O(17W)-H(17B)	0.8500
O(18W)-H(18A)	0.8500
O(18W)-H(18B)	0.8500
O(19W)-H(19A)	0.8500
O(19W)-H(19B)	0.8500
O(1)-Tb(1)-O(5)	81.1(4)
O(1)-Tb(1)-O(7)	79.5(4)
O(1)-Tb(1)-N(1)	62.9(4)
O(1)-Tb(1)-N(5)	73.6(4)
O(1)-Tb(1)-O(9)#1	80.7(4)
O(1)-Tb(1)-O(10)#1	131.5(4)
O(1)-Tb(1)-O(11)#2	144.4(4)
O(1)-Tb(1)-O(4)#3	123.0(4)
O(5)-Tb(1)-O(7)	127.7(4)
O(5)-Tb(1)-N(1)	80.3(4)
O(5)-Tb(1)-N(5)	64.9(4)
O(5)-Tb(1)-O(9)#1	148.8(4)
O(5)-Tb(1)-O(10)#1	146.5(4)
O(5)-Tb(1)-O(11)#2	80.4(4)
O(4)#3-Tb(1)-O(5)	81.9(4)
O(7)-Tb(1)-N(1)	129.4(4)
O(7)-Tb(1)-N(5)	63.1(4)

O(7)-Tb(1)-O(9)#1	72.9(4)
O(7)-Tb(1)-O(10)#1	74.4(3)
O(7)-Tb(1)-O(11)#2	88.3(4)
O(4)#3-Tb(1)-O(7)	147.6(4)
N(1)-Tb(1)-N(5)	127.7(4)
O(9)#1-Tb(1)-N(1)	68.8(4)
O(10)#1-Tb(1)-N(1)	105.5(4)
O(11)#2-Tb(1)-N(1)	141.7(4)
O(4)#3-Tb(1)-N(1)	60.7(4)
O(9)#1-Tb(1)-N(5)	132.1(5)
O(10)#1-Tb(1)-N(5)	125.2(4)
O(11)#2-Tb(1)-N(5)	71.0(4)
O(4)#3-Tb(1)-N(5)	140.9(5)
O(9)#1-Tb(1)-O(10)#1	52.9(4)
O(9)#1-Tb(1)-O(11)#2	127.4(4)
O(4)#3-Tb(1)-O(9)#1	87.1(4)
O(10)#1-Tb(1)-O(11)#2	75.0(4)
O(4)#3-Tb(1)-O(10)#1	73.2(4)
O(4)#3-Tb(1)-O(11)#2	84.0(4)
O(1W)-Tb(2)-O(2)	77.5(3)
O(1W)-Tb(2)-O(2W)	99.7(2)
O(1W)-Tb(2)-O(3)	145.2(3)
O(1W)-Tb(2)-O(3W)	87.87(15)
O(1W)-Tb(2)-O(4W)	140.09(14)
O(1W)-Tb(2)-O(13)	78.6(3)
O(1W)-Tb(2)-O(16)#4	70.3(3)
O(2)-Tb(2)-O(2W)	72.1(4)
O(2)-Tb(2)-O(3)	69.4(4)
O(2)-Tb(2)-O(3W)	78.2(3)
O(2)-Tb(2)-O(4W)	139.4(3)
O(2)-Tb(2)-O(13)	143.6(4)
O(2)-Tb(2)-O(16)#4	126.0(4)
O(2W)-Tb(2)-O(3)	80.3(3)
O(2W)-Tb(2)-O(3W)	146.8(3)
O(2W)-Tb(2)-O(4W)	84.0(3)
O(2W)-Tb(2)-O(13)	139.4(4)

O(2W)-Tb(2)-O(16)#4	72.1(4)
O(3)-Tb(2)-O(3W)	75.5(3)
O(3)-Tb(2)-O(4W)	74.7(3)
O(3)-Tb(2)-O(13)	123.6(4)
O(3)-Tb(2)-O(16)#4	139.4(4)
O(3W)-Tb(2)-O(4W)	110.67(16)
O(3W)-Tb(2)-O(13)	73.8(3)
O(3W)-Tb(2)-O(16)#4	139.8(3)
O(4W)-Tb(2)-O(13)	73.7(3)
O(4W)-Tb(2)-O(16)#4	73.3(3)
O(13)-Tb(2)-O(16)#4	69.2(4)
O(9W)-Tb(3)-O(19)	86.9(3)
O(9W)-Tb(3)-O(21)	80.6(3)
O(9W)-Tb(3)-N(3)	73.9(3)
O(9W)-Tb(3)-O(14)#5	149.2(3)
O(9W)-Tb(3)-O(15)#5	82.1(3)
O(9W)-Tb(3)-O(23)#5	73.1(3)
O(9W)-Tb(3)-O(24)#5	126.3(3)
O(9W)-Tb(3)-N(2)#5	142.4(3)
O(19)-Tb(3)-O(21)	126.5(4)
O(19)-Tb(3)-N(3)	63.2(4)
O(14)#5-Tb(3)-O(19)	82.4(4)
O(15)#5-Tb(3)-O(19)	150.0(4)
O(19)-Tb(3)-O(23)#5	77.2(4)
O(19)-Tb(3)-O(24)#5	72.8(4)
O(19)-Tb(3)-N(2)#5	129.1(4)
O(21)-Tb(3)-N(3)	63.3(4)
O(14)#5-Tb(3)-O(21)	82.7(4)
O(15)#5-Tb(3)-O(21)	79.1(4)
O(21)-Tb(3)-O(23)#5	143.7(4)
O(21)-Tb(3)-O(24)#5	150.3(4)
O(21)-Tb(3)-N(2)#5	84.1(4)
O(14)#5-Tb(3)-N(3)	75.5(4)
O(15)#5-Tb(3)-N(3)	137.9(4)
O(23)#5-Tb(3)-N(3)	128.9(4)
O(24)#5-Tb(3)-N(3)	130.7(4)

N(2)#5-Tb(3)-N(3)	127.8(4)
O(14)#5-Tb(3)-O(15)#5	119.8(4)
O(14)#5-Tb(3)-O(23)#5	131.4(3)
O(14)#5-Tb(3)-O(24)#5	77.7(4)
O(14)#5-Tb(3)-N(2)#5	60.1(4)
O(15)#5-Tb(3)-O(23)#5	73.0(4)
O(15)#5-Tb(3)-O(24)#5	91.5(4)
O(15)#5-Tb(3)-N(2)#5	61.3(4)
O(23)#5-Tb(3)-O(24)#5	54.3(4)
O(23)#5-Tb(3)-N(2)#5	101.8(4)
O(24)#5-Tb(3)-N(2)#5	66.9(4)
O(5W)-Tb(4)-O(6W)	65.24(16)
O(5W)-Tb(4)-O(7W)	72.98(14)
O(5W)-Tb(4)-O(8W)	69.97(16)
O(5W)-Tb(4)-O(17)	82.3(3)
O(5W)-Tb(4)-O(20)	136.45(16)
O(5W)-Tb(4)-O(20W)	141.6(3)
O(5W)-Tb(4)-O(21W)	132.9(4)
O(5W)-Tb(4)-O(8)#5	84.5(3)
O(6W)-Tb(4)-O(7W)	71.73(17)
O(6W)-Tb(4)-O(8W)	119.03(15)
O(6W)-Tb(4)-O(17)	139.3(3)
O(6W)-Tb(4)-O(20)	113.34(15)
O(6W)-Tb(4)-O(20W)	135.0(3)
O(6W)-Tb(4)-O(21W)	67.9(4)
O(6W)-Tb(4)-O(8)#5	65.8(3)
O(7W)-Tb(4)-O(8W)	129.62(18)
O(7W)-Tb(4)-O(17)	76.0(3)
O(7W)-Tb(4)-O(20)	66.29(16)
O(7W)-Tb(4)-O(20W)	138.3(4)
O(7W)-Tb(4)-O(21W)	97.0(4)
O(7W)-Tb(4)-O(8)#5	137.2(3)
O(8W)-Tb(4)-O(17)	66.4(3)
O(8W)-Tb(4)-O(20)	127.62(16)
O(8W)-Tb(4)-O(20W)	71.8(3)
O(8W)-Tb(4)-O(21W)	133.3(4)

O(8)#5-Tb(4)-O(8W)	70.9(3)
O(17)-Tb(4)-O(20)	73.8(3)
O(17)-Tb(4)-O(20W)	85.7(4)
O(17)-Tb(4)-O(21W)	141.1(5)
O(8)#5-Tb(4)-O(17)	137.2(4)
O(20)-Tb(4)-O(20W)	72.7(4)
O(20)-Tb(4)-O(21W)	68.6(4)
O(8)#5-Tb(4)-O(20)	136.9(3)
O(20W)-Tb(4)-O(21W)	74.5(4)
O(8)#5-Tb(4)-O(20W)	80.0(4)
O(8)#5-Tb(4)-O(21W)	72.3(4)
Tb(1)-O(1)-C(1)	128.0(11)
Tb(2)-O(2)-C(1)	139.6(11)
Tb(2)-O(3)-C(4)	157.6(12)
Tb(1)#3-O(4)-C(4)	131.8(12)
Tb(1)-O(5)-C(10)	125.5(11)
Tb(1)-O(7)-C(5)	124.7(10)
Tb(4)#1-O(8)-C(5)	144.8(11)
Tb(1)#5-O(9)-C(12)	95.8(10)
Tb(1)#5-O(10)-C(12)	88.6(9)
Tb(1)#2-O(11)-C(11)	133.6(10)
Tb(2)-O(13)-C(13)	141.3(11)
Tb(3)#1-O(14)-C(13)	130.4(10)
Tb(3)#1-O(15)-C(16)	130.7(11)
Tb(2)#4-O(16)-C(16)	148.8(11)
Tb(4)-O(17)-C(17)	130.4(11)
Tb(3)-O(19)-C(24)	129.6(11)
Tb(4)-O(20)-C(24)	136.2(9)
Tb(3)-O(21)-C(23)	128.2(11)
Tb(3)#1-O(23)-C(22)	92.4(10)
Tb(3)#1-O(24)-C(22)	90.8(10)
Tb(1)-N(1)-C(2)	119.1(11)
Tb(1)-N(1)-C(3)#3	120.8(11)
C(2)-N(1)-C(3)#3	118.5(14)
H(1WA)-O(1W)-H(1WB)	104.9(9)
Tb(2)-O(1W)-H(1WA)	132.4(7)

Tb(2)-O(1W)-H(1WB)	120.8(7)
Tb(3)#1-N(2)-C(14)	116.4(11)
C(14)-N(2)-C(15)	125.0(16)
Tb(3)#1-N(2)-C(15)	113.2(11)
H(2WA)-O(2W)-H(2WB)	106.2(11)
Tb(2)-O(2W)-H(2WA)	120.5(9)
Tb(2)-O(2W)-H(2WB)	129.0(11)
Tb(3)-N(3)-C(20)	119.9(11)
Tb(3)-N(3)-C(19)	121.2(11)
C(19)-N(3)-C(20)	119.0(15)
Tb(2)-O(3W)-H(3WA)	126.8(5)
Tb(2)-O(3W)-H(3WB)	123.8(8)
H(3WA)-O(3W)-H(3WB)	105.1(9)
C(18)-N(4)-C(21)	113.6(15)
Tb(2)-O(4W)-H(4WB)	123.5(11)
H(4WA)-O(4W)-H(4WB)	105.1(9)
Tb(2)-O(4W)-H(4WA)	115.7(5)
Tb(1)-N(5)-C(6)	121.5(11)
C(6)-N(5)-C(9)	119.3(14)
Tb(1)-N(5)-C(9)	118.7(11)
Tb(4)-O(5W)-H(5WB)	122.8(4)
H(5WA)-O(5W)-H(5WB)	103.8(7)
Tb(4)-O(5W)-H(5WA)	116.2(6)
C(7)-N(6)-C(8)	115.6(15)
Tb(4)-O(6W)-H(6WB)	113.2(5)
H(6WA)-O(6W)-H(6WB)	105.0(8)
Tb(4)-O(6W)-H(6WA)	123.6(8)
H(7WA)-O(7W)-H(7WB)	104.4(10)
Tb(4)-O(7W)-H(7WA)	133.4(6)
Tb(4)-O(7W)-H(7WB)	115.4(6)
H(8WA)-O(8W)-H(8WB)	105.1(8)
Tb(4)-O(8W)-H(8WB)	115.6(6)
Tb(4)-O(8W)-H(8WA)	99.8(5)
Tb(3)-O(9W)-H(9WA)	135.1(6)
Tb(3)-O(9W)-H(9WB)	121.2(4)
H(9WA)-O(9W)-H(9WB)	103.6(8)

Tb(4)-O(20W)-H(20A)	109.00
Tb(4)-O(20W)-H(20B)	109.00
H(20A)-O(20W)-H(20B)	110.00
Tb(4)-O(21W)-H(21A)	144.00
H(21A)-O(21W)-H(21B)	110.00
Tb(4)-O(21W)-H(21B)	95.00
O(1)-C(1)-C(2)	114.4(15)
O(1)-C(1)-O(2)	124.3(16)
O(2)-C(1)-C(2)	121.3(15)
N(1)-C(2)-C(3)	122.6(16)
C(1)-C(2)-C(3)	126.5(16)
N(1)-C(2)-C(1)	110.9(14)
N(1)#3-C(3)-C(4)	108.4(14)
C(2)-C(3)-C(4)	132.8(16)
N(1)#3-C(3)-C(2)	118.7(16)
O(3)-C(4)-C(3)	119.5(15)
O(4)-C(4)-C(3)	115.9(16)
O(3)-C(4)-O(4)	124.5(17)
O(7)-C(5)-C(6)	116.8(15)
O(8)-C(5)-C(6)	114.7(15)
O(7)-C(5)-O(8)	128.5(16)
N(5)-C(6)-C(7)	116.9(16)
C(5)-C(6)-C(7)	130.5(16)
N(5)-C(6)-C(5)	112.4(14)
N(6)-C(7)-C(11)	111.7(14)
C(6)-C(7)-C(11)	122.1(15)
N(6)-C(7)-C(6)	126.2(16)
N(6)-C(8)-C(9)	125.0(16)
C(9)-C(8)-C(12)	120.6(16)
N(6)-C(8)-C(12)	114.2(15)
N(5)-C(9)-C(8)	116.8(16)
C(8)-C(9)-C(10)	133.6(16)
N(5)-C(9)-C(10)	109.6(14)
O(5)-C(10)-C(9)	120.5(16)
O(6)-C(10)-C(9)	110.2(14)
O(5)-C(10)-O(6)	128.4(17)



O(11)-C(11)-C(7)	112.9(15)
O(12)-C(11)-C(7)	118.6(14)
O(11)-C(11)-O(12)	128.5(15)
O(9)-C(12)-C(8)	119.4(16)
O(10)-C(12)-C(8)	118.6(15)
O(9)-C(12)-O(10)	122.0(16)
O(13)-C(13)-O(14)	125.1(16)
O(14)-C(13)-C(14)	111.4(15)
O(13)-C(13)-C(14)	123.4(16)
N(2)-C(14)-C(13)	116.0(15)
C(13)-C(14)-C(15)#4	123.8(15)
N(2)-C(14)-C(15)#4	119.5(16)
C(14)#4-C(15)-C(16)	129.4(16)
N(2)-C(15)-C(16)	114.6(14)
N(2)-C(15)-C(14)#4	115.0(16)
O(15)-C(16)-C(15)	113.5(15)
O(15)-C(16)-O(16)	127.2(17)
O(16)-C(16)-C(15)	119.2(15)
O(17)-C(17)-C(18)	119.3(15)
O(17)-C(17)-O(18)	121.3(17)
O(18)-C(17)-C(18)	118.0(17)
N(4)-C(18)-C(19)	122.3(17)
C(17)-C(18)-C(19)	128.2(16)
N(4)-C(18)-C(17)	109.5(15)
C(18)-C(19)-C(24)	124.6(16)
N(3)-C(19)-C(18)	120.3(16)
N(3)-C(19)-C(24)	115.0(15)
C(21)-C(20)-C(23)	125.0(16)
N(3)-C(20)-C(23)	114.1(15)
N(3)-C(20)-C(21)	120.9(16)
N(4)-C(21)-C(22)	112.2(15)
N(4)-C(21)-C(20)	123.7(16)
C(20)-C(21)-C(22)	124.1(17)
O(23)-C(22)-C(21)	124.6(16)
O(23)-C(22)-O(24)	122.0(15)
O(24)-C(22)-C(21)	113.2(16)

O(21)-C(23)-C(20)	114.4(15)
O(22)-C(23)-C(20)	118.4(15)
O(21)-C(23)-O(22)	127.1(16)
O(20)-C(24)-C(19)	121.9(14)
O(19)-C(24)-O(20)	126.9(15)
O(19)-C(24)-C(19)	110.9(14)
H(10A)-O(10W)-H(10B)	103.5(11)
H(15A)-O(15W)-H(15B)	110.00
H(16A)-O(16W)-H(16B)	109.00
H(17A)-O(17W)-H(17B)	109.00
H(18A)-O(18W)-H(18B)	110.00
H(19A)-O(19W)-H(19B)	110.00

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Symmetry transformations used to generate equivalent atoms:

#1  $x+1,y,z$  #2  $-x+2,-y+2,-z$  #3  $-x+3,-y+1,-z$

#4  $-x+2,-y+1,-z+1$  #5  $x-1,y,z$

Table S11. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **2**. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Tb(1)	7(1)	14(1)	6(1)	0(1)	0(1)	-1(1)
Tb(2)	19(1)	14(1)	6(1)	1(1)	3(1)	-4(1)
Tb(3)	8(1)	16(1)	7(1)	1(1)	-2(1)	-4(1)
Tb(4)	18(1)	20(1)	17(1)	1(1)	-3(1)	-5(1)
O(1)	8(2)	10(1)	9(2)	1(1)	-2(2)	-3(1)
O(1W)	20(4)	18(4)	19(4)	7(4)	-3(4)	6(3)
O(2)	10(2)	9(1)	8(1)	0(1)	-2(1)	-3(1)
O(2W)	36(5)	37(5)	21(5)	-6(5)	0(5)	-15(4)
O(3)	16(2)	14(2)	10(1)	1(1)	0(1)	1(2)
O(3W)	26(5)	32(5)	20(5)	-6(5)	1(5)	-18(4)
O(4)	10(2)	11(1)	11(2)	1(1)	-1(1)	-3(1)
O(4W)	49(6)	50(6)	39(6)	-6(5)	-3(5)	2(5)
O(5)	15(1)	16(2)	15(2)	-1(1)	-1(1)	-3(1)
O(5W)	33(5)	31(5)	27(6)	-1(5)	0(5)	-1(4)
O(6)	17(1)	20(1)	18(1)	-2(1)	-2(1)	-4(1)
O(6W)	31(5)	28(5)	30(6)	-5(5)	0(5)	1(4)
O(7)	12(1)	11(1)	12(1)	0(1)	-1(1)	-3(1)
O(7W)	22(5)	16(5)	14(5)	5(4)	2(4)	-2(4)
O(8)	14(1)	14(1)	14(1)	-1(1)	-1(1)	-2(1)
O(8W)	18(5)	24(5)	25(5)	-8(4)	4(4)	-8(4)
O(9)	12(1)	12(1)	12(1)	-1(1)	-1(1)	-2(1)
O(9W)	21(5)	18(5)	24(5)	7(4)	-4(5)	-3(4)
O(10)	12(1)	12(1)	12(1)	-1(1)	0(1)	-1(1)
O(11)	12(1)	12(1)	12(1)	0(1)	-1(1)	-2(1)
O(12)	15(1)	15(2)	14(1)	-1(1)	0(1)	-3(1)
O(13)	16(2)	17(2)	15(1)	-1(1)	3(1)	-5(1)
O(14)	16(2)	14(1)	12(2)	2(1)	0(2)	-4(1)
O(15)	10(2)	10(1)	10(2)	1(1)	0(2)	-3(1)
O(16)	21(3)	13(2)	11(1)	1(1)	-1(1)	-9(1)
O(17)	23(2)	21(2)	21(1)	0(1)	-4(1)	-2(2)
O(18)	20(2)	19(1)	19(2)	0(1)	-1(1)	-6(1)

O(19)	13(1)	14(1)	11(2)	0(1)	-2(1)	-3(1)
O(20)	13(2)	15(1)	13(1)	0(1)	0(1)	-2(1)
O(20W)	24(5)	26(5)	25(5)	-7(5)	-2(5)	-1(4)
O(21)	14(1)	19(2)	16(3)	3(2)	-3(1)	-4(1)
O(21W)	39(6)	37(6)	25(6)	-1(5)	-11(5)	6(4)
O(22)	13(1)	16(2)	16(2)	2(2)	-2(1)	-4(1)
O(23)	16(2)	22(2)	18(1)	-2(1)	-3(1)	-4(1)
O(24)	16(2)	17(1)	14(2)	2(1)	-2(1)	-2(1)
N(1)	10(3)	11(2)	9(1)	0(1)	-1(1)	-3(1)
N(2)	10(2)	11(2)	11(1)	1(1)	-1(1)	-1(1)
N(3)	13(1)	11(1)	11(1)	-4(1)	-1(1)	-2(1)
N(4)	14(1)	17(1)	18(1)	2(1)	-2(1)	-4(1)
N(5)	13(1)	13(1)	14(1)	0(1)	-1(1)	-2(1)
N(6)	12(1)	12(1)	12(1)	1(1)	-1(1)	-2(1)
C(1)	10(1)	10(1)	9(1)	0(1)	-2(1)	-3(1)
C(2)	12(1)	12(1)	10(1)	1(1)	0(1)	-1(1)
C(3)	10(2)	10(1)	9(1)	-1(1)	-2(1)	-4(1)
C(4)	11(2)	12(1)	10(1)	1(1)	-1(1)	-2(1)
C(5)	12(1)	12(1)	12(1)	1(1)	-1(1)	-2(1)
C(6)	12(1)	13(1)	13(1)	0(1)	-1(1)	-2(1)
C(7)	12(1)	12(1)	12(1)	1(1)	-1(1)	-2(1)
C(8)	13(1)	14(1)	14(1)	0(1)	-1(1)	-3(1)
C(9)	13(1)	14(1)	14(1)	0(1)	-1(1)	-3(1)
C(10)	15(1)	15(1)	15(1)	-1(1)	-1(1)	-2(1)
O(10W)	34(5)	38(5)	32(6)	-4(5)	-3(5)	-9(4)
C(11)	13(1)	13(1)	13(1)	0(1)	-1(1)	-2(1)
C(12)	13(1)	13(1)	13(1)	0(1)	-1(1)	-2(1)
C(13)	14(1)	14(1)	13(1)	1(1)	1(1)	-4(1)
C(14)	11(2)	11(1)	11(1)	1(1)	-1(1)	-1(1)
C(15)	9(2)	10(1)	11(1)	1(1)	-2(1)	-1(1)
C(16)	8(2)	10(1)	11(1)	1(1)	-1(1)	-2(1)
C(17)	15(1)	17(1)	19(1)	1(1)	-2(1)	-3(1)
C(18)	14(1)	16(1)	18(1)	0(1)	-2(1)	-4(1)
C(19)	13(1)	12(1)	12(1)	-3(1)	-1(1)	-2(1)
C(20)	13(1)	12(1)	12(1)	-2(1)	-1(1)	-3(1)
C(21)	14(1)	15(1)	15(1)	0(1)	-1(1)	-4(1)

C(22)	14(1)	17(1)	16(1)	1(1)	-2(1)	-4(1)
C(23)	13(1)	12(1)	12(1)	-2(1)	-1(1)	-3(1)
C(24)	13(1)	13(1)	12(1)	-1(1)	-1(1)	-3(1)
O(11W)	55(6)	48(6)	67(6)	-1(5)	-10(5)	-20(5)
O(12W)	27(5)	19(5)	17(5)	-9(4)	-3(5)	-5(4)
O(13W)	61(6)	53(6)	51(6)	0(5)	-5(5)	-14(5)
O(14W)	42(6)	44(6)	47(6)	-1(5)	-5(5)	-2(5)
O(15W)	24(5)	29(5)	21(5)	-3(5)	9(5)	-4(4)
O(16W)	42(6)	43(6)	38(6)	-2(5)	7(5)	-5(5)
O(17W)	64(6)	64(6)	64(6)	-5(5)	-7(5)	-10(5)
O(18W)	63(6)	61(6)	59(6)	-10(5)	-5(5)	-14(5)
O(19W)	36(5)	35(5)	32(6)	10(5)	-3(5)	-4(4)

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Table S12. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for **2**.

	x	y	z	U(eq)
H(3WA)	14202(12)	6481(3)	2668(2)	32
H(9WA)	2344(5)	9074(7)	6091(5)	32
H(9WB)	514(3)	9271(4)	6083(4)	32
H(1WA)	9301(5)	6253(8)	2975(2)	30
H(1WB)	10219(13)	6770(3)	2429(3)	30
H(2WA)	10015(4)	3615(9)	2138(3)	45
H(2WB)	11167(12)	3538(15)	1516(3)	45
H(3WB)	14959(5)	5957(10)	2038(2)	37
H(4WA)	14544(6)	3088(6)	2817(3)	70
H(4WB)	13926(12)	3459(12)	3511(2)	70
H(5WA)	4293(6)	11261(6)	1413(3)	47
H(5WB)	2812(6)	12038(3)	1463(3)	47
H(6WA)	-504(7)	11521(7)	1594(2)	45
H(6WB)	-404(11)	12024(5)	2257(2)	45
H(7WA)	2540(8)	12318(3)	3069(5)	27
H(7WB)	1797(15)	11651(7)	3577(2)	27
H(8WA)	3774(6)	9356(6)	1312(2)	33
H(8WB)	5130(5)	9865(4)	1535(5)	33
H(20A)	2851	8415	2851	38
H(20B)	2466	8337	2203	38
H(21A)	-1476	10158	2470	52
H(21B)	-631	10263	3018	52
H(10A)	3835(6)	7010(7)	3609(3)	51
H(10B)	5596(5)	7004(12)	3379(7)	51
H(14W)	6396	7618	1972	67
H(15A)	6329	6896	1216	38
H(15B)	7042	5950	1294	38
H(16A)	10982	7438	1528	62
H(16B)	9420	7533	1770	62
H(17A)	8415	4756	1240	96

H(17B)	9770	4917	871	96
H(18A)	-1980	13469	2400	90
H(18B)	-1827	13021	3015	90
H(19A)	5774	11800	2909	52
H(19B)	5737	11938	2231	52

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Table S13. Hydrogen bonds lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **2**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(9W)-H(9WA)...O(18)#6	0.985(5)	1.862(10)	2.802(11)	158.4(8)
O(1W)-H(1WA)...O(12W)#7	0.978(4)	1.784(10)	2.762(10)	178.3(7)
O(1W)-H(1WB)...O(16W)	0.976(3)	1.714(12)	2.658(12)	161.9(8)
O(2W)-H(2WA)...O(18W)#7	0.975(4)	1.862(18)	2.791(17)	158.3(10)
O(2W)-H(2WB)...O(6)#8	0.959(12)	1.699(8)	2.627(12)	161.7(12)
O(3W)-H(3WB)...O(15W)#1	0.975(4)	1.780(15)	2.694(13)	154.7(12)
O(4W)-H(4WA)...O(19W)#7	0.975(4)	1.701(11)	2.641(12)	160.8(9)
O(4W)-H(4WB)...O(22)#4	0.975(4)	1.705(11)	2.621(10)	154.9(14)
O(5W)-H(5WA)...O(10)#9	0.977(4)	1.922(11)	2.730(10)	138.4(7)
O(6W)-H(6WA)...O(11)#5	0.977(4)	1.833(11)	2.805(11)	172.7(9)
O(6W)-H(6WB)...O(18W)	0.975(4)	1.690(13)	2.627(13)	160.0(9)
O(8W)-H(8WB)...O(12)	0.975(5)	1.904(11)	2.757(11)	144.6(9)
O(20W)-H(20A)...O(10W)	0.85	2.17	2.940(13)	149.9
O(21W)-H(21A)...O(12)#5	0.85	2.03	2.822(17)	154.8
O(21W)-H(21B)...O(20)	0.85	2.25	2.773(16)	120.2
O(15W)-H(15A)...O(9)	0.85	2.22	2.797(18)	125.3
O(15W)-H(15B)...O(17W)	0.85	1.90	2.75(2)	170.6
O(10W)-H(10A)...O(14)#5	0.985(5)	1.855(9)	2.829(10)	169.0(7)
O(10W)-H(10B)...O(12W)#7	0.988(5)	1.874(9)	2.861(9)	177.3(16)
O(16W)-H(16A)...O(1)	0.84	1.93	2.761(17)	167.4
O(16W)-H(16B)...O(14W)	0.85	2.06	2.77(2)	139.8
O(19W)-H(19A)...O(18)	0.85	1.97	2.809(19)	172.4
O(17W)-H(17A)...O(5)#8	0.85	2.70	2.84(2)	90.4
O(18W)-H(18B)...O(15)#6	0.85	2.27	2.83(2)	123.6
O(14W)-H(14W)...O(15W)	0.85	2.18	2.88(2)	139.8

Symmetry transformations used to generate equivalent atoms:

#1  $x+1, y, z$  #2  $-x+2, -y+2, -z$  #3  $-x+3, -y+1, -z$ #4  $-x+2, -y+1, -z+1$  #5  $x-1, y, z$  #6  $-x+1, -y+2, -z+1$ #7  $x+1, y-1, z$  #8  $-x+2, -y+1, -z$  #9  $-x+1, -y+2, -z$