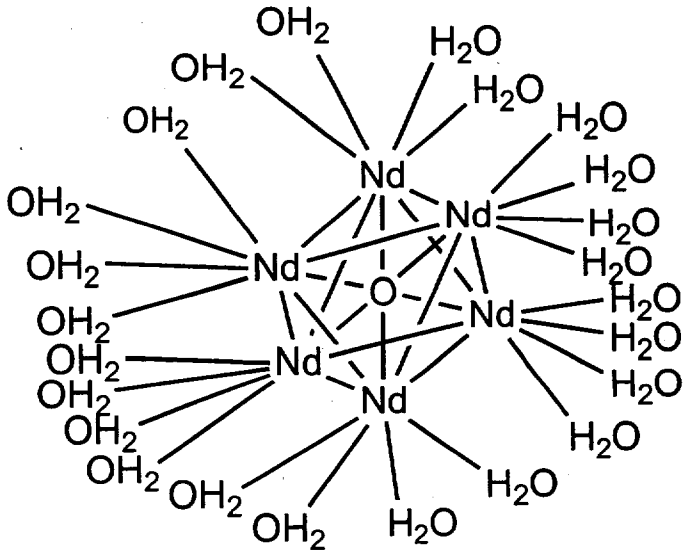
STRUCTURAL REPORT

$[Nd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(H_2O)_{24}](ClO_4)_8 \cdot 8H_2O$ (**2**)



EXPERIMENTAL

A light purple block of $[Nd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(H_2O)_{24}](ClO_4)_8 \bullet 8H_2O$ having approximate dimensions of 0.02 x 0.04 x 0.10 mm was mounted on a glass fiber in a random orientation. Examination of the crystal on a Bruker SMART 1000 CCD detector X-ray diffractometer at 298(2)K and a power setting of 50KV, 40mA showed measurable diffraction to at least theta = 28.23deg. All crystals examined at lower temperatures were cracked beyond use. Data were collected on the SMART1000 system using graphite monochromated Mo Kα radiation (λ=0.71073Å).

Cell constants and an orientation matrix for integration were determined from reflections obtained in three orthogonal 5 deg wedges of reciprocal space. A total of 1868 frames at 1 detector setting covering 0 < 2theta < 60 deg were collected, having an omega scan width of -0.3 and an exposure time of 10 seconds. The frames were integrated using the Bruker SAINT software package's narrow frame algorithm. A total of 26470 reflections were integrated and retained of which 2052 were unique (<redundancy> = 12.9, Rint = 3.8%, Rsig = 1.6%). Of the unique reflections, 1789 (87.2%) were observed >2sigma(I). The final Tetragonal cell parameters of a = 14.4999(8), b = 14.4999(8), c = 15.2489(12), alpha = 90, beta = 90, gamma = 90, volume = 3206.0(4) A^3 are based on the refinement of the XYZ-centroids of 5888 reflections with I > 10 sigma(I) covering the range of 2.67 < theta < 28.23. Empirical absorption and decay corrections were applied using the program SADABS (Sheldrick). The absorption coefficient is 5.243 mm-1, Tmin = 0.591797, and Tmax = 0.962223. For Z = 2 and F.W. = 2389.62 the calculated density is 2.475g/cm3. Systematic absences and intensity statistics indicate the space group to be P4/mnc (#128) which was consistent with refinement.

The structure was solved using SHELXS in the Bruker SHELXTL (Version 5.0) software package[1]. Refinements were performed using SHELXL and illustrations were made using XP. Solution was achieved utilizing direct methods followed by Fourier synthesis. Hydrogen atoms were added to coordinated water at idealized disordered positions, constrained to ride on the atom to which they are bonded and given thermal parameters equal to 1.2 or 1.5 times Uiso of that bonded atom. Positions which lead to short contacts were eliminated. No attempt to place hydrogens on the uncoordinated water was made Perchlorate anions showed large thermal parameters, indicitive of rotational disorder. The Cl-O bond distances were constrained to be approximately 1.44Å, but no further modeling was done. A parameter describing extintion was included. The final anisotropic full-matrix least squares refinement based on F^2 of all reflections converged (maximum shift/esd = 0.005) at R1 = 0.0386, wR2 = 0.1013 and goodness-of-fit = 1.068. "Conventional" refinement indices using the 1789 reflections with F > 4 sigma(F) are R1 = 0.0327, wR2 = 0.0964. The model consisted of 121 variable parameters, 44 constraints and 5 restraints. There were 24 correlation coefficients in the range of 0.86 to 0.64; these were primarily between parameters on the disordered oxygens or between the overall scale factor and the thermal parameters of Nd.. The highest peak on the final difference map was 1.095 e/A^3 located 0.01 A from ND2. The lowest peak on the final difference map was -1.156 e/A^3 located 0.58 A from

CL2_2. Scattering Factors and anomalous dispersion were taken from International Tables Vol C Tables 4.2.6.8 and 6.1.1.4.

EQUATIONS

$R_{int} = \sum|Fo^2-\langle Fo^2\rangle|/\sum[Fo^2]$

$R_{sig} = \sum[\sigma(Fo^2)]/\sum[Fo^2]$

$R_1 = \Sigma||Fo|-|Fc||/\sum|Fo|$

$wR_2 = \{\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]\}^{1/2}$

$w=1/[\sigma^2(Fo^2)+(0.069900\ P)^2+2.788400\ P]$ where $P=(Fo^2+2Fc^2)/3$

$GOF = S = \{\sum[w(Fo^2-Fc^2)^2]/(n-p)\}^{1/2}$

REFERENCES

Bruker (1997) SAINT Reference Manual Version 5.0, Bruker AXS Inc. , Madison, Wisconsin, USA.

Bruker (1997) SHELXTL Reference Manual Version 5.0, Bruker AXS Inc. , Madison, Wisconsin, USA.

Bruker (1997) SMART Reference Manual Version 5.0, Bruker AXS Inc. , Madison, Wisconsin, USA.

Table 1. Crystal data and structure refinement for $[Nd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(H_2O)_{24}](ClO_4)_8 \cdot 8H_2O$ (**2**).

Empirical formula	H72Cl8Nd6O73	
Formula weight	2389.62	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	P4/mnc	
Unit cell dimensions	a = 14.4999(8) Å	a= 90°.
	b = 14.4999(8) Å	b= 90°.
	c = 15.2489(12) Å	g = 90°.
Volume	3206.0(4) $Å^3$	
Z	2	
Density (calculated)	2.475 Mg/m^3	
Absorption coefficient	5.243 mm^{-1}	
F(000)	2304	
Crystal size	0.10 x 0.04 x 0.02 mm^3	
Theta range for utilized data	1.94 to 28.55°.	
Limiting Indices	-18<=h<=19, -18<=k<=19, -20<=l<=19	
Reflections utilized	26470	
Independent reflections	2052 [R(int) = 0.0382]	
Completeness to theta = 28.55°	96.2 %	
Absorption correction	Empirical SADABS (Sheldrick)	
Max. and min. transmission	0.962223 and 0.591797	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2052 / 5 / 121	
Goodness-of-fit on F^2	1.068	
Final R indices [I>2sigma(I)]	R1 = 0.0327, wR2 = 0.0964	
R indices (all data)	R1 = 0.0386, wR2 = 0.1013	
Extinction coefficient	0.00093(16)	
Largest diff. peak and hole	1.095 and -1.156 $e.Å^{-3}$	
RMS difference density	0.145$e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2x 10^3) for $[Nd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(H_2O)_{24}](ClO_4)_8 \cdot 8H_2O$ (**2**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Nd(1)	4328(1)	3325(1)	5000	38(1)
Nd(2)	5000	5000	3283(1)	40(1)
O(1)	5000	5000	5000	36(2)
O(2M)	3615(2)	4407(2)	3991(2)	40(1)
O(3T)	5242(5)	1814(4)	5000	78(2)
O(4T)	3945(3)	2350(3)	3650(3)	76(1)
O(5T)	2607(4)	2855(4)	5000	69(2)
O(6T)	6321(4)	4505(4)	2260(4)	104(2)
Cl11	1781(1)	3219(1)	2500	91(1)
O111	2530(6)	3106(10)	1893(7)	222(6)
O121	989(5)	3090(6)	2009(7)	168(4)
Cl22	2482(6)	5149(4)	0	180(3)
O212	3351(13)	4670(19)	0	840(60)
O222	2425(16)	5750(11)	748(8)	298(10)
O232	1665(11)	4594(15)	0	262(11)
O1013	450(40)	5470(30)	-1350(40)	260(20)
O1023	1010(40)	5561(17)	-1970(40)	250(20)

Table 3. Bond lengths [Å] and angles [°] for $[Nd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(H_2O)_{24}](ClO_4)_8 \cdot 8H_2O$ (**2**).

Nd(1)-O(2M)#1	2.428(3)	O(2M)#1-Nd(1)-O(2M)#2	78.97(15)
Nd(1)-O(2M)	2.428(3)	O(2M)-Nd(1)-O(2M)#2	127.64(14)
Nd(1)-O(2M)#2	2.430(3)	O(2M)#1-Nd(1)-O(2M)#3	127.64(14)
Nd(1)-O(2M)#3	2.430(3)	O(2M)-Nd(1)-O(2M)#3	78.97(15)
Nd(1)-O(4T)	2.558(4)	O(2M)#2-Nd(1)-O(2M)#3	78.54(14)
Nd(1)-O(4T)#1	2.558(4)	O(2M)#1-Nd(1)-O(4T)	140.73(14)
Nd(1)-O(3T)	2.560(5)	O(2M)-Nd(1)-O(4T)	75.79(14)
Nd(1)-O(5T)	2.587(5)	O(2M)#2-Nd(1)-O(4T)	140.25(13)
Nd(1)-O(1)	2.6166(3)	O(2M)#3-Nd(1)-O(4T)	75.52(13)
Nd(1)-Nd(1)#4	3.7004(5)	O(2M)#1-Nd(1)-O(4T)#1	75.79(14)
Nd(1)-Nd(1)#3	3.7004(5)	O(2M)-Nd(1)-O(4T)#1	140.73(14)
Nd(1)-Nd(2)#5	3.7014(4)	O(2M)#2-Nd(1)-O(4T)#1	75.52(13)
Nd(2)-O(2M)#6	2.437(3)	O(2M)#3-Nd(1)-O(4T)#1	140.25(13)
Nd(2)-O(2M)#7	2.437(3)	O(4T)-Nd(1)-O(4T)#1	107.2(2)
Nd(2)-O(2M)	2.437(3)	O(2M)#1-Nd(1)-O(3T)	140.64(7)
Nd(2)-O(2M)#3	2.437(3)	O(2M)-Nd(1)-O(3T)	140.64(7)
Nd(2)-O(6T)#7	2.573(5)	O(2M)#2-Nd(1)-O(3T)	75.97(15)
Nd(2)-O(6T)#6	2.573(5)	O(2M)#3-Nd(1)-O(3T)	75.97(15)
Nd(2)-O(6T)	2.573(5)	O(4T)-Nd(1)-O(3T)	68.87(14)
Nd(2)-O(6T)#3	2.573(5)	O(4T)#1-Nd(1)-O(3T)	68.87(14)
Nd(2)-O(1)	2.6179(5)	O(2M)#1-Nd(1)-O(5T)	76.07(13)
Nd(2)-Nd(1)#5	3.7014(4)	O(2M)-Nd(1)-O(5T)	76.07(13)
Nd(2)-Nd(1)#4	3.7014(4)	O(2M)#2-Nd(1)-O(5T)	140.67(7)
Nd(2)-Nd(1)#3	3.7014(4)	O(2M)#3-Nd(1)-O(5T)	140.67(7)
O(1)-Nd(1)#4	2.6166(3)	O(4T)-Nd(1)-O(5T)	69.20(13)
O(1)-Nd(1)#5	2.6166(3)	O(4T)#1-Nd(1)-O(5T)	69.20(13)
O(1)-Nd(1)#3	2.6166(3)	O(3T)-Nd(1)-O(5T)	105.9(2)
O(1)-Nd(2)#5	2.6179(5)	O(2M)#1-Nd(1)-O(1)	63.83(7)
O(2M)-Nd(1)#4	2.430(3)	O(2M)-Nd(1)-O(1)	63.83(7)
O(2M)-H(2M)	0.9800	O(2M)#2-Nd(1)-O(1)	63.81(8)
O(3T)-H(3T1)	0.9600	O(2M)#3-Nd(1)-O(1)	63.81(8)
O(3T)-H(3T2)	0.9600	O(4T)-Nd(1)-O(1)	126.41(12)
O(3T)-H(3T3)	0.9600	O(4T)#1-Nd(1)-O(1)	126.41(12)
O(4T)-H(4T1)	0.9600	O(3T)-Nd(1)-O(1)	126.99(17)
O(4T)-H(4T2)	0.9600	O(5T)-Nd(1)-O(1)	127.13(14)
O(5T)-H(5T1)	0.9600	O(2M)#1-Nd(1)-Nd(1)#4	40.41(7)
O(5T)-H(5T2)	0.9600	O(2M)-Nd(1)-Nd(1)#4	40.41(7)
O(5T)-H(5T3)	0.9600	O(2M)#2-Nd(1)-Nd(1)#4	97.91(8)
O(6T)-H(6T2)	0.9600	O(2M)#3-Nd(1)-Nd(1)#4	97.91(8)
O(6T)-H(6T3)	0.9600	O(4T)-Nd(1)-Nd(1)#4	115.00(12)
Cl11-O121#8	1.384(4)	O(4T)#1-Nd(1)-Nd(1)#4	115.00(12)
Cl11-O121	1.384(4)	O(3T)-Nd(1)-Nd(1)#4	171.99(17)
Cl11-O111#8	1.436(5)	O(5T)-Nd(1)-Nd(1)#4	82.13(14)
Cl11-O111	1.436(5)	O(1)-Nd(1)-Nd(1)#4	45.0
Cl22-O232	1.433(5)	O(2M)#1-Nd(1)-Nd(1)#3	97.92(8)
Cl22-O222#9	1.437(5)	O(2M)-Nd(1)-Nd(1)#3	97.92(8)
Cl22-O222	1.437(5)	O(2M)#2-Nd(1)-Nd(1)#3	40.37(7)
Cl22-O212	1.438(5)	O(2M)#3-Nd(1)-Nd(1)#3	40.37(7)
O1013-O1023	1.25(5)	O(4T)-Nd(1)-Nd(1)#3	114.64(11)
		O(4T)#1-Nd(1)-Nd(1)#3	114.64(11)
O(2M)#1-Nd(1)-O(2M)	78.62(14)	O(3T)-Nd(1)-Nd(1)#3	81.99(17)

O(5T)-Nd(1)-Nd(1)#3	172.13(14)
O(1)-Nd(1)-Nd(1)#3	45.0
Nd(1)#4-Nd(1)-Nd(1)#3	90.0
O(2M)#1-Nd(1)-Nd(2)#5	40.55(8)
O(2M)-Nd(1)-Nd(2)#5	97.84(7)
O(2M)#2-Nd(1)-Nd(2)#5	40.56(8)
O(2M)#3-Nd(1)-Nd(2)#5	97.80(7)
O(4T)-Nd(1)-Nd(2)#5	171.42(12)
O(4T)#1-Nd(1)-Nd(2)#5	81.40(12)
O(3T)-Nd(1)-Nd(2)#5	115.17(10)
O(5T)-Nd(1)-Nd(2)#5	115.26(9)
O(1)-Nd(1)-Nd(2)#5	45.015(6)
Nd(1)#4-Nd(1)-Nd(2)#5	60.009(4)
Nd(1)#3-Nd(1)-Nd(2)#5	60.009(4)
O(2M)#6-Nd(2)-O(2M)#7	78.68(6)
O(2M)#6-Nd(2)-O(2M)	78.68(6)
O(2M)#7-Nd(2)-O(2M)	127.41(14)
O(2M)#6-Nd(2)-O(2M)#3	127.41(14)
O(2M)#7-Nd(2)-O(2M)#3	78.68(6)
O(2M)-Nd(2)-O(2M)#3	78.68(6)
O(2M)#6-Nd(2)-O(6T)#7	77.08(16)
O(2M)#7-Nd(2)-O(6T)#7	141.62(14)
O(2M)-Nd(2)-O(6T)#7	75.73(17)
O(2M)#3-Nd(2)-O(6T)#7	139.57(15)
O(2M)#6-Nd(2)-O(6T)#6	141.62(14)
O(2M)#7-Nd(2)-O(6T)#6	139.57(15)
O(2M)-Nd(2)-O(6T)#6	77.08(16)
O(2M)#3-Nd(2)-O(6T)#6	75.73(17)
O(6T)#7-Nd(2)-O(6T)#6	68.40(17)
O(2M)#6-Nd(2)-O(6T)	139.57(15)
O(2M)#7-Nd(2)-O(6T)	75.73(17)
O(2M)-Nd(2)-O(6T)	141.62(14)
O(2M)#3-Nd(2)-O(6T)	77.08(16)
O(6T)#7-Nd(2)-O(6T)	105.3(3)
O(6T)#6-Nd(2)-O(6T)	68.40(17)
O(2M)#6-Nd(2)-O(6T)#3	75.73(17)
O(2M)#7-Nd(2)-O(6T)#3	77.08(16)
O(2M)-Nd(2)-O(6T)#3	139.57(15)
O(2M)#3-Nd(2)-O(6T)#3	141.62(14)
O(6T)#7-Nd(2)-O(6T)#3	68.40(17)
O(6T)#6-Nd(2)-O(6T)#3	105.3(3)
O(6T)-Nd(2)-O(6T)#3	68.40(17)
O(2M)#6-Nd(2)-O(1)	63.70(7)
O(2M)#7-Nd(2)-O(1)	63.70(7)
O(2M)-Nd(2)-O(1)	63.70(7)
O(2M)#3-Nd(2)-O(1)	63.70(7)
O(6T)#7-Nd(2)-O(1)	127.35(16)
O(6T)#6-Nd(2)-O(1)	127.35(16)
O(6T)-Nd(2)-O(1)	127.35(16)
O(6T)#3-Nd(2)-O(1)	127.35(16)
O(2M)#6-Nd(2)-Nd(1)#5	40.43(7)
O(2M)#7-Nd(2)-Nd(1)#5	40.38(7)
O(2M)-Nd(2)-Nd(1)#5	97.76(7)
O(2M)#3-Nd(2)-Nd(1)#5	97.73(7)
O(6T)#7-Nd(2)-Nd(1)#5	116.24(13)
O(6T)#6-Nd(2)-Nd(1)#5	172.27(16)
O(6T)-Nd(2)-Nd(1)#5	114.59(15)
O(6T)#3-Nd(2)-Nd(1)#5	82.37(16)
O(1)-Nd(2)-Nd(1)#5	44.985(6)
O(2M)#6-Nd(2)-Nd(1)#4	40.38(7)
O(2M)#7-Nd(2)-Nd(1)#4	97.73(7)
O(2M)-Nd(2)-Nd(1)#4	40.43(7)
O(2M)#3-Nd(2)-Nd(1)#4	97.76(7)
O(6T)#7-Nd(2)-Nd(1)#4	82.37(16)
O(6T)#6-Nd(2)-Nd(1)#4	116.24(13)
O(6T)-Nd(2)-Nd(1)#4	172.27(16)
O(6T)#3-Nd(2)-Nd(1)#4	114.59(15)
O(1)-Nd(2)-Nd(1)#4	44.985(6)
Nd(1)#5-Nd(2)-Nd(1)#4	59.983(7)
O(2M)#6-Nd(2)-Nd(1)#3	97.76(7)
O(2M)#7-Nd(2)-Nd(1)#3	40.43(7)
O(2M)-Nd(2)-Nd(1)#3	97.73(7)
O(2M)#3-Nd(2)-Nd(1)#3	40.38(7)
O(6T)#7-Nd(2)-Nd(1)#3	172.27(16)
O(6T)#6-Nd(2)-Nd(1)#3	114.59(15)
O(6T)-Nd(2)-Nd(1)#3	82.37(16)
O(6T)#3-Nd(2)-Nd(1)#3	116.24(13)
O(1)-Nd(2)-Nd(1)#3	44.985(6)
Nd(1)#5-Nd(2)-Nd(1)#3	59.983(7)
Nd(1)#4-Nd(2)-Nd(1)#3	89.970(12)
Nd(1)-O(1)-Nd(1)#4	90.0
Nd(1)-O(1)-Nd(1)#5	180.0
Nd(1)#4-O(1)-Nd(1)#5	90.0
Nd(1)-O(1)-Nd(1)#3	90.0
Nd(1)#4-O(1)-Nd(1)#3	180.0
Nd(1)#5-O(1)-Nd(1)#3	90.0
Nd(1)-O(1)-Nd(2)#5	90.0
Nd(1)#4-O(1)-Nd(2)#5	90.0
Nd(1)#5-O(1)-Nd(2)#5	90.0
Nd(1)#3-O(1)-Nd(2)#5	90.0
Nd(1)-O(1)-Nd(2)	90.0
Nd(1)#4-O(1)-Nd(2)	90.0
Nd(1)#5-O(1)-Nd(2)	90.0
Nd(1)#3-O(1)-Nd(2)	90.0
Nd(2)#5-O(1)-Nd(2)	180.0
Nd(1)-O(2M)-Nd(1)#4	99.21(11)
Nd(1)-O(2M)-Nd(2)	99.07(11)
Nd(1)#4-O(2M)-Nd(2)	99.01(11)
Nd(1)-O(2M)-H(2M)	118.5
Nd(1)#4-O(2M)-H(2M)	118.5
Nd(2)-O(2M)-H(2M)	118.5
Nd(1)-O(3T)-H(3T1)	109.5
Nd(1)-O(3T)-H(3T2)	109.5
H(3T1)-O(3T)-H(3T2)	109.5
Nd(1)-O(3T)-H(3T3)	109.5
H(3T1)-O(3T)-H(3T3)	109.5

H(3T2)-O(3T)-H(3T3)	109.5
Nd(1)-O(4T)-H(4T1)	109.3
Nd(1)-O(4T)-H(4T2)	109.4
H(4T1)-O(4T)-H(4T2)	109.5
Nd(1)-O(5T)-H(5T1)	109.5
Nd(1)-O(5T)-H(5T2)	109.5
H(5T1)-O(5T)-H(5T2)	109.5
Nd(1)-O(5T)-H(5T3)	109.5
H(5T1)-O(5T)-H(5T3)	109.5
H(5T2)-O(5T)-H(5T3)	109.5
Nd(2)-O(6T)-H(6T2)	109.2
Nd(2)-O(6T)-H(6T3)	109.4
H(6T2)-O(6T)-H(6T3)	109.5
O121#8-Cl11-O121	121.0(7)
O121#8-Cl11-O111#8	105.3(6)
O121-Cl11-O111#8	110.0(7)
O121#8-Cl11-O111	110.0(7)
O121-Cl11-O111	105.3(6)
O111#8-Cl11-O111	104.1(13)
O232-Cl22-O222#9	107.0(13)
O232-Cl22-O222	107.0(13)
O222#9-Cl22-O222	105.0(15)
O232-Cl22-O212	116.9(14)
O222#9-Cl22-O212	110.1(11)
O222-Cl22-O212	110.1(11)

Symmetry transformations used to generate equivalent atoms:
#1 x,y,-z+1 #2 -y+1,x,-z+1 #3 -y+1,x,z #4 y,-x+1,-z+1
#5 -x+1,-y+1,-z+1 #6 y,-x+1,z #7 -x+1,-y+1,z
#8 -y+1/2,-x+1/2,-z+1/2 #9 x,y,-z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Nd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(H_2O)_{24}](ClO_4)_8 \cdot 8H_2O$ (**2**). The anisotropic displacement factor exponent takes the form: $-2p^2[\, h^2\, a^{*2}U^{11} + \ldots + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Nd(1)	38(1)	35(1)	41(1)	0	0	-1(1)
Nd(2)	46(1)	46(1)	29(1)	0	0	0
O(1)	40(2)	40(2)	27(3)	0	0	0
O(2M)	42(2)	42(2)	37(2)	-1(1)	-8(1)	-3(1)
O(3T)	80(4)	49(3)	104(5)	0	0	16(3)
O(4T)	79(3)	65(2)	85(3)	-25(2)	-5(2)	-4(2)
O(5T)	53(3)	71(4)	82(4)	0	0	-14(3)
O(6T)	119(4)	118(4)	76(3)	-9(3)	42(3)	22(4)
Cl11	90(1)	90(1)	94(2)	-32(1)	-32(1)	-13(1)
O111	168(9)	293(15)	204(11)	-119(10)	15(9)	-44(9)
O121	140(6)	165(7)	200(9)	-96(7)	-98(6)	19(6)
Cl22	251(8)	99(3)	191(6)	0	0	-32(4)
O212	1160(110)	200(20)	1170(120)	0	0	390(50)
O222	400(20)	277(17)	216(16)	-64(13)	-73(17)	136(16)
O232	240(20)	220(20)	320(30)	0	0	-111(17)
O1013	240(40)	170(20)	360(50)	-120(30)	0(40)	40(20)
O1023	270(40)	74(13)	410(60)	30(20)	140(50)	27(17)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[Nd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(H_2O)_{24}](ClO_4)_8 \cdot 8H_2O$ (**2**).

	x	y	z	U(eq)
H(2M)	3107	4190	3621	48
H(3T1)	5358	1627	5594	116
H(3T2)	5817	1904	4701	116
H(3T3)	4892	1345	4705	116
H(4T1)	3392	2006	3758	114
H(4T2)	4444	1933	3535	114
H(5T1)	2544	2251	4748	103
H(5T2)	2259	3290	4660	103
H(5T3)	2380	2848	5591	103
H(6T2)	6107	4022	1880	156
H(6T3)	6829	4284	2604	156

Table 6. Torsion angles [°] for $[Nd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(H_2O)_{24}](ClO_4)_8 \cdot 8H_2O$ (**2**).

O(2M)#1-Nd(1)-O(1)-Nd(1)#4	-44.90(8)	Nd(2)#5-Nd(1)-O(1)-Nd(2)	180.0
O(2M)-Nd(1)-O(1)-Nd(1)#4	44.90(8)	O(2M)#6-Nd(2)-O(1)-Nd(1)	134.96(7)
O(2M)#2-Nd(1)-O(1)-Nd(1)#4	-135.14(8)	O(2M)#7-Nd(2)-O(1)-Nd(1)	-135.04(7)
O(2M)#3-Nd(1)-O(1)-Nd(1)#4	135.14(8)	O(2M)-Nd(2)-O(1)-Nd(1)	44.96(7)
O(4T)-Nd(1)-O(1)-Nd(1)#4	90.29(14)	O(2M)#3-Nd(2)-O(1)-Nd(1)	-45.04(7)
O(4T)#1-Nd(1)-O(1)-Nd(1)#4	-90.29(14)	O(6T)#7-Nd(2)-O(1)-Nd(1)	88.67(16)
O(3T)-Nd(1)-O(1)-Nd(1)#4	180.0	O(6T)#6-Nd(2)-O(1)-Nd(1)	-1.33(16)
O(5T)-Nd(1)-O(1)-Nd(1)#4	0.0	O(6T)-Nd(2)-O(1)-Nd(1)	-91.33(16)
Nd(1)#3-Nd(1)-O(1)-Nd(1)#4	180.0	O(6T)#3-Nd(2)-O(1)-Nd(1)	178.67(16)
Nd(2)#5-Nd(1)-O(1)-Nd(1)#4	-90.0	Nd(1)#5-Nd(2)-O(1)-Nd(1)	180.0
O(2M)#1-Nd(1)-O(1)-Nd(1)#5	135.10(8)	Nd(1)#4-Nd(2)-O(1)-Nd(1)	90.0
O(2M)-Nd(1)-O(1)-Nd(1)#5	-135.10(8)	Nd(1)#3-Nd(2)-O(1)-Nd(1)	-90.0
O(2M)#2-Nd(1)-O(1)-Nd(1)#5	44.86(8)	O(2M)#6-Nd(2)-O(1)-Nd(1)#4	44.96(7)
O(2M)#3-Nd(1)-O(1)-Nd(1)#5	-44.86(8)	O(2M)#7-Nd(2)-O(1)-Nd(1)#4	134.96(7)
O(4T)-Nd(1)-O(1)-Nd(1)#5	-89.71(14)	O(2M)-Nd(2)-O(1)-Nd(1)#4	-45.04(7)
O(4T)#1-Nd(1)-O(1)-Nd(1)#5	89.71(14)	O(2M)#3-Nd(2)-O(1)-Nd(1)#4	-135.04(7)
O(3T)-Nd(1)-O(1)-Nd(1)#5	0.0	O(6T)#7-Nd(2)-O(1)-Nd(1)#4	-1.33(16)
O(5T)-Nd(1)-O(1)-Nd(1)#5	180.0	O(6T)#6-Nd(2)-O(1)-Nd(1)#4	-91.33(16)
Nd(1)#4-Nd(1)-O(1)-Nd(1)#5	180.0	O(6T)-Nd(2)-O(1)-Nd(1)#4	178.67(16)
Nd(1)#3-Nd(1)-O(1)-Nd(1)#5	0.0	O(6T)#3-Nd(2)-O(1)-Nd(1)#4	88.67(16)
Nd(2)#5-Nd(1)-O(1)-Nd(1)#5	90.0	Nd(1)#5-Nd(2)-O(1)-Nd(1)#4	90.0
O(2M)#1-Nd(1)-O(1)-Nd(1)#3	135.10(8)	Nd(1)#3-Nd(2)-O(1)-Nd(1)#4	180.0
O(2M)-Nd(1)-O(1)-Nd(1)#3	-135.10(8)	O(2M)#6-Nd(2)-O(1)-Nd(1)#5	-45.04(7)
O(2M)#2-Nd(1)-O(1)-Nd(1)#3	44.86(8)	O(2M)#7-Nd(2)-O(1)-Nd(1)#5	44.96(7)
O(2M)#3-Nd(1)-O(1)-Nd(1)#3	-44.86(8)	O(2M)-Nd(2)-O(1)-Nd(1)#5	-135.04(7)
O(4T)-Nd(1)-O(1)-Nd(1)#3	-89.71(14)	O(2M)#3-Nd(2)-O(1)-Nd(1)#5	134.96(7)
O(4T)#1-Nd(1)-O(1)-Nd(1)#3	89.71(14)	O(6T)#7-Nd(2)-O(1)-Nd(1)#5	-91.33(16)
O(3T)-Nd(1)-O(1)-Nd(1)#3	0.0	O(6T)#6-Nd(2)-O(1)-Nd(1)#5	178.67(16)
O(5T)-Nd(1)-O(1)-Nd(1)#3	180.0	O(6T)-Nd(2)-O(1)-Nd(1)#5	88.67(16)
Nd(1)#4-Nd(1)-O(1)-Nd(1)#3	180.0	O(6T)#3-Nd(2)-O(1)-Nd(1)#5	-1.33(16)
Nd(2)#5-Nd(1)-O(1)-Nd(1)#3	90.0	Nd(1)#4-Nd(2)-O(1)-Nd(1)#5	-90.0
O(2M)#1-Nd(1)-O(1)-Nd(2)#5	45.10(8)	Nd(1)#3-Nd(2)-O(1)-Nd(1)#5	90.0
O(2M)-Nd(1)-O(1)-Nd(2)#5	134.90(8)	O(2M)#6-Nd(2)-O(1)-Nd(1)#3	-135.04(7)
O(2M)#2-Nd(1)-O(1)-Nd(2)#5	-45.14(8)	O(2M)#7-Nd(2)-O(1)-Nd(1)#3	-45.04(7)
O(2M)#3-Nd(1)-O(1)-Nd(2)#5	-134.86(8)	O(2M)-Nd(2)-O(1)-Nd(1)#3	134.96(7)
O(4T)-Nd(1)-O(1)-Nd(2)#5	-179.71(14)	O(2M)#3-Nd(2)-O(1)-Nd(1)#3	44.96(7)
O(4T)#1-Nd(1)-O(1)-Nd(2)#5	-0.29(14)	O(6T)#7-Nd(2)-O(1)-Nd(1)#3	178.67(16)
O(3T)-Nd(1)-O(1)-Nd(2)#5	-90.0	O(6T)#6-Nd(2)-O(1)-Nd(1)#3	88.67(16)
O(5T)-Nd(1)-O(1)-Nd(2)#5	90.0	O(6T)-Nd(2)-O(1)-Nd(1)#3	-1.33(16)
Nd(1)#4-Nd(1)-O(1)-Nd(2)#5	90.0	O(6T)#3-Nd(2)-O(1)-Nd(1)#3	-91.33(16)
Nd(1)#3-Nd(1)-O(1)-Nd(2)#5	-90.0	Nd(1)#5-Nd(2)-O(1)-Nd(1)#3	-90.0
O(2M)#1-Nd(1)-O(1)-Nd(2)	-134.90(8)	Nd(1)#4-Nd(2)-O(1)-Nd(1)#3	180.0
O(2M)-Nd(1)-O(1)-Nd(2)	-45.10(8)	O(2M)#6-Nd(2)-O(1)-Nd(2)#5	-113(3)
O(2M)#2-Nd(1)-O(1)-Nd(2)	134.86(8)	O(2M)#7-Nd(2)-O(1)-Nd(2)#5	-23(3)
O(2M)#3-Nd(1)-O(1)-Nd(2)	45.14(8)	O(2M)-Nd(2)-O(1)-Nd(2)#5	157(37)
O(4T)-Nd(1)-O(1)-Nd(2)	0.29(14)	O(2M)#3-Nd(2)-O(1)-Nd(2)#5	67(3)
O(4T)#1-Nd(1)-O(1)-Nd(2)	179.71(14)	O(6T)#7-Nd(2)-O(1)-Nd(2)#5	-159(3)
O(3T)-Nd(1)-O(1)-Nd(2)	90.0	O(6T)#6-Nd(2)-O(1)-Nd(2)#5	111(3)
O(5T)-Nd(1)-O(1)-Nd(2)	-90.0	O(6T)-Nd(2)-O(1)-Nd(2)#5	21(3)
Nd(1)#4-Nd(1)-O(1)-Nd(2)	-90.0	O(6T)#3-Nd(2)-O(1)-Nd(2)#5	-69(3)
Nd(1)#3-Nd(1)-O(1)-Nd(2)	90.0	Nd(1)#5-Nd(2)-O(1)-Nd(2)#5	-68(3)

Nd(1)#4-Nd(2)-O(1)-Nd(2)#5	-158(3)
Nd(1)#3-Nd(2)-O(1)-Nd(2)#5	22(3)
O(2M)#1-Nd(1)-O(2M)-Nd(1)#4	15.94(15)
O(2M)#2-Nd(1)-O(2M)-Nd(1)#4	-50.38(10)
O(2M)#3-Nd(1)-O(2M)-Nd(1)#4	-116.43(9)
O(4T)-Nd(1)-O(2M)-Nd(1)#4	165.89(16)
O(4T)#1-Nd(1)-O(2M)-Nd(1)#4	66.0(2)
O(3T)-Nd(1)-O(2M)-Nd(1)#4	-167.6(3)
O(5T)-Nd(1)-O(2M)-Nd(1)#4	94.23(14)
O(1)-Nd(1)-O(2M)-Nd(1)#4	-50.34(7)
Nd(1)#3-Nd(1)-O(2M)-Nd(1)#4	-80.60(9)
Nd(2)#5-Nd(1)-O(2M)-Nd(1)#4	-19.96(10)
O(2M)#1-Nd(1)-O(2M)-Nd(2)	116.69(8)
O(2M)#2-Nd(1)-O(2M)-Nd(2)	50.37(13)
O(2M)#3-Nd(1)-O(2M)-Nd(2)	-15.68(11)
O(4T)-Nd(1)-O(2M)-Nd(2)	-93.36(14)
O(4T)#1-Nd(1)-O(2M)-Nd(2)	166.77(19)
O(3T)-Nd(1)-O(2M)-Nd(2)	-66.9(3)
O(5T)-Nd(1)-O(2M)-Nd(2)	-165.02(14)
O(1)-Nd(1)-O(2M)-Nd(2)	50.41(7)
Nd(1)#4-Nd(1)-O(2M)-Nd(2)	100.75(13)
Nd(1)#3-Nd(1)-O(2M)-Nd(2)	20.15(9)
Nd(2)#5-Nd(1)-O(2M)-Nd(2)	80.79(8)
O(2M)#6-Nd(2)-O(2M)-Nd(1)	-116.56(2)
O(2M)#7-Nd(2)-O(2M)-Nd(1)	-50.45(7)
O(2M)#3-Nd(2)-O(2M)-Nd(1)	15.65(12)
O(6T)#7-Nd(2)-O(2M)-Nd(1)	164.07(17)
O(6T)#6-Nd(2)-O(2M)-Nd(1)	93.42(17)
O(6T)-Nd(2)-O(2M)-Nd(1)	67.3(3)
O(6T)#3-Nd(2)-O(2M)-Nd(1)	-168.1(3)
O(1)-Nd(2)-O(2M)-Nd(1)	-50.45(7)
Nd(1)#5-Nd(2)-O(2M)-Nd(1)	-80.73(8)
Nd(1)#4-Nd(2)-O(2M)-Nd(1)	-100.92(13)
Nd(1)#3-Nd(2)-O(2M)-Nd(1)	-20.14(9)
O(2M)#6-Nd(2)-O(2M)-Nd(1)#4	-15.64(12)
O(2M)#7-Nd(2)-O(2M)-Nd(1)#4	50.47(7)
O(2M)#3-Nd(2)-O(2M)-Nd(1)#4	116.57(2)
O(6T)#7-Nd(2)-O(2M)-Nd(1)#4	-95.01(17)
O(6T)#6-Nd(2)-O(2M)-Nd(1)#4	-165.66(18)
O(6T)-Nd(2)-O(2M)-Nd(1)#4	168.2(3)
O(6T)#3-Nd(2)-O(2M)-Nd(1)#4	-67.1(3)
O(1)-Nd(2)-O(2M)-Nd(1)#4	50.47(7)
Nd(1)#5-Nd(2)-O(2M)-Nd(1)#4	20.19(9)
Nd(1)#3-Nd(2)-O(2M)-Nd(1)#4	80.78(8)

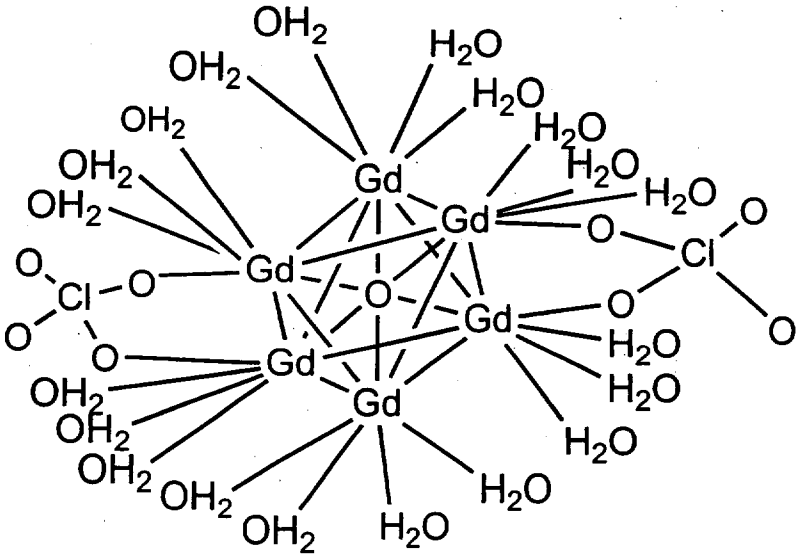
Symmetry transformations used to generate equivalent atoms:
#1 x,y,-z+1 #2 -y+1,x,-z+1 #3 -y+1,x,z #4 y,-x+1,-z+1
#5 -x+1,-y+1,-z+1 #6 y,-x+1,z #7 -x+1,-y+1,z
#8 -y+1/2,-x+1/2,-z+1/2 #9 x,y,-z

Table 7. Hydrogen bonds for $[Nd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(H_2O)_{24}](ClO_4)_8 \cdot 8H_2O$ (**2**) [Å and °].

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O2M-H2M	0.980	2.001	165.95	2.961	O12_1 [-y+1/2, -x+1/2, -z+1/2]
O2M-H2M	0.980	2.932	169.36	3.900	Cl1_1
O3T-H3T1	0.960	2.346	125.17	3.003	O101_3 [-x+1/2, y-1/2, -z+1/2]
O3T-H3T1	0.960	2.379	150.92	3.252	O12_1 [x+1/2, -y+1/2, z+1/2]
O3T-H3T2	0.960	2.226	135.83	2.990	O5T [-y+1, x, z]
O3T-H3T2	0.960	2.619	123.76	3.252	O12_1 [x+1/2, -y+1/2, -z+1/2]
O3T-H3T3	0.960	2.104	155.28	3.003	O101_3 [-x+1/2, y-1/2, z+1/2]
O4T-H4T1	0.960	2.299	154.10	3.190	O22_2 [-x+1/2, y-1/2, -z+1/2]
O4T-H4T1	0.960	2.481	121.45	3.093	O11_1 [-y+1/2, -x+1/2, -z+1/2]
O4T-H4T2	0.960	2.130	131.67	2.860	O101_3 [-x+1/2, y-1/2, z+1/2]
O4T-H4T2	0.960	2.232	113.65	2.761	O102_3 [-x+1/2, y-1/2, z+1/2]
O4T-H4T2	0.960	2.388	141.22	3.193	O12_1 [x+1/2, -y+1/2, -z+1/2]
O5T-H5T1	0.960	2.305	171.95	3.259	O22_2 [-x+1/2, y-1/2, -z+1/2]
O5T-H5T1	0.960	2.658	121.06	3.259	O22_2 [-x+1/2, y-1/2, z+1/2]
O5T-H5T2	0.960	2.284	129.73	2.990	O3T [y, -x+1, -z+1]
O5T-H5T3	0.960	2.177	165.96	3.117	O11_1 [-y+1/2, -x+1/2, z+1/2]
O6T-H6T2	0.960	2.445	119.36	3.034	O11_1 [-y+1, x, z]
O6T-H6T3	0.960	2.049	162.08	2.978	O4T [-y+1, x, z]

STRUCTURAL REPORT

$[Gd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(\eta^2\text{-}ClO_4)_2(H_2O)_{20}](ClO_4)_6 \cdot 4H_2O$ (3)



EXPERIMENTAL

A colorless faceted egg of $[Gd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(\eta^2\text{-}ClO_4)_2(H_2O)_{20}](ClO_4)_6 \cdot 4H_2O$ having approximate dimensions of 0.20 x 0.20 x 0.30 mm was mounted on a glass fiber in a random orientation using a drop of paratone oil. Examination of the crystal on a Bruker SMART 1000 CCD detector X-ray diffractometer at 170(2)K and a power setting of 50KV, 40mA showed measurable diffraction to at least theta = 28.3deg. Data were collected on the SMART1000 system using graphite monochromated Mo Kα radiation (λ=0.71073Å).

Cell constants and an orientation matrix for integration were determined from reflections obtained in three orthogonal 5 deg wedges of reciprocal space. A total of 1868 frames at 1 detector setting covering 0 < 2theta < 60 deg were collected, having an omega scan width of 0.3 and an exposure time of 10 seconds. The frames were integrated using the Bruker SAINT software package's narrow frame algorithm. A total of 24740 reflections were integrated and retained (reflections due to C centering were removed) of which 6716 were unique (<redundancy> = 3.7, Rint = 2.6%, Rsig = 2.4%). Of the unique reflections, 6263 (93.3%) were observed >2sigma(I). The final Monoclinic cell parameters of a = 23.1490(16), b = 11.9086(6), c = 21.0097(15), alpha = 90, beta = 110.220(4), gamma = 90, volume = 5434.9(6) A^3 are based on the refinement of the XYZ-centroids of 6705 reflections with I > 10 sigma(I) covering the range of 3.01 < theta < 28.3. Empirical absorption and decay corrections were applied using the program SADABS (Sheldrick). The absorption coefficient is 7.755 mm-1, Tmin = 0.794169, and Tmax = 0.982808. For Z = 4 and F.W. = 2323.55 the calculated density is 2.840g/cm3. Systematic absences and intensity statistics indicate the space group to be C2/c (#15) which was consistent with refinement.

The structure was solved using SHELXS in the Bruker SHELXTL (Version 5.0) software package[1]. Refinements were performed using SHELXL and illustrations were made using XP. Solution was achieved utilizing direct methods followed by Fourier synthesis. Hydrogen atoms were added at idealized, disordered positions(as though they were .66 occupied methyl groups for coordinated water), constrained to ride on the atom to which they are bonded and given thermal parameters equal to 1.2 or 1.5 times Uiso of that bonded atom. Hydrogens giving rise to close contacts were removed in favor of those making hydrogen bonds. Hydrogens on uncoordinated water were found from a difference map and restrained to a distance of approximately 1.0Å. Several of the uncoordinated perchlorate anions showed rotational disorder. They were lightly constrained to show the same geometry as well behaved perchlorate #4. The final anisotropic full-matrix least squares refinement based on F^2 of all reflections converged (maximum shift/esd = 0.007) at R1 = 0.0235, wR2 = 0.0520 and goodness-of-fit = 1.107. "Conventional" refinement indices using the 6263 reflections with F > 4 sigma(F) are R1 = 0.0209, wR2 = 0.0511. The model consisted of 401 variable parameters, 136 constraints and 60 restraints. There were 24 correlation coefficients between .87 and .60, all were between parameters describing the same disordered perchlorate site. The highest peak on the final difference map was 1.351 e/A^3 located 2.14 A from O22P. The lowest peak on the final difference map was -1.051 e/A^3 located

0.62 A from GD2. Scattering Factors and anomalous dispersion were taken from International Tables Vol C Tables 4.2.6.8 and 6.1.1.4.

EQUATIONS

$R_{int} = \sum|Fo^2-\langle Fo^2\rangle|/\sum[Fo^2]$

$R_{sig} = \sum[\sigma(Fo^2)]/\sum[Fo^2]$

$R_1 = \Sigma||Fo|-|Fc||/\sum|Fo|$

$wR_2 = \{\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]\}^{1/2}$

$w=1/[\sigma^2(Fo^2)+(0.0253P)^2+10.888P]$ where $P=(Fo^2+2Fc^2)/3$

$GOF = S = \{\sum[w(Fo^2-Fc^2)^2]/(n-p)\}^{1/2}$

REFERENCES

Bruker (1997) SAINT Reference Manual Version 5.0, Bruker AXS Inc. , Madison, Wisconsin, USA.

Bruker (1997) SHELXTL Reference Manual Version 5.0, Bruker AXS Inc. , Madison, Wisconsin, USA.

Bruker (1997) SMART Reference Manual Version 5.0, Bruker AXS Inc. , Madison, Wisconsin, USA.

Table 1. Crystal data and structure refinement for $[Gd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(\eta^2\text{-}ClO_4)_2(H_2O)_{20}](ClO_4)_6 \cdot 4H_2O$ (**3**).

Empirical formula	$H_{56}Cl_8Gd_6O_{65}$	
Formula weight	2323.55	
Temperature	170(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 23.1490(16) Å	a= 90°.
	b = 11.9086(6) Å	b= 110.220(4)°.
	c = 21.0097(15) Å	g = 90°.
Volume	5434.9(6) $Å^3$	
Z	4	
Density (calculated)	2.840 Mg/m^3	
Absorption coefficient	7.755 mm^{-1}	
F(000)	4384	
Crystal size	0.30 x 0.20 x 0.20 mm^3	
Theta range for utilized data	2.35 to 28.30°.	
Limiting Indices	-30<=h<=29, -15<=k<=15, -27<=l<=28	
Reflections utilized	24740	
Independent reflections	6716 [R(int) = 0.0258]	
Completeness to theta = 28.30°	99.4 %	
Absorption correction	Empirical	
Max. and min. transmission	0.982808 and 0.794169	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6716 / 60 / 401	
Goodness-of-fit on F^2	1.107	
Final R indices [I>2sigma(I)]	R1 = 0.0209, wR2 = 0.0511	
R indices (all data)	R1 = 0.0235, wR2 = 0.0520	
Largest diff. peak and hole	1.351 and -1.051 $e.Å^{-3}$	
RMS difference density	0.160$e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[Gd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(\eta^2\text{-}ClO_4)_2(H_2O)_{20}](ClO_4)_6 \cdot 4H_2O$ (**3**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Gd(1)	3141(1)	11351(1)	4433(1)	11(1)
Gd(2)	1735(1)	10903(1)	4791(1)	12(1)
Gd(3)	1892(1)	13333(1)	3866(1)	12(1)
O(1)	2500	12500	5000	14(1)
O(2M)	2055(1)	11367(2)	3867(1)	14(1)
O(3M)	2960(1)	13270(2)	4114(1)	14(1)
O(4M)	2790(1)	10386(2)	5229(1)	14(1)
O(5M)	3703(1)	12279(2)	5484(1)	14(1)
O(11T)	2991(1)	11329(2)	3170(1)	25(1)
O(12T)	4073(1)	12033(2)	4277(1)	22(1)
O(13T)	2915(1)	9392(2)	4016(2)	30(1)
O(14T)	4005(1)	10098(2)	5010(1)	26(1)
O(21T)	792(1)	10557(3)	3744(1)	32(1)
O(22T)	1807(1)	9021(2)	4288(1)	27(1)
O(23T)	808(1)	10771(2)	5101(1)	22(1)
O(31T)	2008(1)	13140(2)	2756(1)	26(1)
O(32T)	876(1)	12506(2)	3043(1)	28(1)
O(33T)	1139(1)	14823(2)	3408(1)	29(1)
Cl(1)	2288(1)	8763(1)	6133(1)	21(1)
O(11P)	2662(1)	9614(2)	6571(1)	30(1)
O(12P)	2637(2)	8181(2)	5787(2)	36(1)
O(13P)	2065(2)	7986(3)	6512(2)	40(1)
O(14P)	1765(1)	9305(2)	5628(1)	23(1)
Cl(4)	470(1)	3777(1)	1407(1)	22(1)
O(41P)	41(2)	3569(3)	742(2)	42(1)
O(42P)	807(2)	2767(3)	1667(2)	61(1)
O(43P)	153(2)	4108(3)	1853(2)	51(1)
O(44P)	885(2)	4642(3)	1394(2)	59(1)
Cl(2)	1263(2)	9628(2)	2289(2)	24(1)
O(21P)	1744(3)	10422(6)	2546(3)	54(2)
O(22P)	687(3)	10234(6)	2106(3)	71(2)
Cl(2A)	1493(5)	9463(6)	2366(3)	29(1)
O(22A)	2154(8)	9401(17)	2640(7)	93(7)
O(21A)	1344(14)	10619(13)	2431(11)	100(11)
O(23P)	1306(2)	9084(3)	1701(2)	41(1)
O(24P)	1264(3)	8839(3)	2792(2)	79(2)
Cl(3A)	503(1)	7444(1)	4074(1)	25(1)
O(31A)	101(1)	6481(2)	3877(2)	40(1)
O(32A)	725(6)	7695(10)	3531(5)	34(2)
O(33A)	153(5)	8370(7)	4193(7)	26(2)
O(34A)	1030(4)	7209(8)	4677(5)	24(2)
Cl(3B)	503(1)	7444(1)	4074(1)	25(1)
O(31B)	101(1)	6481(2)	3877(2)	40(1)
O(32B)	1115(4)	7104(8)	4476(5)	33(2)
O(33B)	551(5)	8018(10)	3483(5)	46(3)
O(34B)	273(5)	8255(8)	4445(6)	41(3)
Cl(3C)	503(1)	7444(1)	4074(1)	25(1)

O(31C)	101(1)	6481(2)	3877(2)	40(1)
O(32C)	929(5)	7459(10)	3725(6)	52(3)
O(33C)	165(6)	8448(8)	3986(7)	48(4)
O(34C)	847(5)	7291(9)	4799(4)	43(3)
O(1W)	3929(1)	11464(2)	2576(1)	30(1)
O(2W)	5412(2)	5982(3)	680(2)	50(1)

Table 3. Bond lengths [Å] and angles [°] for $[Gd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(\eta^2\text{-}ClO_4)_2(H_2O)_{20}](ClO_4)_6 \cdot 4H_2O$ (**3**).

Gd(1)-O(3M)	2.378(2)	O(13T)-H(13B)	0.9988
Gd(1)-O(2M)	2.380(2)	O(13T)-H(13C)	0.9735
Gd(1)-O(4M)	2.390(2)	O(14T)-H(14A)	0.9800
Gd(1)-O(5M)	2.408(2)	O(14T)-H(14B)	0.9800
Gd(1)-O(12T)	2.433(2)	O(14T)-H(14C)	0.9800
Gd(1)-O(14T)	2.453(2)	O(21T)-H(21A)	0.9800
Gd(1)-O(13T)	2.483(3)	O(21T)-H(21B)	0.9800
Gd(1)-O(11T)	2.555(3)	O(21T)-H(21C)	0.9800
Gd(1)-O(1)	2.59025(18)	O(22T)-H(22A)	0.9800
Gd(1)-Gd(3)	3.6002(3)	O(22T)-H(22B)	0.9800
Gd(1)-Gd(3)#1	3.6192(3)	O(22T)-H(22C)	0.9800
Gd(1)-Gd(2)#1	3.6204(3)	O(23T)-H(23B)	0.9688
Gd(2)-O(2M)	2.370(2)	O(23T)-H(23C)	0.9746
Gd(2)-O(3M)#1	2.374(2)	O(31T)-H(31A)	0.9800
Gd(2)-O(4M)	2.375(2)	O(31T)-H(31B)	0.9800
Gd(2)-O(5M)#1	2.376(2)	O(32T)-H(32A)	0.9712
Gd(2)-O(23T)	2.454(2)	O(32T)-H(32B)	0.9834
Gd(2)-O(22T)	2.508(2)	O(33T)-H(33A)	0.9800
Gd(2)-O(1)	2.53113(19)	O(33T)-H(33B)	0.9800
Gd(2)-O(21T)	2.541(3)	O(33T)-H(33C)	0.9800
Gd(2)-O(14P)	2.576(2)	Cl(1)-O(13P)	1.429(3)
Gd(2)-Gd(3)#1	3.5612(3)	Cl(1)-O(12P)	1.438(3)
Gd(2)-Gd(3)	3.5738(3)	Cl(1)-O(11P)	1.441(3)
Gd(2)-Gd(1)#1	3.6204(3)	Cl(1)-O(14P)	1.456(3)
Gd(3)-O(3M)	2.345(2)	O(11P)-Gd(3)#1	2.922(3)
Gd(3)-O(4M)#1	2.347(2)	Cl(4)-O(44P)	1.414(3)
Gd(3)-O(5M)#1	2.365(2)	Cl(4)-O(41P)	1.429(3)
Gd(3)-O(2M)	2.372(2)	Cl(4)-O(43P)	1.431(3)
Gd(3)-O(33T)	2.440(3)	Cl(4)-O(42P)	1.434(3)
Gd(3)-O(31T)	2.450(3)	Cl(2)-Cl(2A)	0.538(7)
Gd(3)-O(1)	2.5141(2)	Cl(2)-O(21A)	1.215(16)
Gd(3)-O(32T)	2.586(3)	Cl(2)-O(24P)	1.414(5)
Gd(3)-O(11P)#1	2.922(3)	Cl(2)-O(21P)	1.418(6)
Gd(3)-Gd(2)#1	3.5612(3)	Cl(2)-O(23P)	1.428(4)
O(1)-Gd(3)#1	2.5141(2)	Cl(2)-O(22P)	1.446(7)
O(1)-Gd(2)#1	2.53113(18)	Cl(2)-O(22A)	1.954(18)
O(1)-Gd(1)#1	2.59025(18)	O(21P)-O(21A)	0.90(3)
O(2M)-H(2M)	1.0000	O(21P)-Cl(2A)	1.279(9)
O(3M)-Gd(2)#1	2.374(2)	O(21P)-O(22A)	1.51(2)
O(3M)-H(3M)	1.0000	O(22P)-O(21A)	1.51(3)
O(4M)-Gd(3)#1	2.347(2)	O(22P)-Cl(2A)	1.980(11)
O(4M)-H(4M)	1.0000	Cl(2A)-O(23P)	1.388(7)
O(5M)-Gd(3)#1	2.365(2)	Cl(2A)-O(24P)	1.401(8)
O(5M)-Gd(2)#1	2.376(2)	Cl(2A)-O(21A)	1.437(17)
O(5M)-H(5M)	1.0000	Cl(2A)-O(22A)	1.438(19)
O(11T)-H(11A)	0.9800	Cl(3A)-O(33C)	1.406(9)
O(11T)-H(11B)	0.9800	Cl(3A)-O(32C)	1.418(9)
O(11T)-H(11C)	0.9800	Cl(3A)-O(32B)	1.435(8)
O(12T)-H(12A)	0.9800	Cl(3A)-O(32A)	1.435(8)
O(12T)-H(12B)	0.9800	Cl(3A)-O(33A)	1.440(8)
O(12T)-H(12C)	0.9800	Cl(3A)-O(31A)	1.444(3)

Cl(3A)-O(34A)	1.451(7)
Cl(3A)-O(34B)	1.453(9)
Cl(3A)-O(33B)	1.455(9)
Cl(3A)-O(34C)	1.465(8)
O(32A)-O(33B)	0.540(15)
O(32A)-O(32C)	0.580(15)
O(33A)-O(34B)	0.525(14)
O(34A)-O(32B)	0.540(12)
O(34A)-O(34C)	0.573(12)
O(1W)-H(1WA)	0.9783
O(1W)-H(1WB)	0.9751
O(2W)-H(2WA)	0.9825
O(2W)-H(2WB)	0.9835
O(3M)-Gd(1)-O(2M)	78.43(7)
O(3M)-Gd(1)-O(4M)	126.20(8)
O(2M)-Gd(1)-O(4M)	78.39(8)
O(3M)-Gd(1)-O(5M)	78.70(7)
O(2M)-Gd(1)-O(5M)	126.69(7)
O(4M)-Gd(1)-O(5M)	77.63(7)
O(3M)-Gd(1)-O(12T)	73.64(8)
O(2M)-Gd(1)-O(12T)	139.70(8)
O(4M)-Gd(1)-O(12T)	141.87(8)
O(5M)-Gd(1)-O(12T)	75.35(8)
O(3M)-Gd(1)-O(14T)	139.24(8)
O(2M)-Gd(1)-O(14T)	142.31(8)
O(4M)-Gd(1)-O(14T)	77.17(8)
O(5M)-Gd(1)-O(14T)	74.72(8)
O(12T)-Gd(1)-O(14T)	70.11(9)
O(3M)-Gd(1)-O(13T)	143.94(9)
O(2M)-Gd(1)-O(13T)	76.92(8)
O(4M)-Gd(1)-O(13T)	73.40(8)
O(5M)-Gd(1)-O(13T)	137.36(9)
O(12T)-Gd(1)-O(13T)	110.75(9)
O(14T)-Gd(1)-O(13T)	68.85(9)
O(3M)-Gd(1)-O(11T)	76.66(8)
O(2M)-Gd(1)-O(11T)	74.93(8)
O(4M)-Gd(1)-O(11T)	139.91(8)
O(5M)-Gd(1)-O(11T)	142.45(8)
O(12T)-Gd(1)-O(11T)	70.79(8)
O(14T)-Gd(1)-O(11T)	107.53(9)
O(13T)-Gd(1)-O(11T)	71.79(9)
O(3M)-Gd(1)-O(1)	63.22(5)
O(2M)-Gd(1)-O(1)	63.41(5)
O(4M)-Gd(1)-O(1)	62.98(5)
O(5M)-Gd(1)-O(1)	63.28(5)
O(12T)-Gd(1)-O(1)	124.17(6)
O(14T)-Gd(1)-O(1)	126.36(6)
O(13T)-Gd(1)-O(1)	125.04(6)
O(11T)-Gd(1)-O(1)	126.10(6)
O(3M)-Gd(1)-Gd(3)	40.00(5)
O(2M)-Gd(1)-Gd(3)	40.66(5)
O(4M)-Gd(1)-Gd(3)	96.85(5)
O(5M)-Gd(1)-Gd(3)	96.90(5)
O(12T)-Gd(1)-Gd(3)	112.62(6)
O(14T)-Gd(1)-Gd(3)	170.49(6)
O(13T)-Gd(1)-Gd(3)	116.88(7)
O(11T)-Gd(1)-Gd(3)	81.83(6)
O(1)-Gd(1)-Gd(3)	44.291(5)
O(3M)-Gd(1)-Gd(3)#1	96.72(5)
O(2M)-Gd(1)-Gd(3)#1	96.54(5)
O(4M)-Gd(1)-Gd(3)#1	39.75(5)
O(5M)-Gd(1)-Gd(3)#1	40.26(5)
O(12T)-Gd(1)-Gd(3)#1	114.91(6)
O(14T)-Gd(1)-Gd(3)#1	82.39(6)
O(13T)-Gd(1)-Gd(3)#1	111.85(7)
O(11T)-Gd(1)-Gd(3)#1	170.00(6)
O(1)-Gd(1)-Gd(3)#1	43.999(4)
Gd(3)-Gd(1)-Gd(3)#1	88.290(6)
O(3M)-Gd(1)-Gd(2)#1	40.33(5)
O(2M)-Gd(1)-Gd(2)#1	97.11(5)
O(4M)-Gd(1)-Gd(2)#1	96.47(5)
O(5M)-Gd(1)-Gd(2)#1	40.49(5)
O(12T)-Gd(1)-Gd(2)#1	79.82(6)
O(14T)-Gd(1)-Gd(2)#1	113.75(6)
O(13T)-Gd(1)-Gd(2)#1	168.99(6)
O(11T)-Gd(1)-Gd(2)#1	115.97(6)
O(1)-Gd(1)-Gd(2)#1	44.358(4)
Gd(3)-Gd(1)-Gd(2)#1	59.102(5)
Gd(3)#1-Gd(1)-Gd(2)#1	59.162(4)
O(2M)-Gd(2)-O(3M)#1	128.67(8)
O(2M)-Gd(2)-O(4M)	78.89(8)
O(3M)#1-Gd(2)-O(4M)	79.09(8)
O(2M)-Gd(2)-O(5M)#1	79.43(7)
O(3M)#1-Gd(2)-O(5M)#1	79.42(7)
O(4M)-Gd(2)-O(5M)#1	128.75(7)
O(2M)-Gd(2)-O(23T)	141.44(8)
O(3M)#1-Gd(2)-O(23T)	76.32(8)
O(4M)-Gd(2)-O(23T)	139.23(8)
O(5M)#1-Gd(2)-O(23T)	77.52(8)
O(2M)-Gd(2)-O(22T)	77.17(8)
O(3M)#1-Gd(2)-O(22T)	137.60(8)
O(4M)-Gd(2)-O(22T)	73.91(8)
O(5M)#1-Gd(2)-O(22T)	142.82(8)
O(23T)-Gd(2)-O(22T)	104.23(9)
O(2M)-Gd(2)-O(1)	64.47(5)
O(3M)#1-Gd(2)-O(1)	64.20(5)
O(4M)-Gd(2)-O(1)	64.11(5)
O(5M)#1-Gd(2)-O(1)	64.64(5)
O(23T)-Gd(2)-O(1)	128.74(6)
O(22T)-Gd(2)-O(1)	126.89(6)
O(2M)-Gd(2)-O(21T)	75.36(8)
O(3M)#1-Gd(2)-O(21T)	141.65(9)
O(4M)-Gd(2)-O(21T)	139.02(9)
O(5M)#1-Gd(2)-O(21T)	76.72(9)
O(23T)-Gd(2)-O(21T)	69.52(9)

O(22T)-Gd(2)-O(21T)	69.68(10)
O(1)-Gd(2)-O(21T)	127.76(7)
O(2M)-Gd(2)-O(14P)	142.12(8)
O(3M)#1-Gd(2)-O(14P)	73.51(8)
O(4M)-Gd(2)-O(14P)	76.28(8)
O(5M)#1-Gd(2)-O(14P)	138.38(8)
O(23T)-Gd(2)-O(14P)	65.84(8)
O(22T)-Gd(2)-O(14P)	68.75(9)
O(1)-Gd(2)-O(14P)	125.79(6)
O(21T)-Gd(2)-O(14P)	106.44(9)
O(2M)-Gd(2)-Gd(3)#1	98.25(5)
O(3M)#1-Gd(2)-Gd(3)#1	40.70(5)
O(4M)-Gd(2)-Gd(3)#1	40.76(5)
O(5M)#1-Gd(2)-Gd(3)#1	98.56(5)
O(23T)-Gd(2)-Gd(3)#1	115.40(6)
O(22T)-Gd(2)-Gd(3)#1	113.03(7)
O(1)-Gd(2)-Gd(3)#1	44.907(4)
O(21T)-Gd(2)-Gd(3)#1	172.57(7)
O(14P)-Gd(2)-Gd(3)#1	80.92(6)
O(2M)-Gd(2)-Gd(3)	41.11(5)
O(3M)#1-Gd(2)-Gd(3)	97.98(5)
O(4M)-Gd(2)-Gd(3)	97.84(5)
O(5M)#1-Gd(2)-Gd(3)	40.97(5)
O(23T)-Gd(2)-Gd(3)	117.32(6)
O(22T)-Gd(2)-Gd(3)	117.42(6)
O(1)-Gd(2)-Gd(3)	44.706(5)
O(21T)-Gd(2)-Gd(3)	83.06(7)
O(14P)-Gd(2)-Gd(3)	170.32(6)
Gd(3)#1-Gd(2)-Gd(3)	89.613(6)
O(2M)-Gd(2)-Gd(1)#1	99.18(5)
O(3M)#1-Gd(2)-Gd(1)#1	40.40(5)
O(4M)-Gd(2)-Gd(1)#1	98.55(5)
O(5M)#1-Gd(2)-Gd(1)#1	41.16(5)
O(23T)-Gd(2)-Gd(1)#1	83.06(6)
O(22T)-Gd(2)-Gd(1)#1	172.05(6)
O(1)-Gd(2)-Gd(1)#1	45.681(4)
O(21T)-Gd(2)-Gd(1)#1	116.53(7)
O(14P)-Gd(2)-Gd(1)#1	112.38(6)
Gd(3)#1-Gd(2)-Gd(1)#1	60.167(4)
Gd(3)-Gd(2)-Gd(1)#1	60.402(6)
O(3M)-Gd(3)-O(4M)#1	80.23(8)
O(3M)-Gd(3)-O(5M)#1	129.92(8)
O(4M)#1-Gd(3)-O(5M)#1	79.32(7)
O(3M)-Gd(3)-O(2M)	79.22(8)
O(4M)#1-Gd(3)-O(2M)	129.48(8)
O(5M)#1-Gd(3)-O(2M)	79.60(7)
O(3M)-Gd(3)-O(33T)	131.76(8)
O(4M)#1-Gd(3)-O(33T)	80.10(9)
O(5M)#1-Gd(3)-O(33T)	88.39(8)
O(2M)-Gd(3)-O(33T)	144.06(9)
O(3M)-Gd(3)-O(31T)	75.81(8)
O(4M)#1-Gd(3)-O(31T)	136.50(8)
O(5M)#1-Gd(3)-O(31T)	142.94(8)
O(2M)-Gd(3)-O(31T)	80.69(8)
O(33T)-Gd(3)-O(31T)	89.48(9)
O(3M)-Gd(3)-O(1)	64.86(5)
O(4M)#1-Gd(3)-O(1)	64.76(5)
O(5M)#1-Gd(3)-O(1)	65.05(5)
O(2M)-Gd(3)-O(1)	64.72(5)
O(33T)-Gd(3)-O(1)	138.60(7)
O(31T)-Gd(3)-O(1)	131.00(6)
O(3M)-Gd(3)-O(32T)	141.46(8)
O(4M)#1-Gd(3)-O(32T)	138.30(8)
O(5M)#1-Gd(3)-O(32T)	72.02(8)
O(2M)-Gd(3)-O(32T)	74.44(8)
O(33T)-Gd(3)-O(32T)	69.64(9)
O(31T)-Gd(3)-O(32T)	72.59(9)
O(1)-Gd(3)-O(32T)	124.39(6)
O(3M)-Gd(3)-O(11P)#1	68.73(8)
O(4M)#1-Gd(3)-O(11P)#1	70.47(7)
O(5M)#1-Gd(3)-O(11P)#1	141.15(7)
O(2M)-Gd(3)-O(11P)#1	138.83(8)
O(33T)-Gd(3)-O(11P)#1	63.24(8)
O(31T)-Gd(3)-O(11P)#1	67.18(8)
O(1)-Gd(3)-O(11P)#1	119.06(5)
O(32T)-Gd(3)-O(11P)#1	116.55(8)
O(3M)-Gd(3)-Gd(2)#1	41.31(5)
O(4M)#1-Gd(3)-Gd(2)#1	41.33(5)
O(5M)#1-Gd(3)-Gd(2)#1	99.19(5)
O(2M)-Gd(3)-Gd(2)#1	98.84(5)
O(33T)-Gd(3)-Gd(2)#1	116.56(7)
O(31T)-Gd(3)-Gd(2)#1	114.67(6)
O(1)-Gd(3)-Gd(2)#1	45.295(5)
O(32T)-Gd(3)-Gd(2)#1	169.59(6)
O(11P)#1-Gd(3)-Gd(2)#1	73.77(5)
O(3M)-Gd(3)-Gd(2)	98.68(5)
O(4M)#1-Gd(3)-Gd(2)	98.52(5)
O(5M)#1-Gd(3)-Gd(2)	41.19(5)
O(2M)-Gd(3)-Gd(2)	41.08(5)
O(33T)-Gd(3)-Gd(2)	127.57(6)
O(31T)-Gd(3)-Gd(2)	120.47(6)
O(1)-Gd(3)-Gd(2)	45.092(4)
O(32T)-Gd(3)-Gd(2)	79.32(6)
O(11P)#1-Gd(3)-Gd(2)	164.11(5)
Gd(2)#1-Gd(3)-Gd(2)	90.387(6)
O(3M)-Gd(3)-Gd(1)	40.66(5)
O(4M)#1-Gd(3)-Gd(1)	99.64(5)
O(5M)#1-Gd(3)-Gd(1)	99.67(5)
O(2M)-Gd(3)-Gd(1)	40.82(5)
O(33T)-Gd(3)-Gd(1)	171.76(6)
O(31T)-Gd(3)-Gd(1)	85.09(6)
O(1)-Gd(3)-Gd(1)	46.010(4)
O(32T)-Gd(3)-Gd(1)	114.34(6)
O(11P)#1-Gd(3)-Gd(1)	108.81(6)
Gd(2)#1-Gd(3)-Gd(1)	60.731(5)
Gd(2)-Gd(3)-Gd(1)	60.660(5)

Gd(3)-O(1)-Gd(3)#1	180.0
Gd(3)-O(1)-Gd(2)#1	89.798(6)
Gd(3)#1-O(1)-Gd(2)#1	90.202(6)
Gd(3)-O(1)-Gd(2)	90.202(6)
Gd(3)#1-O(1)-Gd(2)	89.798(6)
Gd(2)#1-O(1)-Gd(2)	180.000(7)
Gd(3)-O(1)-Gd(1)	89.699(7)
Gd(3)#1-O(1)-Gd(1)	90.301(7)
Gd(2)#1-O(1)-Gd(1)	89.961(6)
Gd(2)-O(1)-Gd(1)	90.039(6)
Gd(3)-O(1)-Gd(1)#1	90.301(7)
Gd(3)#1-O(1)-Gd(1)#1	89.699(7)
Gd(2)#1-O(1)-Gd(1)#1	90.039(6)
Gd(2)-O(1)-Gd(1)#1	89.961(6)
Gd(1)-O(1)-Gd(1)#1	180.0
Gd(2)-O(2M)-Gd(3)	97.81(8)
Gd(2)-O(2M)-Gd(1)	99.41(8)
Gd(3)-O(2M)-Gd(1)	98.52(8)
Gd(2)-O(2M)-H(2M)	118.9
Gd(3)-O(2M)-H(2M)	118.9
Gd(1)-O(2M)-H(2M)	118.9
Gd(3)-O(3M)-Gd(2)#1	97.98(8)
Gd(3)-O(3M)-Gd(1)	99.34(8)
Gd(2)#1-O(3M)-Gd(1)	99.27(8)
Gd(3)-O(3M)-H(3M)	118.7
Gd(2)#1-O(3M)-H(3M)	118.7
Gd(1)-O(3M)-H(3M)	118.7
Gd(3)#1-O(4M)-Gd(2)	97.91(8)
Gd(3)#1-O(4M)-Gd(1)	99.62(8)
Gd(2)-O(4M)-Gd(1)	98.99(8)
Gd(3)#1-O(4M)-H(4M)	118.7
Gd(2)-O(4M)-H(4M)	118.7
Gd(1)-O(4M)-H(4M)	118.7
Gd(3)#1-O(5M)-Gd(2)#1	97.84(8)
Gd(3)#1-O(5M)-Gd(1)	98.60(8)
Gd(2)#1-O(5M)-Gd(1)	98.35(8)
Gd(3)#1-O(5M)-H(5M)	119.2
Gd(2)#1-O(5M)-H(5M)	119.2
Gd(1)-O(5M)-H(5M)	119.2
Gd(1)-O(11T)-H(11A)	109.5
Gd(1)-O(11T)-H(11B)	109.5
H(11A)-O(11T)-H(11B)	109.5
Gd(1)-O(11T)-H(11C)	109.5
H(11A)-O(11T)-H(11C)	109.5
H(11B)-O(11T)-H(11C)	109.5
Gd(1)-O(12T)-H(12A)	109.5
Gd(1)-O(12T)-H(12B)	109.5
H(12A)-O(12T)-H(12B)	109.5
Gd(1)-O(12T)-H(12C)	109.5
H(12A)-O(12T)-H(12C)	109.5
H(12B)-O(12T)-H(12C)	109.5
Gd(1)-O(13T)-H(13B)	118.0
Gd(1)-O(13T)-H(13C)	137.0
H(13B)-O(13T)-H(13C)	71.4
Gd(1)-O(14T)-H(14A)	109.5
Gd(1)-O(14T)-H(14B)	109.5
H(14A)-O(14T)-H(14B)	109.5
Gd(1)-O(14T)-H(14C)	109.5
H(14A)-O(14T)-H(14C)	109.5
H(14B)-O(14T)-H(14C)	109.5
Gd(2)-O(21T)-H(21A)	109.5
Gd(2)-O(21T)-H(21B)	109.5
H(21A)-O(21T)-H(21B)	109.5
Gd(2)-O(21T)-H(21C)	109.5
H(21A)-O(21T)-H(21C)	109.5
H(21B)-O(21T)-H(21C)	109.5
Gd(2)-O(22T)-H(22A)	109.5
Gd(2)-O(22T)-H(22B)	109.5
H(22A)-O(22T)-H(22B)	109.5
Gd(2)-O(22T)-H(22C)	109.5
H(22A)-O(22T)-H(22C)	109.5
H(22B)-O(22T)-H(22C)	109.5
Gd(2)-O(23T)-H(23B)	125.0
Gd(2)-O(23T)-H(23C)	124.1
H(23B)-O(23T)-H(23C)	94.8
Gd(3)-O(31T)-H(31A)	109.4
Gd(3)-O(31T)-H(31B)	109.4
H(31A)-O(31T)-H(31B)	109.5
Gd(3)-O(32T)-H(32A)	119.4
Gd(3)-O(32T)-H(32B)	104.4
H(32A)-O(32T)-H(32B)	102.2
Gd(3)-O(33T)-H(33A)	109.5
Gd(3)-O(33T)-H(33B)	109.5
H(33A)-O(33T)-H(33B)	109.5
Gd(3)-O(33T)-H(33C)	109.5
H(33A)-O(33T)-H(33C)	109.5
H(33B)-O(33T)-H(33C)	109.5
O(13P)-Cl(1)-O(12P)	110.13(18)
O(13P)-Cl(1)-O(11P)	110.62(18)
O(12P)-Cl(1)-O(11P)	110.09(19)
O(13P)-Cl(1)-O(14P)	108.86(18)
O(12P)-Cl(1)-O(14P)	108.46(17)
O(11P)-Cl(1)-O(14P)	108.63(16)
Cl(1)-O(11P)-Gd(3)#1	125.94(15)
Cl(1)-O(14P)-Gd(2)	130.06(14)
O(44P)-Cl(4)-O(41P)	110.7(2)
O(44P)-Cl(4)-O(43P)	108.5(2)
O(41P)-Cl(4)-O(43P)	110.3(2)
O(44P)-Cl(4)-O(42P)	109.6(3)
O(41P)-Cl(4)-O(42P)	109.22(19)
O(43P)-Cl(4)-O(42P)	108.5(2)
Cl(2A)-Cl(2)-O(21A)	103.2(17)
Cl(2A)-Cl(2)-O(24P)	77.6(10)
O(21A)-Cl(2)-O(24P)	120.1(9)
Cl(2A)-Cl(2)-O(21P)	64.1(10)
O(21A)-Cl(2)-O(21P)	39.1(13)

O(24P)-Cl(2)-O(21P)	111.1(4)	Cl(2)-O(21A)-O(22P)	63.1(12)
Cl(2A)-Cl(2)-O(23P)	74.8(9)	Cl(2A)-O(21A)-O(22P)	84.4(12)
O(21A)-Cl(2)-O(23P)	127.0(7)	Cl(2A)-O(23P)-Cl(2)	22.0(3)
O(24P)-Cl(2)-O(23P)	111.2(3)	Cl(2A)-O(24P)-Cl(2)	22.0(3)
O(21P)-Cl(2)-O(23P)	110.6(4)	O(33C)-Cl(3A)-O(32C)	112.1(7)
Cl(2A)-Cl(2)-O(22P)	171.5(11)	O(33C)-Cl(3A)-O(32B)	135.1(7)
O(21A)-Cl(2)-O(22P)	68.4(14)	O(32C)-Cl(3A)-O(32B)	65.5(7)
O(24P)-Cl(2)-O(22P)	107.0(4)	O(33C)-Cl(3A)-O(32A)	93.1(8)
O(21P)-Cl(2)-O(22P)	107.4(5)	O(32C)-Cl(3A)-O(32A)	23.4(6)
O(23P)-Cl(2)-O(22P)	109.3(3)	O(32B)-Cl(3A)-O(32A)	88.5(7)
Cl(2A)-Cl(2)-O(22A)	13.9(11)	O(33C)-Cl(3A)-O(33A)	18.3(7)
O(21A)-Cl(2)-O(22A)	89.3(15)	O(32C)-Cl(3A)-O(33A)	127.8(7)
O(24P)-Cl(2)-O(22A)	84.1(6)	O(32B)-Cl(3A)-O(33A)	128.0(6)
O(21P)-Cl(2)-O(22A)	50.3(7)	O(32A)-Cl(3A)-O(33A)	110.8(7)
O(23P)-Cl(2)-O(22A)	83.3(6)	O(33C)-Cl(3A)-O(31A)	111.4(5)
O(22P)-Cl(2)-O(22A)	157.7(7)	O(32C)-Cl(3A)-O(31A)	110.8(5)
O(21A)-O(21P)-Cl(2A)	80.4(13)	O(32B)-Cl(3A)-O(31A)	110.6(4)
O(21A)-O(21P)-Cl(2)	58.2(12)	O(32A)-Cl(3A)-O(31A)	108.0(5)
Cl(2A)-O(21P)-Cl(2)	22.2(3)	O(33A)-Cl(3A)-O(31A)	108.2(4)
O(21A)-O(21P)-O(22A)	141.4(15)	O(33C)-Cl(3A)-O(34A)	122.7(7)
Cl(2A)-O(21P)-O(22A)	61.4(8)	O(32C)-Cl(3A)-O(34A)	85.9(7)
Cl(2)-O(21P)-O(22A)	83.6(7)	O(32B)-Cl(3A)-O(34A)	21.6(5)
Cl(2)-O(22P)-O(21A)	48.5(6)	O(32A)-Cl(3A)-O(34A)	108.1(7)
Cl(2)-O(22P)-Cl(2A)	2.3(3)	O(33A)-Cl(3A)-O(34A)	110.5(7)
O(21A)-O(22P)-Cl(2A)	46.2(6)	O(31A)-Cl(3A)-O(34A)	111.2(4)
Cl(2)-Cl(2A)-O(21P)	93.6(12)	O(33C)-Cl(3A)-O(34B)	38.3(7)
Cl(2)-Cl(2A)-O(23P)	83.3(10)	O(32C)-Cl(3A)-O(34B)	135.9(6)
O(21P)-Cl(2A)-O(23P)	122.7(6)	O(32B)-Cl(3A)-O(34B)	110.0(6)
Cl(2)-Cl(2A)-O(24P)	80.4(11)	O(32A)-Cl(3A)-O(34B)	125.9(7)
O(21P)-Cl(2A)-O(24P)	121.3(6)	O(33A)-Cl(3A)-O(34B)	20.9(6)
O(23P)-Cl(2A)-O(24P)	114.6(5)	O(31A)-Cl(3A)-O(34B)	111.3(5)
Cl(2)-Cl(2A)-O(21A)	55.5(15)	O(34A)-Cl(3A)-O(34B)	90.8(6)
O(21P)-Cl(2A)-O(21A)	38.3(10)	O(33C)-Cl(3A)-O(33B)	72.0(7)
O(23P)-Cl(2A)-O(21A)	113.9(11)	O(32C)-Cl(3A)-O(33B)	44.0(7)
O(24P)-Cl(2A)-O(21A)	107.0(9)	O(32B)-Cl(3A)-O(33B)	106.4(6)
Cl(2)-Cl(2A)-O(22A)	160.9(15)	O(32A)-Cl(3A)-O(33B)	21.5(6)
O(21P)-Cl(2A)-O(22A)	67.4(10)	O(33A)-Cl(3A)-O(33B)	90.1(7)
O(23P)-Cl(2A)-O(22A)	107.8(9)	O(31A)-Cl(3A)-O(33B)	111.1(5)
O(24P)-Cl(2A)-O(22A)	107.6(8)	O(34A)-Cl(3A)-O(33B)	123.1(6)
O(21A)-Cl(2A)-O(22A)	105.5(15)	O(34B)-Cl(3A)-O(33B)	107.2(6)
Cl(2)-Cl(2A)-O(22P)	6.2(8)	O(33C)-Cl(3A)-O(34C)	108.7(7)
O(21P)-Cl(2A)-O(22P)	87.5(7)	O(32C)-Cl(3A)-O(34C)	108.2(7)
O(23P)-Cl(2A)-O(22P)	86.4(5)	O(32B)-Cl(3A)-O(34C)	44.1(6)
O(24P)-Cl(2A)-O(22P)	83.9(5)	O(32A)-Cl(3A)-O(34C)	129.5(7)
O(21A)-Cl(2A)-O(22P)	49.3(13)	O(33A)-Cl(3A)-O(34C)	93.0(7)
O(22A)-Cl(2A)-O(22P)	154.8(10)	O(31A)-Cl(3A)-O(34C)	105.4(4)
Cl(2A)-O(22A)-O(21P)	51.3(8)	O(34A)-Cl(3A)-O(34C)	22.7(5)
Cl(2A)-O(22A)-Cl(2)	5.2(4)	O(34B)-Cl(3A)-O(34C)	72.2(6)
O(21P)-O(22A)-Cl(2)	46.1(5)	O(33B)-Cl(3A)-O(34C)	140.4(6)
O(21P)-O(21A)-Cl(2)	82.7(14)	O(33B)-O(32A)-O(32C)	148(3)
O(21P)-O(21A)-Cl(2A)	61.3(11)	O(33B)-O(32A)-Cl(3A)	81.3(15)
Cl(2)-O(21A)-Cl(2A)	21.4(4)	O(32C)-O(32A)-Cl(3A)	76.7(13)
O(21P)-O(21A)-O(22P)	145.4(17)	O(34B)-O(33A)-Cl(3A)	80.9(14)

O(32B)-O(34A)-O(34C)	156(2)
O(32B)-O(34A)-Cl(3A)	77.5(13)
O(34C)-O(34A)-Cl(3A)	80.1(12)
O(34A)-O(32B)-Cl(3A)	80.9(13)
O(32A)-O(33B)-Cl(3A)	77.2(15)
O(33A)-O(34B)-Cl(3A)	78.2(15)
O(32A)-O(32C)-Cl(3A)	79.9(13)
O(34A)-O(34C)-Cl(3A)	77.3(12)
H(1WA)-O(1W)-H(1WB)	90.8
H(2WA)-O(2W)-H(2WB)	93.6

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,-y+5/2,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Gd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(\eta^2\text{-}ClO_4)_2(H_2O)_{20}](ClO_4)_6 \cdot 4H_2O$ (**3**). The anisotropic displacement factor exponent takes the form: $-2p^2[\, h^2 a^{*2} U^{11} + \ldots + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Gd(1)	10(1)	12(1)	11(1)	0(1)	3(1)	0(1)
Gd(2)	11(1)	12(1)	12(1)	-1(1)	4(1)	-1(1)
Gd(3)	12(1)	14(1)	11(1)	1(1)	2(1)	2(1)
O(1)	12(2)	14(2)	14(2)	1(1)	4(1)	1(1)
O(2M)	13(1)	16(1)	12(1)	-2(1)	3(1)	0(1)
O(3M)	13(1)	14(1)	15(1)	-1(1)	6(1)	-2(1)
O(4M)	14(1)	12(1)	16(1)	2(1)	5(1)	0(1)
O(5M)	11(1)	15(1)	14(1)	-1(1)	1(1)	1(1)
O(11T)	21(1)	32(1)	22(1)	-8(1)	9(1)	-5(1)
O(12T)	17(1)	23(1)	26(1)	2(1)	9(1)	-2(1)
O(13T)	30(2)	21(1)	42(2)	-13(1)	16(1)	-1(1)
O(14T)	19(1)	22(1)	34(2)	3(1)	5(1)	6(1)
O(21T)	24(1)	47(2)	23(1)	0(1)	3(1)	-8(1)
O(22T)	30(2)	18(1)	36(2)	-6(1)	16(1)	-6(1)
O(23T)	14(1)	27(1)	24(1)	7(1)	5(1)	-3(1)
O(31T)	28(1)	33(2)	16(1)	-3(1)	6(1)	-5(1)
O(32T)	23(1)	31(1)	24(1)	0(1)	0(1)	-3(1)
O(33T)	22(1)	29(1)	34(2)	12(1)	8(1)	7(1)
Cl(1)	27(1)	17(1)	22(1)	4(1)	11(1)	6(1)
O(11P)	28(1)	36(2)	23(1)	-3(1)	2(1)	-1(1)
O(12P)	49(2)	23(1)	45(2)	4(1)	29(2)	16(1)
O(13P)	61(2)	29(2)	38(2)	13(1)	29(2)	2(1)
O(14P)	21(1)	19(1)	26(1)	4(1)	5(1)	-2(1)
Cl(4)	18(1)	24(1)	21(1)	0(1)	2(1)	2(1)
O(41P)	39(2)	44(2)	27(2)	-1(1)	-10(1)	7(1)
O(42P)	72(3)	42(2)	40(2)	-10(2)	-16(2)	31(2)
O(43P)	45(2)	77(3)	39(2)	10(2)	26(2)	16(2)
O(44P)	54(2)	68(3)	61(2)	-10(2)	27(2)	-34(2)
Cl(2)	32(1)	25(1)	17(1)	-8(1)	10(1)	-8(1)
O(21P)	62(4)	70(5)	37(3)	-30(3)	28(3)	-41(4)
O(22P)	52(4)	96(5)	59(4)	-23(3)	13(3)	23(4)
Cl(2A)	36(3)	31(2)	19(2)	-5(2)	9(2)	-4(2)
O(22A)	80(12)	118(16)	52(9)	15(9)	-16(8)	-38(11)
O(21A)	220(30)	28(7)	119(18)	3(8)	140(20)	3(13)
O(23P)	46(2)	52(2)	29(2)	-19(1)	18(1)	-7(2)
O(24P)	167(5)	38(2)	48(2)	-1(2)	58(3)	-26(3)
Cl(3A)	20(1)	22(1)	36(1)	-2(1)	12(1)	-5(1)
O(31A)	28(2)	26(2)	63(2)	-8(1)	11(2)	-8(1)
Cl(3B)	20(1)	22(1)	36(1)	-2(1)	12(1)	-5(1)
O(31B)	28(2)	26(2)	63(2)	-8(1)	11(2)	-8(1)
Cl(3C)	20(1)	22(1)	36(1)	-2(1)	12(1)	-5(1)
O(31C)	28(2)	26(2)	63(2)	-8(1)	11(2)	-8(1)
O(1W)	31(2)	29(1)	28(1)	-1(1)	9(1)	-3(1)
O(2W)	30(2)	52(2)	57(2)	-31(2)	3(2)	4(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[Gd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(\eta^2\text{-}ClO_4)_2(H_2O)_{20}](ClO_4)_6 \cdot 4H_2O$ (**3**).

	x	y	z	U(eq)
H(2M)	1877	10942	3432	16
H(3M)	3133	13579	3775	16
H(4M)	2898	9575	5323	17
H(5M)	4161	12200	5675	17
H(11A)	2741	10678	2955	37
H(11B)	3393	11282	3114	37
H(11C)	2782	12019	2958	37
H(12A)	4052	11881	3811	32
H(12B)	4431	11649	4595	32
H(12C)	4111	12843	4361	32
H(13B)	3161	9065	3754	45
H(13C)	2635	9018	3616	45
H(14A)	3882	9571	5298	38
H(14B)	4356	10544	5290	38
H(14C)	4121	9678	4671	38
H(21A)	720	11210	3443	48
H(21B)	432	10438	3881	48
H(21C)	859	9891	3506	48
H(22A)	1497	8972	3832	40
H(22B)	1733	8429	4574	40
H(22C)	2218	8928	4261	40
H(23B)	688	10117	5300	33
H(23C)	393	10935	4792	33
H(31A)	2193	13826	2653	39
H(31B)	1602	13023	2408	39
H(32A)	858	12243	2599	42
H(32B)	589	13145	2928	42
H(33A)	1020	15147	3774	43
H(33B)	774	14511	3059	43
H(33C)	1320	15408	3208	43
H(1WA)	4356	11421	2883	44
H(1WB)	3973	12265	2510	44
H(2WA)	5617	6687	876	75
H(2WB)	5366	5734	1106	75

Table 6. Torsion angles [°] for $[Gd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(\eta^2\text{-}ClO_4)_2(H_2O)_{20}](ClO_4)_6 \cdot 4H_2O$ (**3**).

O(2M)-Gd(2)-Gd(3)-O(3M)	-62.42(10)	Gd(3)#1-Gd(2)-Gd(3)-O(33T)	-124.71(9)
O(3M)#1-Gd(2)-Gd(3)-O(3M)	80.60(8)	Gd(1)#1-Gd(2)-Gd(3)-O(33T)	-69.34(9)
O(4M)-Gd(2)-Gd(3)-O(3M)	0.60(7)	O(2M)-Gd(2)-Gd(3)-O(31T)	16.16(11)
O(5M)#1-Gd(2)-Gd(3)-O(3M)	144.22(10)	O(3M)#1-Gd(2)-Gd(3)-O(31T)	159.19(9)
O(23T)-Gd(2)-Gd(3)-O(3M)	159.28(9)	O(4M)-Gd(2)-Gd(3)-O(31T)	79.19(9)
O(22T)-Gd(2)-Gd(3)-O(3M)	-75.29(9)	O(5M)#1-Gd(2)-Gd(3)-O(31T)	-137.19(11)
O(1)-Gd(2)-Gd(3)-O(3M)	40.64(5)	O(23T)-Gd(2)-Gd(3)-O(31T)	-122.13(10)
O(21T)-Gd(2)-Gd(3)-O(3M)	-138.08(9)	O(22T)-Gd(2)-Gd(3)-O(31T)	3.30(10)
O(14P)-Gd(2)-Gd(3)-O(3M)	52.5(4)	O(1)-Gd(2)-Gd(3)-O(31T)	119.23(7)
Gd(3)#1-Gd(2)-Gd(3)-O(3M)	40.64(5)	O(21T)-Gd(2)-Gd(3)-O(31T)	-59.49(10)
Gd(1)#1-Gd(2)-Gd(3)-O(3M)	96.01(5)	O(14P)-Gd(2)-Gd(3)-O(31T)	131.1(4)
O(2M)-Gd(2)-Gd(3)-O(4M)#1	-143.75(10)	Gd(3)#1-Gd(2)-Gd(3)-O(31T)	119.23(7)
O(3M)#1-Gd(2)-Gd(3)-O(4M)#1	-0.73(8)	Gd(1)#1-Gd(2)-Gd(3)-O(31T)	174.60(7)
O(4M)-Gd(2)-Gd(3)-O(4M)#1	-80.73(8)	O(2M)-Gd(2)-Gd(3)-O(1)	-103.06(8)
O(5M)#1-Gd(2)-Gd(3)-O(4M)#1	62.89(10)	O(3M)#1-Gd(2)-Gd(3)-O(1)	39.96(5)
O(23T)-Gd(2)-Gd(3)-O(4M)#1	77.95(9)	O(4M)-Gd(2)-Gd(3)-O(1)	-40.04(5)
O(22T)-Gd(2)-Gd(3)-O(4M)#1	-156.62(9)	O(5M)#1-Gd(2)-Gd(3)-O(1)	103.58(8)
O(1)-Gd(2)-Gd(3)-O(4M)#1	-40.69(5)	O(23T)-Gd(2)-Gd(3)-O(1)	118.64(7)
O(21T)-Gd(2)-Gd(3)-O(4M)#1	140.59(9)	O(22T)-Gd(2)-Gd(3)-O(1)	-115.93(7)
O(14P)-Gd(2)-Gd(3)-O(4M)#1	-28.8(4)	O(21T)-Gd(2)-Gd(3)-O(1)	-178.72(7)
Gd(3)#1-Gd(2)-Gd(3)-O(4M)#1	-40.69(5)	O(14P)-Gd(2)-Gd(3)-O(1)	11.9(4)
Gd(1)#1-Gd(2)-Gd(3)-O(4M)#1	14.68(5)	Gd(3)#1-Gd(2)-Gd(3)-O(1)	0.0
O(2M)-Gd(2)-Gd(3)-O(5M)#1	153.36(11)	Gd(1)#1-Gd(2)-Gd(3)-O(1)	55.368(5)
O(3M)#1-Gd(2)-Gd(3)-O(5M)#1	-63.62(9)	O(2M)-Gd(2)-Gd(3)-O(32T)	78.51(10)
O(4M)-Gd(2)-Gd(3)-O(5M)#1	-143.62(10)	O(3M)#1-Gd(2)-Gd(3)-O(32T)	-138.46(8)
O(23T)-Gd(2)-Gd(3)-O(5M)#1	15.06(10)	O(4M)-Gd(2)-Gd(3)-O(32T)	141.53(8)
O(22T)-Gd(2)-Gd(3)-O(5M)#1	140.49(11)	O(5M)#1-Gd(2)-Gd(3)-O(32T)	-74.85(10)
O(1)-Gd(2)-Gd(3)-O(5M)#1	-103.58(8)	O(23T)-Gd(2)-Gd(3)-O(32T)	-59.78(9)
O(21T)-Gd(2)-Gd(3)-O(5M)#1	77.70(11)	O(22T)-Gd(2)-Gd(3)-O(32T)	65.65(10)
O(14P)-Gd(2)-Gd(3)-O(5M)#1	-91.7(4)	O(1)-Gd(2)-Gd(3)-O(32T)	-178.42(6)
Gd(3)#1-Gd(2)-Gd(3)-O(5M)#1	-103.58(8)	O(21T)-Gd(2)-Gd(3)-O(32T)	2.86(9)
Gd(1)#1-Gd(2)-Gd(3)-O(5M)#1	-48.21(8)	O(14P)-Gd(2)-Gd(3)-O(32T)	-166.5(4)
O(3M)#1-Gd(2)-Gd(3)-O(2M)	143.02(10)	Gd(3)#1-Gd(2)-Gd(3)-O(32T)	-178.42(6)
O(4M)-Gd(2)-Gd(3)-O(2M)	63.02(10)	Gd(1)#1-Gd(2)-Gd(3)-O(32T)	-123.06(6)
O(5M)#1-Gd(2)-Gd(3)-O(2M)	-153.36(11)	O(2M)-Gd(2)-Gd(3)-O(11P)#1	-98.9(2)
O(23T)-Gd(2)-Gd(3)-O(2M)	-138.29(11)	O(3M)#1-Gd(2)-Gd(3)-O(11P)#1	44.2(2)
O(22T)-Gd(2)-Gd(3)-O(2M)	-12.87(11)	O(4M)-Gd(2)-Gd(3)-O(11P)#1	-35.8(2)
O(1)-Gd(2)-Gd(3)-O(2M)	103.06(8)	O(5M)#1-Gd(2)-Gd(3)-O(11P)#1	107.8(2)
O(21T)-Gd(2)-Gd(3)-O(2M)	-75.65(11)	O(23T)-Gd(2)-Gd(3)-O(11P)#1	122.8(2)
O(14P)-Gd(2)-Gd(3)-O(2M)	115.0(4)	O(22T)-Gd(2)-Gd(3)-O(11P)#1	-111.7(2)
Gd(3)#1-Gd(2)-Gd(3)-O(2M)	103.06(8)	O(1)-Gd(2)-Gd(3)-O(11P)#1	4.2(2)
Gd(1)#1-Gd(2)-Gd(3)-O(2M)	158.43(8)	O(21T)-Gd(2)-Gd(3)-O(11P)#1	-174.5(2)
O(2M)-Gd(2)-Gd(3)-O(33T)	132.23(12)	O(14P)-Gd(2)-Gd(3)-O(11P)#1	16.1(4)
O(3M)#1-Gd(2)-Gd(3)-O(33T)	-84.75(10)	Gd(3)#1-Gd(2)-Gd(3)-O(11P)#1	4.2(2)
O(4M)-Gd(2)-Gd(3)-O(33T)	-164.75(10)	Gd(1)#1-Gd(2)-Gd(3)-O(11P)#1	59.6(2)
O(5M)#1-Gd(2)-Gd(3)-O(33T)	-21.13(12)	O(2M)-Gd(2)-Gd(3)-Gd(2)#1	-103.06(8)
O(23T)-Gd(2)-Gd(3)-O(33T)	-6.07(11)	O(3M)#1-Gd(2)-Gd(3)-Gd(2)#1	39.96(5)
O(22T)-Gd(2)-Gd(3)-O(33T)	119.36(11)	O(4M)-Gd(2)-Gd(3)-Gd(2)#1	-40.04(5)
O(1)-Gd(2)-Gd(3)-O(33T)	-124.71(9)	O(5M)#1-Gd(2)-Gd(3)-Gd(2)#1	103.58(8)
O(21T)-Gd(2)-Gd(3)-O(33T)	56.57(11)		
O(14P)-Gd(2)-Gd(3)-O(33T)	-112.8(4)		

O(23T)-Gd(2)-Gd(3)-Gd(2)#1	118.64(7)
O(22T)-Gd(2)-Gd(3)-Gd(2)#1	-115.93(7)
O(1)-Gd(2)-Gd(3)-Gd(2)#1	0.0
O(21T)-Gd(2)-Gd(3)-Gd(2)#1	-178.72(7)
O(14P)-Gd(2)-Gd(3)-Gd(2)#1	11.9(4)
Gd(3)#1-Gd(2)-Gd(3)-Gd(2)#1	0.0
Gd(1)#1-Gd(2)-Gd(3)-Gd(2)#1	55.368(5)
O(2M)-Gd(2)-Gd(3)-Gd(1)	-47.44(8)
O(3M)#1-Gd(2)-Gd(3)-Gd(1)	95.58(5)
O(4M)-Gd(2)-Gd(3)-Gd(1)	15.58(5)
O(5M)#1-Gd(2)-Gd(3)-Gd(1)	159.20(8)
O(23T)-Gd(2)-Gd(3)-Gd(1)	174.26(7)
O(22T)-Gd(2)-Gd(3)-Gd(1)	-60.31(7)
O(1)-Gd(2)-Gd(3)-Gd(1)	55.621(6)
O(21T)-Gd(2)-Gd(3)-Gd(1)	-123.10(7)
O(14P)-Gd(2)-Gd(3)-Gd(1)	67.5(4)
Gd(3)#1-Gd(2)-Gd(3)-Gd(1)	55.621(6)
Gd(1)#1-Gd(2)-Gd(3)-Gd(1)	110.989(6)
O(2M)-Gd(1)-Gd(3)-O(3M)	-155.32(12)
O(4M)-Gd(1)-Gd(3)-O(3M)	141.47(10)
O(5M)-Gd(1)-Gd(3)-O(3M)	63.17(10)
O(12T)-Gd(1)-Gd(3)-O(3M)	-13.79(10)
O(14T)-Gd(1)-Gd(3)-O(3M)	91.0(4)
O(13T)-Gd(1)-Gd(3)-O(3M)	-143.70(11)
O(11T)-Gd(1)-Gd(3)-O(3M)	-78.96(10)
O(1)-Gd(1)-Gd(3)-O(3M)	102.57(8)
Gd(3)#1-Gd(1)-Gd(3)-O(3M)	102.57(8)
Gd(2)#1-Gd(1)-Gd(3)-O(3M)	48.01(8)
O(3M)-Gd(1)-Gd(3)-O(4M)#1	-62.49(10)
O(2M)-Gd(1)-Gd(3)-O(4M)#1	142.19(10)
O(4M)-Gd(1)-Gd(3)-O(4M)#1	78.98(8)
O(5M)-Gd(1)-Gd(3)-O(4M)#1	0.68(8)
O(12T)-Gd(1)-Gd(3)-O(4M)#1	-76.28(8)
O(14T)-Gd(1)-Gd(3)-O(4M)#1	28.6(4)
O(13T)-Gd(1)-Gd(3)-O(4M)#1	153.81(9)
O(11T)-Gd(1)-Gd(3)-O(4M)#1	-141.45(8)
O(1)-Gd(1)-Gd(3)-O(4M)#1	40.08(5)
Gd(3)#1-Gd(1)-Gd(3)-O(4M)#1	40.08(5)
Gd(2)#1-Gd(1)-Gd(3)-O(4M)#1	-14.48(5)
O(3M)-Gd(1)-Gd(3)-O(5M)#1	-143.19(10)
O(2M)-Gd(1)-Gd(3)-O(5M)#1	61.49(10)
O(4M)-Gd(1)-Gd(3)-O(5M)#1	-1.72(7)
O(5M)-Gd(1)-Gd(3)-O(5M)#1	-80.02(8)
O(12T)-Gd(1)-Gd(3)-O(5M)#1	-156.98(8)
O(14T)-Gd(1)-Gd(3)-O(5M)#1	-52.1(4)
O(13T)-Gd(1)-Gd(3)-O(5M)#1	73.11(9)
O(11T)-Gd(1)-Gd(3)-O(5M)#1	137.85(8)
O(1)-Gd(1)-Gd(3)-O(5M)#1	-40.61(5)
Gd(3)#1-Gd(1)-Gd(3)-O(5M)#1	-40.61(5)
Gd(2)#1-Gd(1)-Gd(3)-O(5M)#1	-95.18(5)
O(3M)-Gd(1)-Gd(3)-O(2M)	155.32(12)
O(4M)-Gd(1)-Gd(3)-O(2M)	-63.21(10)
O(5M)-Gd(1)-Gd(3)-O(2M)	-141.51(10)
O(12T)-Gd(1)-Gd(3)-O(2M)	141.53(10)
O(14T)-Gd(1)-Gd(3)-O(2M)	-113.6(4)
O(13T)-Gd(1)-Gd(3)-O(2M)	11.62(11)
O(11T)-Gd(1)-Gd(3)-O(2M)	76.36(10)
O(1)-Gd(1)-Gd(3)-O(2M)	-102.11(8)
Gd(3)#1-Gd(1)-Gd(3)-O(2M)	-102.11(8)
Gd(2)#1-Gd(1)-Gd(3)-O(2M)	-156.67(8)
O(3M)-Gd(1)-Gd(3)-O(33T)	24.9(5)
O(2M)-Gd(1)-Gd(3)-O(33T)	-130.4(5)
O(4M)-Gd(1)-Gd(3)-O(33T)	166.4(5)
O(5M)-Gd(1)-Gd(3)-O(33T)	88.1(5)
O(12T)-Gd(1)-Gd(3)-O(33T)	11.1(5)
O(14T)-Gd(1)-Gd(3)-O(33T)	116.0(6)
O(13T)-Gd(1)-Gd(3)-O(33T)	-118.8(5)
O(11T)-Gd(1)-Gd(3)-O(33T)	-54.0(5)
O(1)-Gd(1)-Gd(3)-O(33T)	127.5(5)
Gd(3)#1-Gd(1)-Gd(3)-O(33T)	127.5(5)
Gd(2)#1-Gd(1)-Gd(3)-O(33T)	72.9(5)
O(3M)-Gd(1)-Gd(3)-O(31T)	73.89(10)
O(2M)-Gd(1)-Gd(3)-O(31T)	-81.43(10)
O(4M)-Gd(1)-Gd(3)-O(31T)	-144.64(8)
O(5M)-Gd(1)-Gd(3)-O(31T)	137.06(8)
O(12T)-Gd(1)-Gd(3)-O(31T)	60.09(9)
O(14T)-Gd(1)-Gd(3)-O(31T)	164.9(4)
O(13T)-Gd(1)-Gd(3)-O(31T)	-69.81(10)
O(11T)-Gd(1)-Gd(3)-O(31T)	-5.07(8)
O(1)-Gd(1)-Gd(3)-O(31T)	176.46(6)
Gd(3)#1-Gd(1)-Gd(3)-O(31T)	176.46(6)
Gd(2)#1-Gd(1)-Gd(3)-O(31T)	121.90(6)
O(3M)-Gd(1)-Gd(3)-O(1)	-102.57(8)
O(2M)-Gd(1)-Gd(3)-O(1)	102.11(8)
O(4M)-Gd(1)-Gd(3)-O(1)	38.90(5)
O(5M)-Gd(1)-Gd(3)-O(1)	-39.41(5)
O(12T)-Gd(1)-Gd(3)-O(1)	-116.37(6)
O(14T)-Gd(1)-Gd(3)-O(1)	-11.5(4)
O(13T)-Gd(1)-Gd(3)-O(1)	113.72(7)
O(11T)-Gd(1)-Gd(3)-O(1)	178.46(6)
Gd(3)#1-Gd(1)-Gd(3)-O(1)	0.0
Gd(2)#1-Gd(1)-Gd(3)-O(1)	-54.564(5)
O(3M)-Gd(1)-Gd(3)-O(32T)	142.27(11)
O(2M)-Gd(1)-Gd(3)-O(32T)	-13.05(11)
O(4M)-Gd(1)-Gd(3)-O(32T)	-76.26(9)
O(5M)-Gd(1)-Gd(3)-O(32T)	-154.56(9)
O(12T)-Gd(1)-Gd(3)-O(32T)	128.48(9)
O(14T)-Gd(1)-Gd(3)-O(32T)	-126.7(4)
O(13T)-Gd(1)-Gd(3)-O(32T)	-1.43(10)
O(11T)-Gd(1)-Gd(3)-O(32T)	63.31(9)
O(1)-Gd(1)-Gd(3)-O(32T)	-115.15(7)
Gd(3)#1-Gd(1)-Gd(3)-O(32T)	-115.15(7)
Gd(2)#1-Gd(1)-Gd(3)-O(32T)	-169.72(7)
O(3M)-Gd(1)-Gd(3)-O(11P)#1	10.03(10)
O(2M)-Gd(1)-Gd(3)-O(11P)#1	-145.29(10)
O(4M)-Gd(1)-Gd(3)-O(11P)#1	151.50(8)

O(5M)-Gd(1)-Gd(3)-O(11P)#1	73.19(8)
O(12T)-Gd(1)-Gd(3)-O(11P)#1	-3.77(8)
O(14T)-Gd(1)-Gd(3)-O(11P)#1	101.1(4)
O(13T)-Gd(1)-Gd(3)-O(11P)#1	-133.68(9)
O(11T)-Gd(1)-Gd(3)-O(11P)#1	-68.94(8)
O(1)-Gd(1)-Gd(3)-O(11P)#1	112.60(5)
Gd(3)#1-Gd(1)-Gd(3)-O(11P)#1	112.60(5)
Gd(2)#1-Gd(1)-Gd(3)-O(11P)#1	58.04(5)
O(3M)-Gd(1)-Gd(3)-Gd(2)#1	-48.01(8)
O(2M)-Gd(1)-Gd(3)-Gd(2)#1	156.67(8)
O(4M)-Gd(1)-Gd(3)-Gd(2)#1	93.46(5)
O(5M)-Gd(1)-Gd(3)-Gd(2)#1	15.16(5)
O(12T)-Gd(1)-Gd(3)-Gd(2)#1	-61.80(6)
O(14T)-Gd(1)-Gd(3)-Gd(2)#1	43.0(4)
O(13T)-Gd(1)-Gd(3)-Gd(2)#1	168.29(7)
O(11T)-Gd(1)-Gd(3)-Gd(2)#1	-126.97(6)
O(1)-Gd(1)-Gd(3)-Gd(2)#1	54.564(5)
Gd(3)#1-Gd(1)-Gd(3)-Gd(2)#1	54.564(5)
O(3M)-Gd(1)-Gd(3)-Gd(2)	-156.91(8)
O(2M)-Gd(1)-Gd(3)-Gd(2)	47.77(8)
O(4M)-Gd(1)-Gd(3)-Gd(2)	-15.44(5)
O(5M)-Gd(1)-Gd(3)-Gd(2)	-93.74(5)
O(12T)-Gd(1)-Gd(3)-Gd(2)	-170.70(6)
O(14T)-Gd(1)-Gd(3)-Gd(2)	-65.9(4)
O(13T)-Gd(1)-Gd(3)-Gd(2)	59.39(7)
O(11T)-Gd(1)-Gd(3)-Gd(2)	124.13(6)
O(1)-Gd(1)-Gd(3)-Gd(2)	-54.336(5)
Gd(3)#1-Gd(1)-Gd(3)-Gd(2)	-54.336(5)
Gd(2)#1-Gd(1)-Gd(3)-Gd(2)	-108.900(6)
O(3M)-Gd(3)-O(1)-Gd(3)#1	-179(100)
O(4M)#1-Gd(3)-O(1)-Gd(3)#1	90(48)
O(5M)#1-Gd(3)-O(1)-Gd(3)#1	0(48)
O(2M)-Gd(3)-O(1)-Gd(3)#1	-90(48)
O(33T)-Gd(3)-O(1)-Gd(3)#1	55(48)
O(31T)-Gd(3)-O(1)-Gd(3)#1	-139(48)
O(32T)-Gd(3)-O(1)-Gd(3)#1	-43(48)
O(11P)#1-Gd(3)-O(1)-Gd(3)#1	137(48)
Gd(2)#1-Gd(3)-O(1)-Gd(3)#1	135(48)
Gd(2)-Gd(3)-O(1)-Gd(3)#1	-45(48)
Gd(1)-Gd(3)-O(1)-Gd(3)#1	-135(48)
O(3M)-Gd(3)-O(1)-Gd(2)#1	45.33(6)
O(4M)#1-Gd(3)-O(1)-Gd(2)#1	-45.46(6)
O(5M)#1-Gd(3)-O(1)-Gd(2)#1	-135.09(6)
O(2M)-Gd(3)-O(1)-Gd(2)#1	134.94(6)
O(33T)-Gd(3)-O(1)-Gd(2)#1	-80.14(10)
O(31T)-Gd(3)-O(1)-Gd(2)#1	85.29(8)
O(32T)-Gd(3)-O(1)-Gd(2)#1	-178.12(8)
O(11P)#1-Gd(3)-O(1)-Gd(2)#1	1.32(6)
Gd(2)-Gd(3)-O(1)-Gd(2)#1	180.0
Gd(1)-Gd(3)-O(1)-Gd(2)#1	89.962(6)
O(3M)-Gd(3)-O(1)-Gd(2)	-134.67(6)
O(4M)#1-Gd(3)-O(1)-Gd(2)	134.54(6)
O(5M)#1-Gd(3)-O(1)-Gd(2)	44.91(6)
O(2M)-Gd(3)-O(1)-Gd(2)	-45.06(6)
O(33T)-Gd(3)-O(1)-Gd(2)	99.86(10)
O(31T)-Gd(3)-O(1)-Gd(2)	-94.71(8)
O(32T)-Gd(3)-O(1)-Gd(2)	1.88(8)
O(11P)#1-Gd(3)-O(1)-Gd(2)	-178.68(6)
Gd(2)#1-Gd(3)-O(1)-Gd(2)	180.0
Gd(1)-Gd(3)-O(1)-Gd(2)	-90.038(6)
O(3M)-Gd(3)-O(1)-Gd(1)	-44.63(6)
O(4M)#1-Gd(3)-O(1)-Gd(1)	-135.43(6)
O(5M)#1-Gd(3)-O(1)-Gd(1)	134.95(6)
O(2M)-Gd(3)-O(1)-Gd(1)	44.98(6)
O(33T)-Gd(3)-O(1)-Gd(1)	-170.10(10)
O(31T)-Gd(3)-O(1)-Gd(1)	-4.67(8)
O(32T)-Gd(3)-O(1)-Gd(1)	91.91(8)
O(11P)#1-Gd(3)-O(1)-Gd(1)	-88.65(6)
Gd(2)#1-Gd(3)-O(1)-Gd(1)	-89.962(6)
Gd(2)-Gd(3)-O(1)-Gd(1)	90.038(6)
O(3M)-Gd(3)-O(1)-Gd(1)#1	135.37(6)
O(4M)#1-Gd(3)-O(1)-Gd(1)#1	44.57(6)
O(5M)#1-Gd(3)-O(1)-Gd(1)#1	-45.05(6)
O(2M)-Gd(3)-O(1)-Gd(1)#1	-135.02(6)
O(33T)-Gd(3)-O(1)-Gd(1)#1	9.90(10)
O(31T)-Gd(3)-O(1)-Gd(1)#1	175.33(8)
O(32T)-Gd(3)-O(1)-Gd(1)#1	-88.09(8)
O(11P)#1-Gd(3)-O(1)-Gd(1)#1	91.35(6)
Gd(2)#1-Gd(3)-O(1)-Gd(1)#1	90.038(6)
Gd(2)-Gd(3)-O(1)-Gd(1)#1	-89.962(6)
Gd(1)-Gd(3)-O(1)-Gd(1)#1	180.0
O(2M)-Gd(2)-O(1)-Gd(3)	45.22(6)
O(3M)#1-Gd(2)-O(1)-Gd(3)	-135.05(6)
O(4M)-Gd(2)-O(1)-Gd(3)	134.89(6)
O(5M)#1-Gd(2)-O(1)-Gd(3)	-44.86(6)
O(23T)-Gd(2)-O(1)-Gd(3)	-91.48(7)
O(22T)-Gd(2)-O(1)-Gd(3)	93.45(8)
O(21T)-Gd(2)-O(1)-Gd(3)	1.61(9)
O(14P)-Gd(2)-O(1)-Gd(3)	-177.55(7)
Gd(3)#1-Gd(2)-O(1)-Gd(3)	180.0
Gd(1)#1-Gd(2)-O(1)-Gd(3)	-90.301(7)
O(2M)-Gd(2)-O(1)-Gd(3)#1	-134.78(6)
O(3M)#1-Gd(2)-O(1)-Gd(3)#1	44.95(6)
O(4M)-Gd(2)-O(1)-Gd(3)#1	-45.11(6)
O(5M)#1-Gd(2)-O(1)-Gd(3)#1	135.14(6)
O(23T)-Gd(2)-O(1)-Gd(3)#1	88.52(7)
O(22T)-Gd(2)-O(1)-Gd(3)#1	-86.55(8)
O(21T)-Gd(2)-O(1)-Gd(3)#1	-178.39(9)
O(14P)-Gd(2)-O(1)-Gd(3)#1	2.45(7)
Gd(3)-Gd(2)-O(1)-Gd(3)#1	180.0
Gd(1)#1-Gd(2)-O(1)-Gd(3)#1	89.699(7)
O(2M)-Gd(2)-O(1)-Gd(2)#1	175(100)
O(3M)#1-Gd(2)-O(1)-Gd(2)#1	-5(100)
O(4M)-Gd(2)-O(1)-Gd(2)#1	-95(100)
O(5M)#1-Gd(2)-O(1)-Gd(2)#1	85(100)
O(23T)-Gd(2)-O(1)-Gd(2)#1	39(100)

O(22T)-Gd(2)-O(1)-Gd(2)#1	-137(100)	O(13T)-Gd(1)-O(1)-Gd(2)#1	176.08(8)
O(21T)-Gd(2)-O(1)-Gd(2)#1	132(100)	O(11T)-Gd(1)-O(1)-Gd(2)#1	-91.68(7)
O(14P)-Gd(2)-O(1)-Gd(2)#1	-48(100)	Gd(3)-Gd(1)-O(1)-Gd(2)#1	-89.798(6)
Gd(3)#1-Gd(2)-O(1)-Gd(2)#1	-50(100)	Gd(3)#1-Gd(1)-O(1)-Gd(2)#1	90.202(6)
Gd(3)-Gd(2)-O(1)-Gd(2)#1	130(100)	O(3M)-Gd(1)-O(1)-Gd(2)	134.85(6)
Gd(1)#1-Gd(2)-O(1)-Gd(2)#1	40(100)	O(2M)-Gd(1)-O(1)-Gd(2)	44.77(6)
O(2M)-Gd(2)-O(1)-Gd(1)	-44.48(6)	O(4M)-Gd(1)-O(1)-Gd(2)	-45.39(6)
O(3M)#1-Gd(2)-O(1)-Gd(1)	135.25(6)	O(5M)-Gd(1)-O(1)-Gd(2)	-134.67(6)
O(4M)-Gd(2)-O(1)-Gd(1)	45.19(6)	O(12T)-Gd(1)-O(1)-Gd(2)	178.48(7)
O(5M)#1-Gd(2)-O(1)-Gd(1)	-134.56(6)	O(14T)-Gd(1)-O(1)-Gd(2)	-92.15(8)
O(23T)-Gd(2)-O(1)-Gd(1)	178.82(7)	O(13T)-Gd(1)-O(1)-Gd(2)	-3.92(8)
O(22T)-Gd(2)-O(1)-Gd(1)	3.75(8)	O(11T)-Gd(1)-O(1)-Gd(2)	88.32(7)
O(21T)-Gd(2)-O(1)-Gd(1)	-88.09(9)	Gd(3)-Gd(1)-O(1)-Gd(2)	90.202(6)
O(14P)-Gd(2)-O(1)-Gd(1)	92.75(7)	Gd(3)#1-Gd(1)-O(1)-Gd(2)	-89.798(6)
Gd(3)#1-Gd(2)-O(1)-Gd(1)	90.301(7)	Gd(2)#1-Gd(1)-O(1)-Gd(2)	180.0
Gd(3)-Gd(2)-O(1)-Gd(1)	-89.699(7)	O(3M)-Gd(1)-O(1)-Gd(1)#1	-153(58)
Gd(1)#1-Gd(2)-O(1)-Gd(1)	180.0	O(2M)-Gd(1)-O(1)-Gd(1)#1	117(58)
O(2M)-Gd(2)-O(1)-Gd(1)#1	135.52(6)	O(4M)-Gd(1)-O(1)-Gd(1)#1	27(58)
O(3M)#1-Gd(2)-O(1)-Gd(1)#1	-44.75(6)	O(5M)-Gd(1)-O(1)-Gd(1)#1	-62(58)
O(4M)-Gd(2)-O(1)-Gd(1)#1	-134.81(6)	O(12T)-Gd(1)-O(1)-Gd(1)#1	-109(58)
O(5M)#1-Gd(2)-O(1)-Gd(1)#1	45.44(6)	O(14T)-Gd(1)-O(1)-Gd(1)#1	-20(58)
O(23T)-Gd(2)-O(1)-Gd(1)#1	-1.18(7)	O(13T)-Gd(1)-O(1)-Gd(1)#1	68(58)
O(22T)-Gd(2)-O(1)-Gd(1)#1	-176.25(8)	O(11T)-Gd(1)-O(1)-Gd(1)#1	161(58)
O(21T)-Gd(2)-O(1)-Gd(1)#1	91.91(9)	Gd(3)-Gd(1)-O(1)-Gd(1)#1	162(58)
O(14P)-Gd(2)-O(1)-Gd(1)#1	-87.25(7)	Gd(3)#1-Gd(1)-O(1)-Gd(1)#1	-18(58)
Gd(3)#1-Gd(2)-O(1)-Gd(1)#1	-89.699(7)	Gd(2)#1-Gd(1)-O(1)-Gd(1)#1	-108(58)
Gd(3)-Gd(2)-O(1)-Gd(1)#1	90.301(7)	O(3M)#1-Gd(2)-O(2M)-Gd(3)	-49.72(12)
O(3M)-Gd(1)-O(1)-Gd(3)	44.65(6)	O(4M)-Gd(2)-O(2M)-Gd(3)	-115.88(8)
O(2M)-Gd(1)-O(1)-Gd(3)	-45.43(6)	O(5M)#1-Gd(2)-O(2M)-Gd(3)	17.40(7)
O(4M)-Gd(1)-O(1)-Gd(3)	-135.59(6)	O(23T)-Gd(2)-O(2M)-Gd(3)	71.48(14)
O(5M)-Gd(1)-O(1)-Gd(3)	135.12(6)	O(22T)-Gd(2)-O(2M)-Gd(3)	168.30(10)
O(12T)-Gd(1)-O(1)-Gd(3)	88.28(7)	O(1)-Gd(2)-O(2M)-Gd(3)	-49.41(5)
O(14T)-Gd(1)-O(1)-Gd(3)	177.65(8)	O(21T)-Gd(2)-O(2M)-Gd(3)	96.28(10)
O(13T)-Gd(1)-O(1)-Gd(3)	-94.12(8)	O(14P)-Gd(2)-O(2M)-Gd(3)	-165.63(9)
O(11T)-Gd(1)-O(1)-Gd(3)	-1.88(7)	Gd(3)#1-Gd(2)-O(2M)-Gd(3)	-79.83(6)
Gd(3)#1-Gd(1)-O(1)-Gd(3)	180.0	Gd(1)#1-Gd(2)-O(2M)-Gd(3)	-18.89(7)
Gd(2)#1-Gd(1)-O(1)-Gd(3)	89.798(6)	O(3M)#1-Gd(2)-O(2M)-Gd(1)	50.31(12)
O(3M)-Gd(1)-O(1)-Gd(3)#1	-135.35(6)	O(4M)-Gd(2)-O(2M)-Gd(1)	-15.84(7)
O(2M)-Gd(1)-O(1)-Gd(3)#1	134.57(6)	O(5M)#1-Gd(2)-O(2M)-Gd(1)	117.44(8)
O(4M)-Gd(1)-O(1)-Gd(3)#1	44.41(6)	O(23T)-Gd(2)-O(2M)-Gd(1)	171.52(10)
O(5M)-Gd(1)-O(1)-Gd(3)#1	-44.88(6)	O(22T)-Gd(2)-O(2M)-Gd(1)	-91.66(9)
O(12T)-Gd(1)-O(1)-Gd(3)#1	-91.72(7)	O(1)-Gd(2)-O(2M)-Gd(1)	50.63(5)
O(14T)-Gd(1)-O(1)-Gd(3)#1	-2.35(8)	O(21T)-Gd(2)-O(2M)-Gd(1)	-163.68(10)
O(13T)-Gd(1)-O(1)-Gd(3)#1	85.88(8)	O(14P)-Gd(2)-O(2M)-Gd(1)	-65.59(14)
O(11T)-Gd(1)-O(1)-Gd(3)#1	178.12(7)	Gd(3)#1-Gd(2)-O(2M)-Gd(1)	20.21(7)
Gd(3)-Gd(1)-O(1)-Gd(3)#1	180.0	Gd(3)-Gd(2)-O(2M)-Gd(1)	100.04(9)
Gd(2)#1-Gd(1)-O(1)-Gd(3)#1	-90.202(6)	Gd(1)#1-Gd(2)-O(2M)-Gd(1)	81.14(6)
O(3M)-Gd(1)-O(1)-Gd(2)#1	-45.15(6)	O(3M)-Gd(3)-O(2M)-Gd(2)	116.88(9)
O(2M)-Gd(1)-O(1)-Gd(2)#1	-135.23(6)	O(4M)#1-Gd(3)-O(2M)-Gd(2)	49.25(12)
O(4M)-Gd(1)-O(1)-Gd(2)#1	134.61(6)	O(5M)#1-Gd(3)-O(2M)-Gd(2)	-17.47(7)
O(5M)-Gd(1)-O(1)-Gd(2)#1	45.33(6)	O(33T)-Gd(3)-O(2M)-Gd(2)	-89.92(14)
O(12T)-Gd(1)-O(1)-Gd(2)#1	-1.52(7)	O(31T)-Gd(3)-O(2M)-Gd(2)	-165.93(9)
O(14T)-Gd(1)-O(1)-Gd(2)#1	87.85(8)	O(1)-Gd(3)-O(2M)-Gd(2)	49.73(5)

O(32T)-Gd(3)-O(2M)-Gd(2)	-91.53(9)
O(11P)#1-Gd(3)-O(2M)-Gd(2)	155.74(8)
Gd(2)#1-Gd(3)-O(2M)-Gd(2)	80.33(6)
Gd(1)-Gd(3)-O(2M)-Gd(2)	100.80(9)
O(3M)-Gd(3)-O(2M)-Gd(1)	16.08(8)
O(4M)#1-Gd(3)-O(2M)-Gd(1)	-51.54(12)
O(5M)#1-Gd(3)-O(2M)-Gd(1)	-118.27(8)
O(33T)-Gd(3)-O(2M)-Gd(1)	169.29(11)
O(31T)-Gd(3)-O(2M)-Gd(1)	93.28(9)
O(1)-Gd(3)-O(2M)-Gd(1)	-51.07(5)
O(32T)-Gd(3)-O(2M)-Gd(1)	167.67(10)
O(11P)#1-Gd(3)-O(2M)-Gd(1)	54.95(13)
Gd(2)#1-Gd(3)-O(2M)-Gd(1)	-20.46(7)
Gd(2)-Gd(3)-O(2M)-Gd(1)	-100.80(9)
O(3M)-Gd(1)-O(2M)-Gd(2)	-115.34(8)
O(4M)-Gd(1)-O(2M)-Gd(2)	15.76(7)
O(5M)-Gd(1)-O(2M)-Gd(2)	-49.05(11)
O(12T)-Gd(1)-O(2M)-Gd(2)	-162.05(9)
O(14T)-Gd(1)-O(2M)-Gd(2)	66.22(15)
O(13T)-Gd(1)-O(2M)-Gd(2)	91.19(9)
O(11T)-Gd(1)-O(2M)-Gd(2)	165.54(10)
O(1)-Gd(1)-O(2M)-Gd(2)	-49.67(5)
Gd(3)-Gd(1)-O(2M)-Gd(2)	-99.44(9)
Gd(3)#1-Gd(1)-O(2M)-Gd(2)	-19.79(7)
Gd(2)#1-Gd(1)-O(2M)-Gd(2)	-79.41(6)
O(3M)-Gd(1)-O(2M)-Gd(3)	-15.90(8)
O(4M)-Gd(1)-O(2M)-Gd(3)	115.20(8)
O(5M)-Gd(1)-O(2M)-Gd(3)	50.39(11)
O(12T)-Gd(1)-O(2M)-Gd(3)	-62.61(14)
O(14T)-Gd(1)-O(2M)-Gd(3)	165.66(11)
O(13T)-Gd(1)-O(2M)-Gd(3)	-169.37(10)
O(11T)-Gd(1)-O(2M)-Gd(3)	-95.02(9)
O(1)-Gd(1)-O(2M)-Gd(3)	49.78(5)
Gd(3)#1-Gd(1)-O(2M)-Gd(3)	79.65(6)
Gd(2)#1-Gd(1)-O(2M)-Gd(3)	20.03(7)
O(4M)#1-Gd(3)-O(3M)-Gd(2)#1	16.63(7)
O(5M)#1-Gd(3)-O(3M)-Gd(2)#1	-50.47(12)
O(2M)-Gd(3)-O(3M)-Gd(2)#1	-116.97(8)
O(33T)-Gd(3)-O(3M)-Gd(2)#1	83.81(12)
O(31T)-Gd(3)-O(3M)-Gd(2)#1	160.03(10)
O(1)-Gd(3)-O(3M)-Gd(2)#1	-49.97(5)
O(32T)-Gd(3)-O(3M)-Gd(2)#1	-164.33(10)
O(11P)#1-Gd(3)-O(3M)-Gd(2)#1	89.35(8)
Gd(2)-Gd(3)-O(3M)-Gd(2)#1	-80.60(6)
Gd(1)-Gd(3)-O(3M)-Gd(2)#1	-100.83(10)
O(4M)#1-Gd(3)-O(3M)-Gd(1)	117.46(8)
O(5M)#1-Gd(3)-O(3M)-Gd(1)	50.37(12)
O(2M)-Gd(3)-O(3M)-Gd(1)	-16.13(8)
O(33T)-Gd(3)-O(3M)-Gd(1)	-175.36(9)
O(31T)-Gd(3)-O(3M)-Gd(1)	-99.14(9)
O(1)-Gd(3)-O(3M)-Gd(1)	50.86(5)
O(32T)-Gd(3)-O(3M)-Gd(1)	-63.49(15)
O(11P)#1-Gd(3)-O(3M)-Gd(1)	-169.81(10)
Gd(2)#1-Gd(3)-O(3M)-Gd(1)	100.83(10)
Gd(2)-Gd(3)-O(3M)-Gd(1)	20.23(7)
O(2M)-Gd(1)-O(3M)-Gd(3)	16.12(8)
O(4M)-Gd(1)-O(3M)-Gd(3)	-50.03(11)
O(5M)-Gd(1)-O(3M)-Gd(3)	-115.39(9)
O(12T)-Gd(1)-O(3M)-Gd(3)	166.74(10)
O(14T)-Gd(1)-O(3M)-Gd(3)	-165.34(10)
O(13T)-Gd(1)-O(3M)-Gd(3)	63.78(16)
O(11T)-Gd(1)-O(3M)-Gd(3)	93.17(9)
O(1)-Gd(1)-O(3M)-Gd(3)	-49.77(5)
Gd(3)#1-Gd(1)-O(3M)-Gd(3)	-79.21(6)
Gd(2)#1-Gd(1)-O(3M)-Gd(3)	-99.76(10)
O(2M)-Gd(1)-O(3M)-Gd(2)#1	115.88(8)
O(4M)-Gd(1)-O(3M)-Gd(2)#1	49.73(11)
O(5M)-Gd(1)-O(3M)-Gd(2)#1	-15.63(8)
O(12T)-Gd(1)-O(3M)-Gd(2)#1	-93.50(9)
O(14T)-Gd(1)-O(3M)-Gd(2)#1	-65.58(14)
O(13T)-Gd(1)-O(3M)-Gd(2)#1	163.53(11)
O(11T)-Gd(1)-O(3M)-Gd(2)#1	-167.07(9)
O(1)-Gd(1)-O(3M)-Gd(2)#1	49.99(5)
Gd(3)-Gd(1)-O(3M)-Gd(2)#1	99.76(9)
Gd(3)#1-Gd(1)-O(3M)-Gd(2)#1	20.55(7)
O(2M)-Gd(2)-O(4M)-Gd(3)#1	116.87(8)
O(3M)#1-Gd(2)-O(4M)-Gd(3)#1	-16.48(7)
O(5M)#1-Gd(2)-O(4M)-Gd(3)#1	50.29(11)
O(23T)-Gd(2)-O(4M)-Gd(3)#1	-70.15(13)
O(22T)-Gd(2)-O(4M)-Gd(3)#1	-163.44(10)
O(1)-Gd(2)-O(4M)-Gd(3)#1	50.00(5)
O(21T)-Gd(2)-O(4M)-Gd(3)#1	168.63(10)
O(14P)-Gd(2)-O(4M)-Gd(3)#1	-91.97(9)
Gd(3)-Gd(2)-O(4M)-Gd(3)#1	80.20(6)
Gd(1)#1-Gd(2)-O(4M)-Gd(3)#1	19.11(7)
O(2M)-Gd(2)-O(4M)-Gd(1)	15.75(7)
O(3M)#1-Gd(2)-O(4M)-Gd(1)	-117.59(8)
O(5M)#1-Gd(2)-O(4M)-Gd(1)	-50.83(12)
O(23T)-Gd(2)-O(4M)-Gd(1)	-171.27(9)
O(22T)-Gd(2)-O(4M)-Gd(1)	95.45(9)
O(1)-Gd(2)-O(4M)-Gd(1)	-51.12(5)
O(21T)-Gd(2)-O(4M)-Gd(1)	67.51(14)
O(14P)-Gd(2)-O(4M)-Gd(1)	166.91(10)
Gd(3)#1-Gd(2)-O(4M)-Gd(1)	-101.12(9)
Gd(3)-Gd(2)-O(4M)-Gd(1)	-20.92(7)
Gd(1)#1-Gd(2)-O(4M)-Gd(1)	-82.01(6)
O(3M)-Gd(1)-O(4M)-Gd(3)#1	-49.22(11)
O(2M)-Gd(1)-O(4M)-Gd(3)#1	-115.39(9)
O(5M)-Gd(1)-O(4M)-Gd(3)#1	16.63(7)
O(12T)-Gd(1)-O(4M)-Gd(3)#1	62.31(15)
O(14T)-Gd(1)-O(4M)-Gd(3)#1	93.52(9)
O(13T)-Gd(1)-O(4M)-Gd(3)#1	164.97(10)
O(11T)-Gd(1)-O(4M)-Gd(3)#1	-164.40(10)
O(1)-Gd(1)-O(4M)-Gd(3)#1	-49.48(5)
Gd(3)-Gd(1)-O(4M)-Gd(3)#1	-78.97(6)

Gd(2)#1-Gd(1)-O(4M)-Gd(3)#1	-19.43(7)
O(3M)-Gd(1)-O(4M)-Gd(2)	50.45(11)
O(2M)-Gd(1)-O(4M)-Gd(2)	-15.72(7)
O(5M)-Gd(1)-O(4M)-Gd(2)	116.31(8)
O(12T)-Gd(1)-O(4M)-Gd(2)	161.99(10)
O(14T)-Gd(1)-O(4M)-Gd(2)	-166.80(10)
O(13T)-Gd(1)-O(4M)-Gd(2)	-95.35(9)
O(11T)-Gd(1)-O(4M)-Gd(2)	-64.72(14)
O(1)-Gd(1)-O(4M)-Gd(2)	50.19(5)
Gd(3)-Gd(1)-O(4M)-Gd(2)	20.71(7)
Gd(3)#1-Gd(1)-O(4M)-Gd(2)	99.68(9)
Gd(2)#1-Gd(1)-O(4M)-Gd(2)	80.25(6)
O(3M)-Gd(1)-O(5M)-Gd(3)#1	114.88(8)
O(2M)-Gd(1)-O(5M)-Gd(3)#1	48.71(11)
O(4M)-Gd(1)-O(5M)-Gd(3)#1	-16.45(7)
O(12T)-Gd(1)-O(5M)-Gd(3)#1	-169.28(9)
O(14T)-Gd(1)-O(5M)-Gd(3)#1	-96.32(9)
O(13T)-Gd(1)-O(5M)-Gd(3)#1	-64.40(14)
O(11T)-Gd(1)-O(5M)-Gd(3)#1	164.64(10)
O(1)-Gd(1)-O(5M)-Gd(3)#1	49.33(5)
Gd(3)-Gd(1)-O(5M)-Gd(3)#1	79.08(6)
Gd(2)#1-Gd(1)-O(5M)-Gd(3)#1	99.30(9)
O(3M)-Gd(1)-O(5M)-Gd(2)#1	15.58(8)
O(2M)-Gd(1)-O(5M)-Gd(2)#1	-50.59(11)
O(4M)-Gd(1)-O(5M)-Gd(2)#1	-115.75(9)
O(12T)-Gd(1)-O(5M)-Gd(2)#1	91.42(9)
O(14T)-Gd(1)-O(5M)-Gd(2)#1	164.38(10)
O(13T)-Gd(1)-O(5M)-Gd(2)#1	-163.70(9)
O(11T)-Gd(1)-O(5M)-Gd(2)#1	65.34(15)
O(1)-Gd(1)-O(5M)-Gd(2)#1	-49.97(5)
Gd(3)-Gd(1)-O(5M)-Gd(2)#1	-20.22(7)
Gd(3)#1-Gd(1)-O(5M)-Gd(2)#1	-99.30(9)
O(13P)-Cl(1)-O(11P)-Gd(3)#1	-169.52(18)
O(12P)-Cl(1)-O(11P)-Gd(3)#1	68.5(2)
O(14P)-Cl(1)-O(11P)-Gd(3)#1	-50.1(2)
O(13P)-Cl(1)-O(14P)-Gd(2)	175.07(18)
O(12P)-Cl(1)-O(14P)-Gd(2)	-65.1(2)
O(11P)-Cl(1)-O(14P)-Gd(2)	54.5(2)
O(2M)-Gd(2)-O(14P)-Cl(1)	61.4(2)
O(3M)#1-Gd(2)-O(14P)-Cl(1)	-71.50(19)
O(4M)-Gd(2)-O(14P)-Cl(1)	10.98(18)
O(5M)#1-Gd(2)-O(14P)-Cl(1)	-123.07(18)
O(23T)-Gd(2)-O(14P)-Cl(1)	-153.6(2)
O(22T)-Gd(2)-O(14P)-Cl(1)	88.8(2)
O(1)-Gd(2)-O(14P)-Cl(1)	-32.1(2)
O(21T)-Gd(2)-O(14P)-Cl(1)	148.57(19)
Gd(3)#1-Gd(2)-O(14P)-Cl(1)	-30.37(18)
Gd(3)-Gd(2)-O(14P)-Cl(1)	-42.4(5)
Gd(1)#1-Gd(2)-O(14P)-Cl(1)	-82.74(19)
Cl(2A)-Cl(2)-O(21P)-O(21A)	-175.8(19)
O(24P)-Cl(2)-O(21P)-O(21A)	-112.1(15)
O(23P)-Cl(2)-O(21P)-O(21A)	123.8(14)
O(22P)-Cl(2)-O(21P)-O(21A)	4.6(15)
O(22A)-Cl(2)-O(21P)-O(21A)	-174.4(17)
O(21A)-Cl(2)-O(21P)-Cl(2A)	175.8(19)
O(24P)-Cl(2)-O(21P)-Cl(2A)	63.7(10)
O(23P)-Cl(2)-O(21P)-Cl(2A)	-60.3(10)
O(22P)-Cl(2)-O(21P)-Cl(2A)	-179.6(12)
O(22A)-Cl(2)-O(21P)-Cl(2A)	1.4(12)
Cl(2A)-Cl(2)-O(21P)-O(22A)	-1.4(12)
O(21A)-Cl(2)-O(21P)-O(22A)	174.4(17)
O(24P)-Cl(2)-O(21P)-O(22A)	62.3(8)
O(23P)-Cl(2)-O(21P)-O(22A)	-61.7(7)
O(22P)-Cl(2)-O(21P)-O(22A)	179.0(7)
Cl(2A)-Cl(2)-O(22P)-O(21A)	-6(7)
O(24P)-Cl(2)-O(22P)-O(21A)	116.3(9)
O(21P)-Cl(2)-O(22P)-O(21A)	-3.1(10)
O(23P)-Cl(2)-O(22P)-O(21A)	-123.2(9)
O(22A)-Cl(2)-O(22P)-O(21A)	-1.2(17)
O(21A)-Cl(2)-O(22P)-Cl(2A)	6(7)
O(24P)-Cl(2)-O(22P)-Cl(2A)	122(7)
O(21P)-Cl(2)-O(22P)-Cl(2A)	3(7)
O(23P)-Cl(2)-O(22P)-Cl(2A)	-117(7)
O(22A)-Cl(2)-O(22P)-Cl(2A)	4(7)
O(21A)-Cl(2)-Cl(2A)-O(21P)	-2.7(12)
O(24P)-Cl(2)-Cl(2A)-O(21P)	-121.1(5)
O(23P)-Cl(2)-Cl(2A)-O(21P)	122.5(6)
O(22P)-Cl(2)-Cl(2A)-O(21P)	3(8)
O(22A)-Cl(2)-Cl(2A)-O(21P)	-4(4)
O(21A)-Cl(2)-Cl(2A)-O(23P)	-125.2(8)
O(24P)-Cl(2)-Cl(2A)-O(23P)	116.4(3)
O(21P)-Cl(2)-Cl(2A)-O(23P)	-122.5(6)
O(22P)-Cl(2)-Cl(2A)-O(23P)	-120(7)
O(22A)-Cl(2)-Cl(2A)-O(23P)	-127(4)
O(21A)-Cl(2)-Cl(2A)-O(24P)	118.4(9)
O(21P)-Cl(2)-Cl(2A)-O(24P)	121.1(5)
O(23P)-Cl(2)-Cl(2A)-O(24P)	-116.4(3)
O(22P)-Cl(2)-Cl(2A)-O(24P)	124(7)
O(22A)-Cl(2)-Cl(2A)-O(24P)	117(4)
O(24P)-Cl(2)-Cl(2A)-O(21A)	-118.4(9)
O(21P)-Cl(2)-Cl(2A)-O(21A)	2.7(12)
O(23P)-Cl(2)-Cl(2A)-O(21A)	125.2(8)
O(22P)-Cl(2)-Cl(2A)-O(21A)	5(7)
O(22A)-Cl(2)-Cl(2A)-O(21A)	-2(4)
O(21A)-Cl(2)-Cl(2A)-O(22A)	2(4)
O(24P)-Cl(2)-Cl(2A)-O(22A)	-117(4)
O(21P)-Cl(2)-Cl(2A)-O(22A)	4(4)
O(23P)-Cl(2)-Cl(2A)-O(22A)	127(4)
O(22P)-Cl(2)-Cl(2A)-O(22A)	7(11)
O(21A)-Cl(2)-Cl(2A)-O(22P)	-5(7)
O(24P)-Cl(2)-Cl(2A)-O(22P)	-124(7)
O(21P)-Cl(2)-Cl(2A)-O(22P)	-3(8)
O(23P)-Cl(2)-Cl(2A)-O(22P)	120(7)
O(22A)-Cl(2)-Cl(2A)-O(22P)	-7(11)
O(21A)-O(21P)-Cl(2A)-Cl(2)	3.6(16)
O(22A)-O(21P)-Cl(2A)-Cl(2)	178.4(13)

O(21A)-O(21P)-Cl(2A)-O(23P)	88.0(16)
Cl(2)-O(21P)-Cl(2A)-O(23P)	84.4(12)
O(22A)-O(21P)-Cl(2A)-O(23P)	-97.2(11)
O(21A)-O(21P)-Cl(2A)-O(24P)	-77.4(16)
Cl(2)-O(21P)-Cl(2A)-O(24P)	-81.0(13)
O(22A)-O(21P)-Cl(2A)-O(24P)	97.4(11)
Cl(2)-O(21P)-Cl(2A)-O(21A)	-3.6(16)
O(22A)-O(21P)-Cl(2A)-O(21A)	174.8(16)
O(21A)-O(21P)-Cl(2A)-O(22A)	-174.8(16)
Cl(2)-O(21P)-Cl(2A)-O(22A)	-178.4(13)
O(21A)-O(21P)-Cl(2A)-O(22P)	3.9(13)
Cl(2)-O(21P)-Cl(2A)-O(22P)	0.3(8)
O(22A)-O(21P)-Cl(2A)-O(22P)	178.7(8)
O(21A)-O(22P)-Cl(2A)-Cl(2)	174(8)
Cl(2)-O(22P)-Cl(2A)-O(21P)	-177(100)
O(21A)-O(22P)-Cl(2A)-O(21P)	-3.2(10)
Cl(2)-O(22P)-Cl(2A)-O(23P)	60(7)
O(21A)-O(22P)-Cl(2A)-O(23P)	-126.2(10)
Cl(2)-O(22P)-Cl(2A)-O(24P)	-55(7)
O(21A)-O(22P)-Cl(2A)-O(24P)	118.6(10)
Cl(2)-O(22P)-Cl(2A)-O(21A)	-174(8)
Cl(2)-O(22P)-Cl(2A)-O(22A)	-175(8)
O(21A)-O(22P)-Cl(2A)-O(22A)	0(2)
Cl(2)-Cl(2A)-O(22A)-O(21P)	-5(4)
O(23P)-Cl(2A)-O(22A)-O(21P)	118.8(7)
O(24P)-Cl(2A)-O(22A)-O(21P)	-117.2(7)
O(21A)-Cl(2A)-O(22A)-O(21P)	-3.3(10)
O(22P)-Cl(2A)-O(22A)-O(21P)	-3.0(19)
O(21P)-Cl(2A)-O(22A)-Cl(2)	5(4)
O(23P)-Cl(2A)-O(22A)-Cl(2)	124(4)
O(24P)-Cl(2A)-O(22A)-Cl(2)	-112(4)
O(21A)-Cl(2A)-O(22A)-Cl(2)	1(4)
O(22P)-Cl(2A)-O(22A)-Cl(2)	2(3)
O(21A)-O(21P)-O(22A)-Cl(2A)	8(2)
Cl(2)-O(21P)-O(22A)-Cl(2A)	0.6(5)
O(21A)-O(21P)-O(22A)-Cl(2)	8(2)
Cl(2A)-O(21P)-O(22A)-Cl(2)	-0.6(5)
O(21A)-Cl(2)-O(22A)-Cl(2A)	-178(100)
O(24P)-Cl(2)-O(22A)-Cl(2A)	61(4)
O(21P)-Cl(2)-O(22A)-Cl(2A)	-175(4)
O(23P)-Cl(2)-O(22A)-Cl(2A)	-51(4)
O(22P)-Cl(2)-O(22A)-Cl(2A)	-177(4)
Cl(2A)-Cl(2)-O(22A)-O(21P)	175(4)
O(21A)-Cl(2)-O(22A)-O(21P)	-3.5(10)
O(24P)-Cl(2)-O(22A)-O(21P)	-123.8(6)
O(23P)-Cl(2)-O(22A)-O(21P)	123.9(6)
O(22P)-Cl(2)-O(22A)-O(21P)	-2.4(18)
Cl(2A)-O(21P)-O(21A)-Cl(2)	-1.6(7)
O(22A)-O(21P)-O(21A)-Cl(2)	-9(3)
Cl(2)-O(21P)-O(21A)-Cl(2A)	1.6(7)
O(22A)-O(21P)-O(21A)-Cl(2A)	-7(2)
Cl(2A)-O(21P)-O(21A)-O(22P)	-9(3)
Cl(2)-O(21P)-O(21A)-O(22P)	-7(2)
O(22A)-O(21P)-O(21A)-O(22P)	-16(5)
Cl(2A)-Cl(2)-O(21A)-O(21P)	3.9(17)
O(24P)-Cl(2)-O(21A)-O(21P)	87.0(12)
O(23P)-Cl(2)-O(21A)-O(21P)	-77(2)
O(22P)-Cl(2)-O(21A)-O(21P)	-175.3(15)
O(22A)-Cl(2)-O(21A)-O(21P)	4.3(13)
O(24P)-Cl(2)-O(21A)-Cl(2A)	83.1(14)
O(21P)-Cl(2)-O(21A)-Cl(2A)	-3.9(17)
O(23P)-Cl(2)-O(21A)-Cl(2A)	-80.7(15)
O(22P)-Cl(2)-O(21A)-Cl(2A)	-179.1(11)
O(22A)-Cl(2)-O(21A)-Cl(2A)	0.4(11)
Cl(2A)-Cl(2)-O(21A)-O(22P)	179.1(11)
O(24P)-Cl(2)-O(21A)-O(22P)	-97.8(11)
O(21P)-Cl(2)-O(21A)-O(22P)	175.3(15)
O(23P)-Cl(2)-O(21A)-O(22P)	98.5(12)
O(22A)-Cl(2)-O(21A)-O(22P)	179.5(7)
Cl(2)-Cl(2A)-O(21A)-O(21P)	-175.6(19)
O(23P)-Cl(2A)-O(21A)-O(21P)	-113.1(15)
O(24P)-Cl(2A)-O(21A)-O(21P)	119.3(11)
O(22A)-Cl(2A)-O(21A)-O(21P)	4.9(15)
O(22P)-Cl(2A)-O(21A)-O(21P)	-174.9(17)
O(21P)-Cl(2A)-O(21A)-Cl(2)	175.6(19)
O(23P)-Cl(2A)-O(21A)-Cl(2)	62.6(11)
O(24P)-Cl(2A)-O(21A)-Cl(2)	-65.1(13)
O(22A)-Cl(2A)-O(21A)-Cl(2)	-179.4(15)
O(22P)-Cl(2A)-O(21A)-Cl(2)	0.8(10)
Cl(2)-Cl(2A)-O(21A)-O(22P)	-0.8(10)
O(21P)-Cl(2A)-O(21A)-O(22P)	174.9(17)
O(23P)-Cl(2A)-O(21A)-O(22P)	61.8(10)
O(24P)-Cl(2A)-O(21A)-O(22P)	-65.9(10)
O(22A)-Cl(2A)-O(21A)-O(22P)	179.8(9)
Cl(2)-O(22P)-O(21A)-O(21P)	8(3)
Cl(2A)-O(22P)-O(21A)-O(21P)	8(3)
Cl(2A)-O(22P)-O(21A)-Cl(2)	-0.3(4)
Cl(2)-O(22P)-O(21A)-Cl(2A)	0.3(4)
O(21P)-Cl(2A)-O(23P)-Cl(2)	-90.0(14)
O(24P)-Cl(2A)-O(23P)-Cl(2)	76.2(11)
O(21A)-Cl(2A)-O(23P)-Cl(2)	-47.4(14)
O(22A)-Cl(2A)-O(23P)-Cl(2)	-164.1(15)
O(22P)-Cl(2A)-O(23P)-Cl(2)	-5.4(8)
O(21A)-Cl(2)-O(23P)-Cl(2A)	95(2)
O(24P)-Cl(2)-O(23P)-Cl(2A)	-69.8(10)
O(21P)-Cl(2)-O(23P)-Cl(2A)	54.1(10)
O(22P)-Cl(2)-O(23P)-Cl(2A)	172.2(12)
O(22A)-Cl(2)-O(23P)-Cl(2A)	11.2(11)
O(21P)-Cl(2A)-O(24P)-Cl(2)	88.5(13)
O(23P)-Cl(2A)-O(24P)-Cl(2)	-78.0(10)
O(21A)-Cl(2A)-O(24P)-Cl(2)	49.3(16)
O(22A)-Cl(2A)-O(24P)-Cl(2)	162.2(15)
O(22P)-Cl(2A)-O(24P)-Cl(2)	5.2(8)
O(21A)-Cl(2)-O(24P)-Cl(2A)	-98.1(19)
O(21P)-Cl(2)-O(24P)-Cl(2A)	-55.7(10)
O(23P)-Cl(2)-O(24P)-Cl(2A)	68.0(9)

O(22P)-Cl(2)-O(24P)-Cl(2A)	-172.6(11)
O(22A)-Cl(2)-O(24P)-Cl(2A)	-12.5(11)
O(33C)-Cl(3A)-O(32A)-O(33B)	-12(2)
O(32C)-Cl(3A)-O(32A)-O(33B)	-157(3)
O(32B)-Cl(3A)-O(32A)-O(33B)	-147(2)
O(33A)-Cl(3A)-O(32A)-O(33B)	-17(2)
O(31A)-Cl(3A)-O(32A)-O(33B)	102(2)
O(34A)-Cl(3A)-O(32A)-O(33B)	-138(2)
O(34B)-Cl(3A)-O(32A)-O(33B)	-33(2)
O(34C)-Cl(3A)-O(32A)-O(33B)	-129(2)
O(33C)-Cl(3A)-O(32A)-O(32C)	145.4(19)
O(32B)-Cl(3A)-O(32A)-O(32C)	10.3(19)
O(33A)-Cl(3A)-O(32A)-O(32C)	140.7(19)
O(31A)-Cl(3A)-O(32A)-O(32C)	-100.9(18)
O(34A)-Cl(3A)-O(32A)-O(32C)	19(2)
O(34B)-Cl(3A)-O(32A)-O(32C)	124.1(19)
O(33B)-Cl(3A)-O(32A)-O(32C)	157(3)
O(34C)-Cl(3A)-O(32A)-O(32C)	28(2)
O(33C)-Cl(3A)-O(33A)-O(34B)	-155(4)
O(32C)-Cl(3A)-O(33A)-O(34B)	-121(2)
O(32B)-Cl(3A)-O(33A)-O(34B)	-35(2)
O(32A)-Cl(3A)-O(33A)-O(34B)	-139.7(19)
O(31A)-Cl(3A)-O(33A)-O(34B)	102.1(19)
O(34A)-Cl(3A)-O(33A)-O(34B)	-20(2)
O(33B)-Cl(3A)-O(33A)-O(34B)	-146(2)
O(34C)-Cl(3A)-O(33A)-O(34B)	-5(2)
O(33C)-Cl(3A)-O(34A)-O(32B)	-131.8(16)
O(32C)-Cl(3A)-O(34A)-O(32B)	-18.1(17)
O(32A)-Cl(3A)-O(34A)-O(32B)	-25.7(18)
O(33A)-Cl(3A)-O(34A)-O(32B)	-147.1(16)
O(31A)-Cl(3A)-O(34A)-O(32B)	92.7(16)
O(34B)-Cl(3A)-O(34A)-O(32B)	-154.1(17)
O(33B)-Cl(3A)-O(34A)-O(32B)	-42.8(18)
O(34C)-Cl(3A)-O(34A)-O(32B)	172(3)
O(33C)-Cl(3A)-O(34A)-O(34C)	56.6(18)
O(32C)-Cl(3A)-O(34A)-O(34C)	170.3(17)
O(32B)-Cl(3A)-O(34A)-O(34C)	-172(3)
O(32A)-Cl(3A)-O(34A)-O(34C)	162.7(16)
O(33A)-Cl(3A)-O(34A)-O(34C)	41.3(17)
O(31A)-Cl(3A)-O(34A)-O(34C)	-79.0(16)
O(34B)-Cl(3A)-O(34A)-O(34C)	34.3(16)
O(33B)-Cl(3A)-O(34A)-O(34C)	145.5(16)
O(34C)-O(34A)-O(32B)-Cl(3A)	21(7)
O(33C)-Cl(3A)-O(32B)-O(34A)	63(2)
O(32C)-Cl(3A)-O(32B)-O(34A)	160.1(18)
O(32A)-Cl(3A)-O(32B)-O(34A)	155.6(17)
O(33A)-Cl(3A)-O(32B)-O(34A)	40.2(19)
O(31A)-Cl(3A)-O(32B)-O(34A)	-95.7(16)
O(34B)-Cl(3A)-O(32B)-O(34A)	27.7(18)
O(33B)-Cl(3A)-O(32B)-O(34A)	143.6(16)
O(34C)-Cl(3A)-O(32B)-O(34A)	-4.6(16)
O(32C)-O(32A)-O(33B)-Cl(3A)	-46(5)
O(33C)-Cl(3A)-O(33B)-O(32A)	168(2)
O(32C)-Cl(3A)-O(33B)-O(32A)	12.8(19)
O(32B)-Cl(3A)-O(33B)-O(32A)	35(2)
O(33A)-Cl(3A)-O(33B)-O(32A)	165(2)
O(31A)-Cl(3A)-O(33B)-O(32A)	-86(2)
O(34A)-Cl(3A)-O(33B)-O(32A)	50(2)
O(34B)-Cl(3A)-O(33B)-O(32A)	152(2)
O(34C)-Cl(3A)-O(33B)-O(32A)	70(2)
O(33C)-Cl(3A)-O(34B)-O(33A)	12(2)
O(32C)-Cl(3A)-O(34B)-O(33A)	77(2)
O(32B)-Cl(3A)-O(34B)-O(33A)	151.5(19)
O(32A)-Cl(3A)-O(34B)-O(33A)	48(2)
O(31A)-Cl(3A)-O(34B)-O(33A)	-85(2)
O(34A)-Cl(3A)-O(34B)-O(33A)	161(2)
O(33B)-Cl(3A)-O(34B)-O(33A)	36(2)
O(34C)-Cl(3A)-O(34B)-O(33A)	175(2)
O(33B)-O(32A)-O(32C)-Cl(3A)	47(5)
O(33C)-Cl(3A)-O(32C)-O(32A)	-38(2)
O(32B)-Cl(3A)-O(32C)-O(32A)	-169(2)
O(33A)-Cl(3A)-O(32C)-O(32A)	-49(2)
O(31A)-Cl(3A)-O(32C)-O(32A)	87.4(19)
O(34A)-Cl(3A)-O(32C)-O(32A)	-161.5(19)
O(34B)-Cl(3A)-O(32C)-O(32A)	-75(2)
O(33B)-Cl(3A)-O(32C)-O(32A)	-11.8(18)
O(34C)-Cl(3A)-O(32C)-O(32A)	-157.6(18)
O(32B)-O(34A)-O(34C)-Cl(3A)	-20(7)
O(33C)-Cl(3A)-O(34C)-O(34A)	-132.2(16)
O(32C)-Cl(3A)-O(34C)-O(34A)	-10.2(18)
O(32B)-Cl(3A)-O(34C)-O(34A)	4.4(15)
O(32A)-Cl(3A)-O(34C)-O(34A)	-22(2)
O(33A)-Cl(3A)-O(34C)-O(34A)	-141.8(16)
O(31A)-Cl(3A)-O(34C)-O(34A)	108.4(16)
O(34B)-Cl(3A)-O(34C)-O(34A)	-143.7(17)
O(33B)-Cl(3A)-O(34C)-O(34A)	-48(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,-y+5/2,-z+1

Table 7. Hydrogen bonds for $[Gd_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8(\eta^2\text{-}ClO_4)_2(H_2O)_{20}](ClO_4)_6 \cdot 4H_2O$ (**3**). [Å and °].

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O2M-H2M	1.000	1.883	160.76	2.846	O21P
O2M-H2M	1.000	2.073	158.98	3.028	O21A_a
O2M-H2M	1.000	2.745	170.08	3.734	Cl2A_a
O2M-H2M	1.000	2.807	172.17	3.800	Cl2
O3M-H3M	1.000	1.986	164.15	2.961	O23P [-x+1/2, y+1/2, -z+1/2]
O4M-H4M	1.000	2.117	139.17	2.947	O12P
O5M-H5M	1.000	2.194	153.80	3.123	O41P [x+1/2, -y+3/2, z+1/2]
O11T-H11A	0.980	1.993	169.45	2.962	O22A_a
O11T-H11A	0.980	2.188	131.79	2.933	O21P
O11T-H11B	0.980	1.956	151.87	2.858	O1W
O11T-H11B	0.980	2.546	120.84	3.163	O44P [-x+1/2, y+1/2, -z+1/2]
O11T-H11C	0.980	2.156	148.80	3.037	O31T
O12T-H12A	0.980	2.558	176.61	3.537	O1W
O12T-H12B	0.980	2.348	144.94	3.200	O41P [x+1/2, -y+3/2, z+1/2]
O12T-H12C	0.980	1.972	155.88	2.894	O23T [-x+1/2, -y+5/2, -z+1]
O12T-H12C	0.980	2.570	115.19	3.116	O23P [-x+1/2, y+1/2, -z+1/2]
O13T-H13B	0.999	2.434	132.64	3.196	O44P [-x+1/2, y+1/2, -z+1/2]
O13T-H13B	0.999	2.521	112.73	3.049	O13P [-x+1/2, -y+3/2, -z+1]
O13T-H13C	0.974	2.019	137.92	2.818	O22A_a
O13T-H13C	0.974	2.526	113.55	3.049	O13P [-x+1/2, -y+3/2, -z+1]
O14T-H14A	0.980	2.050	141.99	2.886	O32B_b [-x+1/2, -y+3/2, -z+1]
O14T-H14A	0.980	2.128	127.37	2.832	O34A [-x+1/2, -y+3/2, -z+1]
O14T-H14A	0.980	2.332	114.25	2.877	O34C_c [-x+1/2, -y+3/2, -z+1]
O14T-H14A	0.980	2.868	128.00	3.557	Cl3A [-x+1/2, -y+3/2, -z+1]
O14T-H14A	0.980	2.868	128.00	3.557	Cl3B_b [-x+1/2, -y+3/2, -z+1]
O14T-H14A	0.980	2.868	128.00	3.557	Cl3C_c [-x+1/2, -y+3/2, -z+1]
O14T-H14B	0.980	1.869	174.00	2.845	O41P [x+1/2, -y+3/2, z+1/2]
O14T-H14B	0.980	2.937	161.31	3.878	Cl4 [x+1/2, -y+3/2, z+1/2]
O14T-H14C	0.980	2.234	146.02	3.095	O44P [-x+1/2, y+1/2, -z+1/2]
O14T-H14C	0.980	2.943	170.66	3.913	Cl4 [-x+1/2, y+1/2, -z+1/2]
O21T-H21A	0.980	1.850	159.86	2.791	O32T
O21T-H21B	0.980	2.478	115.34	3.030	O33C_c
O21T-H21B	0.980	2.516	156.27	3.436	O2W [-x+1/2, y+1/2, -z+1/2]

O21T-H21C	0.980	2.337	133.03	3.090	O33B_b
O21T-H21C	0.980	2.381	156.27	3.302	O24P
O21T-H21C	0.980	2.635	138.82	3.434	O32A
O22T-H22A	0.980	2.068	150.84	2.962	O24P
O22T-H22A	0.980	2.196	111.03	2.706	O32C_c
O22T-H22A	0.980	2.264	123.60	2.922	O32A
O22T-H22A	0.980	2.348	128.48	3.056	O33B_b
O22T-H22B	0.980	2.091	137.78	2.892	O32B_b
O22T-H22B	0.980	2.247	144.14	3.095	O34A
O22T-H22B	0.980	2.632	142.41	3.461	O34C_c
O22T-H22B	0.980	2.919	115.06	3.450	Cl3A
O22T-H22B	0.980	2.919	115.06	3.450	Cl3B_b
O22T-H22B	0.980	2.919	115.06	3.450	Cl3C_c
O22T-H22C	0.980	1.934	154.02	2.848	O13T
O23T-H23B	0.969	1.764	174.01	2.729	O2W [x-1/2, -y+3/2, z+1/2]
O23T-H23C	0.975	1.784	167.34	2.743	O2W [-x+1/2, y+1/2, -z+1/2]
O31T-H31A	0.980	1.945	144.14	2.799	O22A_a [-x+1/2, y+1/2, -z+1/2]
O31T-H31A	0.980	2.417	117.45	2.998	O11P [-x+1/2, -y+5/2, -z+1]
O31T-H31B	0.980	1.981	176.64	2.960	O42P [x, y+1, z]
O31T-H31B	0.980	2.878	153.60	3.781	Cl4 [x, y+1, z]
O32T-H32A	0.971	2.021	143.23	2.859	O42P [x, y+1, z]
O32T-H32A	0.971	2.325	123.52	2.974	O21A_a
O32T-H32A	0.971	2.583	129.27	3.285	O22P
O32T-H32A	0.971	2.977	120.71	3.572	Cl4 [x, y+1, z]
O32T-H32B	0.983	2.242	147.55	3.117	O43P [-x, y+1, -z+1/2]
O32T-H32B	0.983	2.421	128.73	3.131	O43P [x, y+1, z]
O33T-H33A	0.980	2.592	146.71	3.454	O14T [-x+1/2, -y+5/2, -z+1]
O33T-H33B	0.980	2.268	127.85	2.972	O43P [-x, y+1, -z+1/2]
O33T-H33B	0.980	2.491	151.61	3.386	O43P [x, y+1, z]
O33T-H33C	0.980	1.993	139.46	2.810	O1W [-x+1/2, y+1/2, -z+1/2]
O33T-H33C	0.980	2.240	118.54	2.841	O11P [-x+1/2, -y+5/2, -z+1]
O1W-H1WA	0.978	2.202	154.85	3.115	O31A [x+1/2, y+1/2, z]
O1W-H1WA	0.978	2.202	154.85	3.115	O31B_b [x+1/2, y+1/2, z]
O1W-H1WA	0.978	2.202	154.85	3.115	O31C_c [x+1/2, y+1/2, z]
O1W-H1WB	0.975	1.993	159.21	2.925	O24P [-x+1/2, y+1/2, -z+1/2]
O1W-H1WB	0.975	2.568	112.97	3.082	O32A [-x+1/2, y+1/2, -z+1/2]
O1W-H1WB	0.975	2.876	144.73	3.715	Cl2A_a [-x+1/2, y+1/2, -z+1/2]
O1W-H1WB	0.975	2.925	152.48	3.816	Cl2 [-x+1/2, y+1/2, -z+1/2]

O2W-H2WA	0.982	2.025	145.43	2.888	O42P [x+1/2, y+1/2, z]
O2W-H2WA	0.982	2.573	122.74	3.213	O41P [x+1/2, y+1/2, z]
O2W-H2WA	0.982	2.796	145.10	3.645	Cl4 [x+1/2, y+1/2, z]
O2W-H2WB	0.984	2.059	154.42	2.977	O22P [x+1/2, y-1/2, z]
O2W-H2WB	0.984	2.941	129.57	3.647	Cl2 [x+1/2, y-1/2,z]