Iodine-induced electrical conductivity of novel columnar lanthanide metal–organic frameworks based on a butterfly-shaped π-extended tetrathiafulvalene ligand

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SUPPORTING INFORMATION

Experimental Section

General Materials and Methods

Reagents, starting materials, and solvents were purchased from Sigma-Aldrich, Acros Organic, TCI America and EMD Chemicals and used as received. Ag-paint was procured from Ted Pella. The electrodes (Ag/AgCl, Pt-mesh, Pt-disk, and glassy-carbon disc) and electrochemical cells were procured from BASi.

The single crystal X-ray diffraction (SXRD) data were collected on a Bruker D8 Venture dual source diffractometer equipped with Cu and Mo radiation sources and CMOS detector. The isostructural Ln-MOF structures were solved and refined by using Bruker SHELXTL software package. The powder X-ray diffraction (PXRD) pattern of Tb-MOF crystals were recorded on a Rigaku Ultima IV X-ray diffractometer equipped with Cu Kα radiation source (λ = 1.5406 Å) and a CCD area detector.

The thermogravimetric analysis (TGA) was conducted under N_2 atmosphere using an SDT Q600 instrument.

A Shimadzu UV-2600 spectrophotometer equipped with an integrated sphere (200–1100 nm range) was used to measure the diffuse-reflectance spectra of the pristine and iodine-treated MOFs. The optical band-gaps were determined from Tauc plots.

Electrochemical measurements of Tb-MOFs were conducted on a Princeton Applied Research VersaStat 3-450 instrument using a glassy carbon working electrode, Ag/AgCl reference electrode, Pt-mesh counter electrode, and a 0.1 M Bu_4NPF_6 in MeCN as supporting electrolyte. The pastes of pristine and iodine-treated Tb-MOF made in MeCN were mounted onto the glassy carbon electrode surface to record their solid-state cyclic voltammograms.

The solid- state EPR spectra of pristine and iodine-treated Tb-MOF were recorded on a Bruker EMX EPR X-band spectrometer at room temperature. Powdered samples of each freshly prepared and air-exposed were inserted into precision-bore 4 mm quartz tube, and the sample weight and height were measured in order to determine the amount and volume. The spin was quantified by performing double integration of the obtained spectrum using the following equation, as described in the literature.[S1]

$$n_s = \frac{DI}{\frac{c}{f(B_1, B_m)} \times \{G_R \times C_t \times n\} \times \left\{\sqrt{P} \times B_m \times Q \times n_B \times S(S+1)\right\}}$$

where, c = point sample calibration factor; B_1 = microwave magnetic field; B_m = modulation amplitude; G_R = the receiver gain, C_t = conversion time; n = number of scans; P = microwave power; Q = quality factor of the resonator; n_B = Boltzmann temperature correction; S = electronic spin; and n_s = absolute number of spins.

The current-voltage (*I-V*) relationships of pristine and iodine-treated Tb-MOF pellets sandwiched between two Ag-coated stainless-steel electrodes were recorded under ambient conditions between –1 to +1 V using a Keithley 2400 source-meter. To prepare pristine and iodine-treated MOF pellets for *dc*-sweep measurements, 2.5 mg of respective material was placed inside a Teflon tube (inner diameter 2.7 mm) capped on one side with a snugly fit stainless-steel rod (diameter 2.7 mm) with conductive silver-coated tip. Then the other end of the Teflon tube was capped with another identical stainless-steel rod with conductive silver-coated tip. Finally, the entire setup containing the MOF material, sandwiched between the two rods, was pressed under 200 MPa pressure using a digital Parr Pellet Press. The thickness of the resulting pellets (ca. 0.2 mm) was measured by a digital caliper from the difference in total length of the two steel rods with and without the sandwiched materials. The resistance of each device was extracted from the slope of the linear *I-V* plot and the corresponding conductivity was calculated using the equation $\sigma = L/RA$.; where σ = conductivity, L = thickness of the pellet, R = resistance of the pellet, and A = area of the pellet (πr^2 , r = pellet radius = 1.35 mm).[S1–S3]

Synthesis of Ln-MOFs (Ln= Tb^{3+}, Eu^{3+} and Er^{3+}). To a solution of ExTTFTB ligand[S4] (8.6 mg, 0.010 mmol) in DMF (1.0 mL) placed in a screw-capped vial, a separately prepared solution of $Ln(NO_3)_3 \bullet 5H_2O$ (0.0135 mmol) in a 2:1 DMF/H_2O mixture (1.5 mL) was added slowly to prevent rapid precipitation. To the resulting solution, 0.1 mL of TFA and 1 mL of chlorobenzene were added immediately. This reaction mixture was then heated at 65 °C for 72 h to obtain dark orange to red-colored crystals suitable for SXRD analysis. The crystalline material was washed thoroughly with DMF, then subjected to solvent exchange with EtOH, and finally dried under vacuum for 48 h. to obtain the bulk materials as crystalline dark orange to red-colored powders.

Iodine-Treated Tb-MOF. The dark orange colored evacuated Tb-MOF powder (20 mg) placed in small open vial was placed inside a larger screw-capped vial containing a few iodine chips. The larger vial was capped tightly and sealed with a parafilm tape to expose the MOF crystals to iodine vapor for 4 days, which turned the MOF powder brown. The iodine-treated Tb-MOF was then washed thoroughly with hexanes and kept under vacuum to remove any physisorbed iodide.

Supplementary Figures:

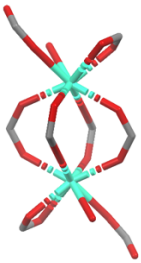

Fig. S1. Tb-MOF secondary building unit, showing the 8-coordinated environment of Tb ions (C, gray, O, red; and Tb, cyan).

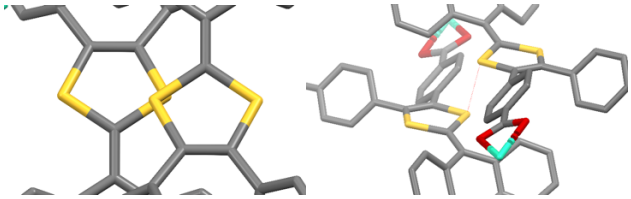

Fig. S2. A section of SXRD structure shows the lack of π–π-overlap between the 1,3-dithiolene rings of ExTTFTB ligands in Ln-MOFs.

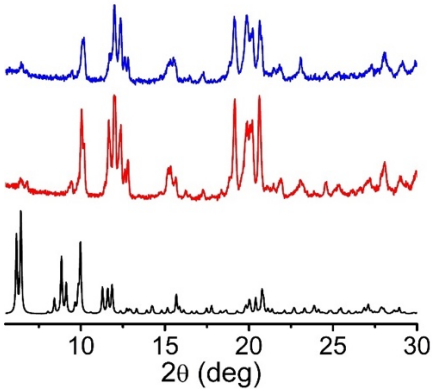

Fig. S3. The experimental PXRD patterns of pristine (red) and iodine-treated (blue) Tb-MOF. The simulated pattern of Tb-MOF is shown at the bottom (black).

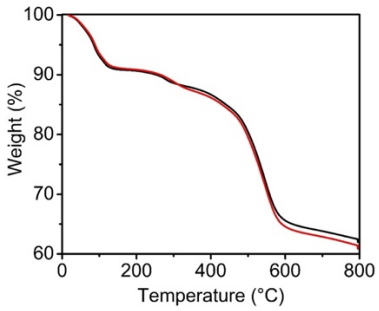

Fig. S4. The TGA profile of pristine (black) and iodine-treated (red) Tb-MOF.

References:

S1. S. Zhang, D. K. Panda, A. Yadav, W. Zhou and S. Saha, *Chem. Sci.*, 2021, **12**, 13379–13391.
S2. D. K.Panda, K. Maity, A. Palukoshka, F. Ibrahim and S. Saha, *ACS Sus. Chem. Eng*. 2019, **7**, 4619–4624.
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S4. M. A. Gordillo, P. A. Benavides, D. K. Panda and S. Saha, *ACS Appl. Mater. Interfaces*, 2020, **12**, 12955–12961.

Crystal Structure Report for $[Tb(C_{48}H_{25}O_8S_4)(H_2O)]n \cdot 2C_3H_7NO$, 0.5 H_2O

A specimen of $C_{54}H_{42}N_2O_{11.50}S_4Tb$, approximate dimensions 0.098 mm x 0.241 mm x 0.279 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The integration of the data using a triclinic unit cell yielded a total of 143920 reflections to a maximum θ angle of 29.15° (0.73 Å resolution), of which 17184 were independent (average redundancy 8.375, completeness = 99.7%, R_{int} = 3.59%, R_{sig} = 2.13%) and 15470 (90.03%) were greater than $2\sigma(F^2)$. The final cell constants of a = 11.6881(7) Å, b = 16.0699(10) Å, c = 19.7107(12) Å, α = 66.845(2)°, β = 76.074(2)°, γ = 71.653(2)°, volume = 3201.8(3) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8937 and 1.0000.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 2 for the formula unit, $C_{54}H_{42}N_2O_{11.50}S_4Tb$. The final anisotropic full-matrix least-squares refinement on F^2 with 802 variables converged at R1 = 4.89%, for the observed data and wR2 = 15.60% for all data. The goodness-of-fit was 1.074. The largest peak in the final difference electron density synthesis was 2.750 $e^-/Å^3$ and the largest hole was -0.934 $e^-/Å^3$ with an RMS deviation of 0.166 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.234 g/cm^3 and F(000), 1202 e^-.

Crystal Structure Report for $[Er(C_{48}H_{25}O_8S_4)(H_2O)]n \cdot 2C_3H_7NO$, H_2O

A specimen of $C_{54}H_{43}ErN_2O_{12}S_4$, approximate dimensions 0.051 mm x 0.064 mm x 0.081 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 111398 reflections to a maximum θ angle of 28.31° (0.75 Å resolution), of which 15744 were independent (average redundancy 7.076, completeness = 99.6%, R_{int} = 2.78%, R_{sig} = 1.60%) and 15000 (95.27%) were greater than $2\sigma(F^2)$. The final cell constants of a = 11.6009(10) Å, b = 16.1085(14) Å, c = 19.5975(17) Å, α = 66.704(3)°, β = 76.136(3)°, γ = 72.168(3)°, volume = 3172.5(5) $Å^3$, are based upon the refinement of the XYZ-centroids of 9241 reflections above 20 σ(I) with 5.469° < 2θ < 56.60°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.931. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9313 and 1.0000.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 2 for the formula unit, $C_{54}H_{43}ErN_2O_{12}S_4$. The final anisotropic full-matrix least-squares refinement on F^2 with 808 variables converged at R1 = 4.66%, for the observed data and wR2 = 14.92% for all data. The goodness-of-fit was 1.096. The largest peak in the final difference electron density synthesis was 2.233 $e^-/Å^3$ and the largest hole was -1.274 $e^-/Å^3$ with an RMS deviation of 0.165 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.264 g/cm^3 and F(000), 1218 e^-.

Crystal Structure Report for $[Eu(C_{48}H_{25}O_8S_4)(H_2O)]n \cdot 2C_3H_7NO$, 1.25 H_2O

A specimen of $C_{54}H_{43.50}EuN_2O_{12.25}S_4$, approximate dimensions 0.170 mm x 0.180 mm x 0.220 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The integration of the data using a triclinic unit cell yielded a total of 105127 reflections to a maximum θ angle of 28.34° (0.75 Å resolution), of which 15974 were independent (average redundancy 6.581, completeness = 99.5%, R_{int} = 3.21%, R_{sig} = 2.17%) and 14485 (90.68%) were greater than $2\sigma(F^2)$. The final cell constants of a = 11.6915(6) Å, b = 16.0431(8) Å, c = 19.7816(10) Å, α = 66.8521(13)°, β = 76.8187(14)°, γ = 71.4086(14)°, volume = 3211.1(3) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I).

The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9409 and 1.0000.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 2 for the formula unit, $C_{54}H_{43.50}EuN_2O_{12.25}S_4$. The final anisotropic full-matrix least-squares refinement on F^2 with 808 variables converged at R1 = 5.08%, for the observed data and wR2 = 15.64% for all data. The goodness-of-fit was 1.119. The largest peak in the final difference electron density synthesis was 2.856 $e^-/Å^3$ and the largest hole was -1.624 $e^-/Å^3$ with an RMS deviation of 0.165 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.238 g/cm^3 and F(000), 1213 e^-.

The geometry of the Ln(III) ions in each MOF were calculated using SHAPE 2.1 software, which revealed that the Tb(III) and Er(III) ions have distorted biaugmented trigonal prims J50 geometry, whereas Eu(III) ions have distorted heptagonal pyramid geometry.

Table S1. Sample and crystal data for Tb-MOF.

Chemical formula	$C_{54}H_{42}N_2O_{11.50}S_4Tb$	
Formula weight	1190.05 g/mol	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal size	0.098 x 0.241 x 0.279 mm	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.6881(7) Å	α = 66.845(2)°
	b = 16.0699(10) Å	β = 76.074(2)°
	c = 19.7107(12) Å	γ = 71.653(2)°
Volume	3201.8(3) $Å^3$	
Z	2	
Density (calculated)	1.234 g/cm^3	
Absorption coefficient	1.286 mm^{-1}	
F(000)	1202	

Table S2. Data collection and structure refinement for Tb-MOF.

Theta range for data collection	3.12 to 29.15°

Index ranges	-16<=h<=16, -22<=k<=21, -27<=l<=26
Reflections collected	143920
Independent reflections	17184 [R(int) = 0.0359]
Max. and min. transmission	1.0000 and 0.8937
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2016/6 (Sheldrick, 2016)
Function minimized	$\Sigma\ w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	17184 / 246 / 802
Goodness-of-fit on F^2	1.074
Final R indices	15470 data; I>2σ(I) R1 = 0.0489, wR2 = 0.1495
	all data R1 = 0.0552, wR2 = 0.1560
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0954P)^2+9.4107P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	2.750 and -0.934 eÅ^{-3}
R.M.S. deviation from mean	0.166 eÅ^{-3}

Table S3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for Tb-MOF.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Tb1	0.05113(2)	0.11463(2)	0.99530(2)	0.01961(7)
S1	0.24622(9)	0.15109(9)	0.42944(7)	0.0334(2)
S2	0.51060(9)	0.09397(7)	0.41110(5)	0.02603(19)
S3	0.26795(8)	0.53564(6)	0.42138(5)	0.02253(17)

	x/a	y/b	z/c	U(eq)
S4	0.53297(8)	0.47824(6)	0.41171(5)	0.02271(17)
O1	0.0489(4)	0.1829(4)	0.0785(3)	0.0638(13)
O2	0.9535(11)	0.3029(7)	0.0998(7)	0.204(6)
O3	0.8036(3)	0.9740(2)	0.07298(17)	0.0316(6)
O4	0.8834(3)	0.0789(3)	0.0811(2)	0.0408(8)
O5	0.0632(3)	0.9110(3)	0.07152(17)	0.0403(8)
O6	0.1620(3)	0.9946(2)	0.08996(17)	0.0373(7)
O7	0.7636(3)	0.8219(3)	0.04544(18)	0.0400(8)
O8	0.8985(3)	0.7701(3)	0.1222(2)	0.0639(14)
O9W	0.8897(6)	0.2617(4)	0.9786(4)	0.096(2)
C1	0.0325(7)	0.2313(6)	0.1127(5)	0.085(3)
C2	0.1025(6)	0.2069(5)	0.1738(4)	0.064(2)
C3	0.1800(5)	0.1208(4)	0.1956(3)	0.0434(12)
C4	0.2481(5)	0.0937(4)	0.2530(3)	0.0403(10)
C5	0.2404(4)	0.1548(3)	0.2887(3)	0.0358(10)
C6	0.1622(7)	0.2430(6)	0.2656(5)	0.087(3)
C7	0.0945(9)	0.2688(6)	0.2096(6)	0.107(4)
C8	0.3185(4)	0.1318(3)	0.3455(2)	0.0296(8)
C9	0.4402(4)	0.1033(3)	0.3383(2)	0.0268(7)
C10	0.5268(3)	0.0854(3)	0.2740(2)	0.0252(7)
C11	0.5594(4)	0.9994(3)	0.2656(3)	0.0375(10)
C12	0.6469(4)	0.9825(3)	0.2069(3)	0.0355(9)
C13	0.7046(3)	0.0516(3)	0.1591(2)	0.0262(7)
C14	0.6735(5)	0.1366(3)	0.1686(3)	0.0383(10)
C15	0.5834(5)	0.1544(3)	0.2248(3)	0.0366(10)
C16	0.8057(4)	0.0328(3)	0.0988(2)	0.0287(8)

	x/a	y/b	z/c	U(eq)
C17	0.3789(3)	0.1488(3)	0.4582(2)	0.0237(7)
C18	0.3809(3)	0.1895(2)	0.5055(2)	0.0225(7)
C19	0.4945(3)	0.1952(2)	0.5217(2)	0.0220(7)
C20	0.5972(4)	0.1201(3)	0.5358(2)	0.0279(8)
C21	0.7014(4)	0.1306(3)	0.5499(3)	0.0321(8)
C22	0.7048(4)	0.2155(3)	0.5508(2)	0.0310(8)
C23	0.6034(4)	0.2911(3)	0.5370(2)	0.0254(7)
C24	0.4986(3)	0.2822(2)	0.52164(19)	0.0204(6)
C25	0.3890(3)	0.3598(2)	0.50359(19)	0.0189(6)
C26	0.2732(3)	0.3322(2)	0.53519(19)	0.0199(6)
C27	0.2698(4)	0.2441(3)	0.5377(2)	0.0236(7)
C28	0.1640(4)	0.2129(3)	0.5695(2)	0.0317(9)
C29	0.0622(4)	0.2675(4)	0.5991(3)	0.0377(10)
C30	0.0658(4)	0.3539(3)	0.5967(3)	0.0334(9)
C31	0.1703(3)	0.3866(3)	0.5648(2)	0.0251(7)
C32	0.3958(3)	0.4458(2)	0.45485(19)	0.0193(6)
C33	0.3496(3)	0.6031(2)	0.3433(2)	0.0215(6)
C34	0.4711(3)	0.5767(2)	0.3390(2)	0.0212(6)
C35	0.2806(3)	0.6859(3)	0.28948(19)	0.0219(7)
C36	0.3053(4)	0.7725(3)	0.2702(2)	0.0284(8)
C37	0.2540(4)	0.8481(3)	0.2124(2)	0.0274(8)
C38	0.1761(3)	0.8392(3)	0.1741(2)	0.0241(7)
C39	0.1443(4)	0.7543(3)	0.1964(2)	0.0285(8)
C40	0.1969(3)	0.6787(3)	0.2537(2)	0.0250(7)
C41	0.1301(4)	0.9194(3)	0.1076(2)	0.0296(8)
C42	0.5582(3)	0.6234(3)	0.2796(2)	0.0245(7)

	x/a	y/b	z/c	U(eq)
C43	0.5464(4)	0.6496(4)	0.2047(2)	0.0362(10)
C44	0.6233(4)	0.6992(4)	0.1497(2)	0.0375(10)
C45	0.7157(4)	0.7197(3)	0.1685(2)	0.0299(8)
C46	0.7302(4)	0.6912(3)	0.2423(3)	0.0361(10)
C47	0.6515(4)	0.6439(3)	0.2977(2)	0.0326(9)
C48	0.7979(4)	0.7736(3)	0.1086(3)	0.0351(9)
N49	0.9204(7)	0.0357(8)	0.3410(6)	0.057(3)
C50	0.9333(12)	0.0007(9)	0.2832(8)	0.060(3)
C51	0.8473(14)	0.1305(14)	0.3342(12)	0.089(5)
C52	0.9661(15)	0.9976(11)	0.4026(10)	0.076(4)
O53	0.0227(9)	0.9161(9)	0.4238(8)	0.093(4)
N54	0.9558(7)	0.4060(6)	0.3596(5)	0.0377(18)
C55	0.8919(16)	0.3479(12)	0.4080(11)	0.086(5)
C57	0.9649(15)	0.4684(11)	0.2878(9)	0.071(4)
C56	0.0505(11)	0.4120(8)	0.3838(9)	0.064(3)
O58	0.0387(19)	0.5142(13)	0.2565(12)	0.158(7)
N59	0.5115(15)	0.2802(9)	0.0186(6)	0.072(4)
C60	0.4083(12)	0.2415(14)	0.0625(7)	0.073(5)
C62	0.6054(12)	0.2352(9)	0.9818(6)	0.053(3)
C61	0.537(3)	0.3547(19)	0.0202(15)	0.131(9)
O63	0.5956(12)	0.1669(10)	0.9765(8)	0.095(4)
O10W	0.5311(9)	0.0141(9)	0.9319(6)	0.029(2)
O11W	0.4311(10)	0.0077(11)	0.9913(8)	0.042(3)
C65B	0.529(3)	0.441(2)	0.1755(18)	0.070(3)
O68B	0.5010(17)	0.3501(12)	0.3092(10)	0.057(2)
C66B	0.760(2)	0.383(2)	0.1600(18)	0.073(4)

	x/a	y/b	z/c	U(eq)
C67B	0.604(2)	0.346(2)	0.2819(14)	0.070(3)
N64B	0.637(2)	0.3901(18)	0.2049(13)	0.072(3)
C65A	0.393(2)	0.3713(17)	0.3043(13)	0.053(3)
C67A	0.6021(19)	0.374(2)	0.257(2)	0.071(3)
N64A	0.4850(18)	0.3978(16)	0.2474(12)	0.068(2)
C66A	0.417(3)	0.463(2)	0.1887(16)	0.073(4)
O68A	0.711(2)	0.3657(17)	0.2385(14)	0.082(3)

Table S4. Bond lengths (Å) for Tb-MOF.

Tb1-O1	2.296(4)	Tb1-O5	2.304(3)
Tb1-O4	2.320(3)	Tb1-O3	2.368(3)
Tb1-O6	2.375(3)	Tb1-O8	2.408(3)
Tb1-O9W	2.476(5)	Tb1-O7	2.506(3)
Tb1-C48	2.810(4)	Tb1-H9B	2.4983(2)
S1-C17	1.760(4)	S1-C8	1.765(4)
S2-C9	1.755(4)	S2-C17	1.764(4)
S3-C33	1.757(4)	S3-C32	1.767(3)
S4-C34	1.754(4)	S4-C32	1.756(4)
O1-C1	1.163(7)	O2-C1	1.207(10)
O2-H2	0.84	O3-C16	1.244(5)
O4-C16	1.250(5)	O5-C41	1.243(5)
O6-C41	1.269(6)	O7-C48	1.264(6)
O8-C48	1.246(6)	O9W-H9A	0.860(5)
O9W-H9B	0.880(7)	C1-C2	1.474(8)
C2-C3	1.360(8)	C2-C7	1.399(7)
C3-C4	1.391(7)	C3-H3	0.95

C4-C5	1.387(6)	C4-H4	0.95
C5-C6	1.389(8)	C5-C8	1.475(6)
C6-C7	1.368(9)	C6-H6	0.95
C7-H7	0.95	C8-C9	1.340(6)
C9-C10	1.484(5)	C10-C11	1.378(6)
C10-C15	1.383(6)	C11-C12	1.400(6)
C11-H11	0.95	C12-C13	1.385(6)
C12-H12	0.95	C13-C14	1.374(6)
C13-C16	1.512(5)	C14-C15	1.384(6)
C14-H14	0.95	C15-H15	0.95
C17-C18	1.340(5)	C18-C19	1.475(5)
C18-C27	1.478(5)	C19-C20	1.400(5)
C19-C24	1.414(5)	C20-C21	1.386(6)
C20-H20	0.95	C21-C22	1.385(6)
C21-H21	0.95	C22-C23	1.395(5)
C22-H22	0.95	C23-C24	1.391(5)
C23-H23	0.95	C24-C25	1.479(5)
C25-C32	1.351(5)	C25-C26	1.474(5)
C26-C31	1.398(5)	C26-C27	1.409(5)
C27-C28	1.394(5)	C28-C29	1.392(6)
C28-H28	0.95	C29-C30	1.385(6)
C29-H29	0.95	C30-C31	1.391(6)
C30-H30	0.95	C31-H31	0.95
C33-C34	1.340(5)	C33-C35	1.474(5)
C34-C42	1.479(5)	C35-C40	1.392(5)
C35-C36	1.396(5)	C36-C37	1.384(5)
C36-H36	0.95	C37-C38	1.384(5)

C37-H37	0.95	C38-C39	1.399(6)
C38-C41	1.499(5)	C39-C40	1.384(5)
C39-H39	0.95	C40-H40	0.95
C42-C47	1.390(5)	C42-C43	1.397(6)
C43-C44	1.385(6)	C43-H43	0.95
C44-C45	1.387(6)	C44-H44	0.95
C45-C46	1.378(6)	C45-C48	1.498(5)
C46-C47	1.386(6)	C46-H46	0.95
C47-H47	0.95	N49-C52	1.286(19)
N49-C50	1.418(19)	N49-C51	1.46(2)
C50-H50A	0.98	C50-H50B	0.98
C50-H50C	0.98	C51-H51A	0.98
C51-H51B	0.98	C51-H51C	0.98
C52-O53	1.218(15)	C52-H52	0.95
N54-C55	1.317(17)	N54-C56	1.350(15)
N54-C57	1.377(18)	C55-H55A	0.98
C55-H55B	0.98	C55-H55C	0.98
C57-O58	1.206(15)	C57-H57	0.95
C56-H56A	0.98	C56-H56B	0.98
C56-H56C	0.98	N59-C61	1.33(3)
N59-C62	1.336(19)	N59-C60	1.46(2)
C60-H60A	0.98	C60-H60B	0.98
C60-H60C	0.98	C62-O63	1.186(14)
C62-H62	0.95	C61-H61A	0.98
C61-H61B	0.98	C61-H61C	0.98
O10W-H10A	0.948(11)	O10W-H10B	0.860(11)
O11W-H11B	0.861(17)	O11W-H11A	0.851(13)

C65B-N64B	1.386(18)	C65B-H65A	0.98
C65B-H65B	0.98	C65B-H65C	0.98
O68B-C67B	1.184(18)	C66B-N64B	1.495(18)
C66B-H66A	0.98	C66B-H66B	0.98
C66B-H66C	0.98	C67B-N64B	1.413(18)
C67B-H67B	0.95	C65A-N64A	1.392(18)
C65A-H65D	0.98	C65A-H65E	0.98
C65A-H65F	0.98	C67A-O68A	1.219(18)
C67A-N64A	1.338(18)	C67A-H67A	0.95
N64A-C66A	1.424(18)	C66A-H66D	0.98
C66A-H66E	0.98	C66A-H66F	0.98

Table S5. Bond angles (°) for Tb-MOF.

O1-Tb1-O5	146.04(15)	O1-Tb1-O4	78.12(15)
O5-Tb1-O4	76.75(12)	O1-Tb1-O3	137.95(15)
O5-Tb1-O3	76.01(12)	O4-Tb1-O3	130.01(12)
O1-Tb1-O6	74.76(17)	O5-Tb1-O6	124.08(13)
O4-Tb1-O6	83.54(13)	O3-Tb1-O6	78.27(12)
O1-Tb1-O8	101.99(19)	O5-Tb1-O8	83.61(14)
O4-Tb1-O8	140.28(14)	O3-Tb1-O8	75.96(15)
O6-Tb1-O8	135.42(12)	O1-Tb1-O9W	68.6(2)
O5-Tb1-O9W	82.3(2)	O4-Tb1-O9W	72.76(19)
O3-Tb1-O9W	141.8(2)	O6-Tb1-O9W	139.5(2)
O8-Tb1-O9W	70.6(2)	O1-Tb1-O7	73.27(14)
O5-Tb1-O7	131.02(11)	O4-Tb1-O7	151.08(12)
O3-Tb1-O7	72.76(12)	O6-Tb1-O7	84.97(12)
O8-Tb1-O7	52.88(12)	O9W-Tb1-O7	100.13(18)

O1-Tb1-C48	88.73(16)	O5-Tb1-C48	106.89(13)
O4-Tb1-C48	157.90(14)	O3-Tb1-C48	71.13(13)
O6-Tb1-C48	110.28(13)	O8-Tb1-C48	26.20(13)
O9W-Tb1-C48	85.97(18)	O7-Tb1-C48	26.74(13)
O1-Tb1-H9B	87.10(14)	O5-Tb1-H9B	62.14(10)
O4-Tb1-H9B	66.95(10)	O3-Tb1-H9B	129.92(8)
O6-Tb1-H9B	148.11(9)	O8-Tb1-H9B	73.36(9)
O9W-Tb1-H9B	20.38(17)	O7-Tb1-H9B	115.03(9)
C48-Tb1-H9B	94.99(9)	C17-S1-C8	96.05(19)
C9-S2-C17	96.10(19)	C33-S3-C32	96.02(17)
C34-S4-C32	96.25(17)	C1-O1-Tb1	167.3(6)
C1-O2-H2	109.5	C16-O3-Tb1	134.9(3)
C16-O4-Tb1	142.8(3)	C41-O5-Tb1	175.9(3)
C41-O6-Tb1	109.7(3)	C48-O7-Tb1	90.1(3)
C48-O8-Tb1	95.2(3)	Tb1-O9W-H9A	167.3(7)
Tb1-O9W-H9B	81.2(3)	H9A-O9W-H9B	95.7(7)
O1-C1-O2	119.7(7)	O1-C1-C2	122.3(6)
O2-C1-C2	118.0(6)	C3-C2-C7	118.4(5)
C3-C2-C1	118.6(5)	C7-C2-C1	123.0(6)
C2-C3-C4	121.1(4)	C2-C3-H3	119.4
C4-C3-H3	119.4	C5-C4-C3	120.7(5)
C5-C4-H4	119.7	C3-C4-H4	119.7
C4-C5-C6	117.9(5)	C4-C5-C8	122.3(4)
C6-C5-C8	119.6(4)	C7-C6-C5	121.1(5)
C7-C6-H6	119.5	C5-C6-H6	119.5
C6-C7-C2	120.8(6)	C6-C7-H7	119.6
C2-C7-H7	119.6	C9-C8-C5	126.8(4)

C9-C8-S1	116.0(3)	C5-C8-S1	117.1(3)
C8-C9-C10	129.0(4)	C8-C9-S2	116.9(3)
C10-C9-S2	113.9(3)	C11-C10-C15	119.3(4)
C11-C10-C9	121.6(4)	C15-C10-C9	118.9(4)
C10-C11-C12	120.5(4)	C10-C11-H11	119.7
C12-C11-H11	119.7	C13-C12-C11	119.4(4)
C13-C12-H12	120.3	C11-C12-H12	120.3
C14-C13-C12	119.9(4)	C14-C13-C16	119.6(4)
C12-C13-C16	120.5(4)	C13-C14-C15	120.5(4)
C13-C14-H14	119.7	C15-C14-H14	119.7
C10-C15-C14	120.3(4)	C10-C15-H15	119.9
C14-C15-H15	119.9	O3-C16-O4	127.6(4)
O3-C16-C13	117.8(4)	O4-C16-C13	114.6(4)
C18-C17-S1	124.7(3)	C18-C17-S2	123.9(3)
S1-C17-S2	111.2(2)	C17-C18-C19	123.0(3)
C17-C18-C27	122.8(4)	C19-C18-C27	113.7(3)
C20-C19-C24	119.1(4)	C20-C19-C18	123.6(3)
C24-C19-C18	117.3(3)	C21-C20-C19	120.5(4)
C21-C20-H20	119.7	C19-C20-H20	119.7
C22-C21-C20	120.3(4)	C22-C21-H21	119.8
C20-C21-H21	119.8	C21-C22-C23	120.0(4)
C21-C22-H22	120.0	C23-C22-H22	120.0
C24-C23-C22	120.4(4)	C24-C23-H23	119.8
C22-C23-H23	119.8	C23-C24-C19	119.6(3)
C23-C24-C25	123.7(3)	C19-C24-C25	116.7(3)
C32-C25-C26	123.1(3)	C32-C25-C24	122.1(3)
C26-C25-C24	114.3(3)	C31-C26-C27	119.2(3)

C31-C26-C25	123.6(3)	C27-C26-C25	117.1(3)
C28-C27-C26	119.6(3)	C28-C27-C18	123.3(3)
C26-C27-C18	117.1(3)	C29-C28-C27	120.7(4)
C29-C28-H28	119.7	C27-C28-H28	119.7
C30-C29-C28	119.7(4)	C30-C29-H29	120.2
C28-C29-H29	120.2	C29-C30-C31	120.5(4)
C29-C30-H30	119.7	C31-C30-H30	119.7
C30-C31-C26	120.3(4)	C30-C31-H31	119.8
C26-C31-H31	119.8	C25-C32-S4	124.0(3)
C25-C32-S3	123.7(3)	S4-C32-S3	112.07(19)
C34-C33-C35	125.0(3)	C34-C33-S3	116.7(3)
C35-C33-S3	118.3(3)	C33-C34-C42	126.4(3)
C33-C34-S4	116.9(3)	C42-C34-S4	116.7(3)
C40-C35-C36	119.1(3)	C40-C35-C33	121.4(3)
C36-C35-C33	119.4(3)	C37-C36-C35	120.1(3)
C37-C36-H36	119.9	C35-C36-H36	119.9
C36-C37-C38	120.5(4)	C36-C37-H37	119.8
C38-C37-H37	119.8	C37-C38-C39	119.7(3)
C37-C38-C41	119.6(4)	C39-C38-C41	120.6(3)
C40-C39-C38	119.5(3)	C40-C39-H39	120.3
C38-C39-H39	120.3	C39-C40-C35	120.9(4)
C39-C40-H40	119.6	C35-C40-H40	119.6
O5-C41-O6	122.2(4)	O5-C41-C38	120.0(4)
O6-C41-C38	117.8(4)	C47-C42-C43	119.0(4)
C47-C42-C34	120.3(3)	C43-C42-C34	120.7(3)
C44-C43-C42	120.1(4)	C44-C43-H43	120.0
C42-C43-H43	120.0	C43-C44-C45	120.3(4)

C43-C44-H44	119.8	C45-C44-H44	119.8
C46-C45-C44	119.7(4)	C46-C45-C48	120.4(4)
C44-C45-C48	119.8(4)	C45-C46-C47	120.3(4)
C45-C46-H46	119.9	C47-C46-H46	119.9
C46-C47-C42	120.5(4)	C46-C47-H47	119.7
C42-C47-H47	119.7	O8-C48-O7	121.5(4)
O8-C48-C45	119.3(4)	O7-C48-C45	119.2(4)
O8-C48-Tb1	58.6(2)	O7-C48-Tb1	63.1(2)
C45-C48-Tb1	174.5(4)	C52-N49-C50	130.2(13)
C52-N49-C51	109.9(15)	C50-N49-C51	119.8(12)
N49-C50-H50A	109.5	N49-C50-H50B	109.5
H50A-C50-H50B	109.5	N49-C50-H50C	109.5
H50A-C50-H50C	109.5	H50B-C50-H50C	109.5
N49-C51-H51A	109.5	N49-C51-H51B	109.5
H51A-C51-H51B	109.5	N49-C51-H51C	109.5
H51A-C51-H51C	109.5	H51B-C51-H51C	109.5
O53-C52-N49	122.3(17)	O53-C52-H52	118.9
N49-C52-H52	118.9	C55-N54-C56	116.0(14)
C55-N54-C57	143.5(14)	C56-N54-C57	100.5(12)
N54-C55-H55A	109.5	N54-C55-H55B	109.5
H55A-C55-H55B	109.5	N54-C55-H55C	109.5
H55A-C55-H55C	109.5	H55B-C55-H55C	109.5
O58-C57-N54	128.7(19)	O58-C57-H57	115.7
N54-C57-H57	115.7	N54-C56-H56A	109.5
N54-C56-H56B	109.5	H56A-C56-H56B	109.5
N54-C56-H56C	109.5	H56A-C56-H56C	109.5
H56B-C56-H56C	109.5	C61-N59-C62	110.2(19)

C61-N59-C60	125.5(18)	C62-N59-C60	123.3(13)
N59-C60-H60A	109.5	N59-C60-H60B	109.5
H60A-C60-H60B	109.5	N59-C60-H60C	109.5
H60A-C60-H60C	109.5	H60B-C60-H60C	109.5
O63-C62-N59	117.3(14)	O63-C62-H62	121.3
N59-C62-H62	121.3	N59-C61-H61A	109.5
N59-C61-H61B	109.5	H61A-C61-H61B	109.5
N59-C61-H61C	109.5	H61A-C61-H61C	109.5
H61B-C61-H61C	109.5	H10A-O10W-H10B	128.0(14)
H11B-O11W-H11A	114.7(15)	N64B-C65B-H65A	109.5
N64B-C65B-H65B	109.5	H65A-C65B-H65B	109.5
N64B-C65B-H65C	109.5	H65A-C65B-H65C	109.5
H65B-C65B-H65C	109.5	N64B-C66B-H66A	109.5
N64B-C66B-H66B	109.5	H66A-C66B-H66B	109.5
N64B-C66B-H66C	109.5	H66A-C66B-H66C	109.5
H66B-C66B-H66C	109.5	O68B-C67B-N64B	122.(3)
O68B-C67B-H67B	118.8	N64B-C67B-H67B	118.8
C65B-N64B-C67B	106.(2)	C65B-N64B-C66B	124.(3)
C67B-N64B-C66B	129.(2)	N64A-C65A-H65D	109.5
N64A-C65A-H65E	109.5	H65D-C65A-H65E	109.5
N64A-C65A-H65F	109.5	H65D-C65A-H65F	109.5
H65E-C65A-H65F	109.5	O68A-C67A-N64A	157.(4)
O68A-C67A-H67A	101.5	N64A-C67A-H67A	101.5
C67A-N64A-C65A	124.(2)	C67A-N64A-C66A	134.(3)
C65A-N64A-C66A	101.(2)	N64A-C66A-H66D	109.5
N64A-C66A-H66E	109.5	H66D-C66A-H66E	109.5

N64A-C66A-H66F 109.5 H66D-C66A-H66F 109.5

H66E-C66A-H66F 109.5

Table S6. Anisotropic atomic displacement parameters (Å^2) for Tb-MOF.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Tb1	0.02177(10)	0.02165(10)	0.01529(9)	-0.00445(6)	0.00105(6)	-0.01030(6)
S1	0.0218(4)	0.0484(6)	0.0419(6)	-0.0325(5)	0.0091(4)	-0.0127(4)
S2	0.0228(4)	0.0301(5)	0.0261(4)	-0.0152(4)	0.0033(3)	-0.0057(3)
S3	0.0166(4)	0.0215(4)	0.0242(4)	-0.0015(3)	-0.0033(3)	-0.0055(3)
S4	0.0173(4)	0.0206(4)	0.0250(4)	0.0002(3)	-0.0042(3)	-0.0070(3)
O1	0.069(3)	0.096(4)	0.062(3)	-0.060(3)	0.005(2)	-0.035(3)
O2	0.242(10)	0.178(8)	0.239(10)	-0.156(8)	-0.198(9)	0.119(7)
O3	0.0283(14)	0.0433(17)	0.0267(14)	-0.0203(13)	0.0058(11)	-0.0098(12)
O4	0.0336(16)	0.054(2)	0.0419(18)	-0.0279(16)	0.0187(14)	-0.0235(15)
O5	0.0301(15)	0.063(2)	0.0208(14)	-0.0032(14)	-0.0117(12)	-0.0105(15)
O6	0.0456(18)	0.0292(15)	0.0257(14)	0.0025(12)	-0.0119(13)	-0.0039(13)
O7	0.0495(19)	0.0460(19)	0.0290(15)	-0.0037(14)	-0.0012(14)	-0.0327(16)
O8	0.0270(16)	0.061(2)	0.064(3)	0.035(2)	-0.0163(17)	-0.0229(17)
O9W	0.078(4)	0.042(3)	0.137(6)	-0.017(3)	-0.020(4)	0.010(2)
C1	0.067(4)	0.104(6)	0.117(7)	-0.089(6)	-0.058(5)	0.034(4)
C2	0.048(3)	0.078(4)	0.096(5)	-0.072(4)	-0.036(3)	0.019(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C3	0.040(2)	0.051(3)	0.060(3)	-0.042(3)	-0.003(2)	-0.012(2)
C4	0.039(2)	0.040(2)	0.054(3)	-0.030(2)	-0.005(2)	-0.0087(19)
C5	0.0274(19)	0.043(2)	0.048(3)	-0.031(2)	-0.0048(18)	-0.0034(17)
C6	0.079(5)	0.085(5)	0.135(7)	-0.096(5)	-0.070(5)	0.045(4)
C7	0.114(7)	0.092(6)	0.157(9)	-0.106(6)	-0.100(7)	0.062(5)
C8	0.0259(18)	0.037(2)	0.033(2)	-0.0231(17)	0.0039(15)	-0.0077(16)
C9	0.0277(18)	0.0295(19)	0.0258(18)	-0.0154(15)	0.0035(14)	-0.0082(15)
C10	0.0229(17)	0.0298(18)	0.0245(17)	-0.0141(15)	0.0021(13)	-0.0066(14)
C11	0.041(2)	0.033(2)	0.038(2)	-0.0179(18)	0.0165(19)	-0.0166(18)
C12	0.037(2)	0.032(2)	0.039(2)	-0.0218(18)	0.0138(18)	-0.0129(17)
C13	0.0211(16)	0.034(2)	0.0235(17)	-0.0135(15)	0.0048(13)	-0.0082(14)
C14	0.046(3)	0.035(2)	0.032(2)	-0.0127(18)	0.0124(19)	-0.019(2)
C15	0.044(2)	0.031(2)	0.034(2)	-0.0178(18)	0.0115(19)	-0.0128(18)
C16	0.0246(17)	0.038(2)	0.0238(17)	-0.0156(16)	0.0043(14)	-0.0067(15)
C17	0.0232(16)	0.0235(16)	0.0256(17)	-0.0115(14)	0.0061(13)	-0.0104(13)
C18	0.0242(17)	0.0199(16)	0.0228(16)	-0.0078(13)	0.0034(13)	-0.0087(13)
C19	0.0257(17)	0.0202(16)	0.0192(15)	-0.0064(13)	0.0000(13)	-0.0072(13)
C20	0.034(2)	0.0214(17)	0.0261(18)	-0.0084(14)	-0.0041(15)	-0.0037(15)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C21	0.032(2)	0.0258(19)	0.035(2)	-0.0086(16)	-0.0117(16)	0.0019(15)
C22	0.0275(19)	0.0286(19)	0.035(2)	-0.0081(16)	-0.0121(16)	-0.0015(15)
C23	0.0253(17)	0.0236(17)	0.0265(18)	-0.0077(14)	-0.0068(14)	-0.0041(14)
C24	0.0226(16)	0.0198(15)	0.0161(14)	-0.0041(12)	-0.0005(12)	-0.0058(13)
C25	0.0184(15)	0.0196(15)	0.0192(15)	-0.0064(12)	-0.0019(12)	-0.0062(12)
C26	0.0197(15)	0.0213(16)	0.0175(15)	-0.0064(12)	0.0020(12)	-0.0074(12)
C27	0.0276(17)	0.0225(16)	0.0214(16)	-0.0098(13)	0.0047(13)	-0.0104(14)
C28	0.034(2)	0.032(2)	0.035(2)	-0.0173(17)	0.0122(17)	-0.0199(17)
C29	0.030(2)	0.045(2)	0.045(3)	-0.025(2)	0.0165(18)	-0.0213(19)
C30	0.0270(19)	0.038(2)	0.039(2)	-0.0216(19)	0.0094(16)	-0.0123(17)
C31	0.0249(17)	0.0244(17)	0.0265(18)	-0.0123(14)	0.0022(14)	-0.0066(14)
C32	0.0163(14)	0.0207(15)	0.0209(15)	-0.0066(13)	-0.0026(12)	-0.0050(12)
C33	0.0224(16)	0.0202(15)	0.0197(15)	-0.0012(12)	-0.0052(12)	-0.0080(13)
C34	0.0218(16)	0.0202(15)	0.0194(15)	-0.0004(12)	-0.0045(12)	-0.0090(13)
C35	0.0217(16)	0.0240(16)	0.0173(15)	-0.0018(13)	-0.0056(12)	-0.0067(13)
C36	0.033(2)	0.0251(18)	0.0278(18)	-0.0029(15)	-0.0175(16)	-0.0067(15)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C37	0.035(2)	0.0212(17)	0.0257(18)	-0.0035(14)	-0.0128(15)	-0.0053(15)
C38	0.0231(16)	0.0280(18)	0.0177(15)	-0.0036(13)	-0.0061(13)	-0.0050(14)
C39	0.0252(18)	0.037(2)	0.0222(17)	-0.0024(15)	-0.0083(14)	-0.0129(16)
C40	0.0245(17)	0.0276(18)	0.0229(17)	-0.0023(14)	-0.0064(14)	-0.0121(14)
C41	0.0253(18)	0.039(2)	0.0158(16)	-0.0037(15)	-0.0056(13)	-0.0010(16)
C42	0.0212(16)	0.0253(17)	0.0229(17)	-0.0010(14)	-0.0029(13)	-0.0100(14)
C43	0.038(2)	0.052(3)	0.0247(19)	-0.0069(18)	-0.0012(17)	-0.029(2)
C44	0.041(2)	0.050(3)	0.0235(19)	-0.0045(18)	0.0008(17)	-0.028(2)
C45	0.0262(18)	0.0269(18)	0.0292(19)	0.0017(15)	-0.0022(15)	-0.0126(15)
C46	0.0277(19)	0.041(2)	0.036(2)	0.0053(18)	-0.0116(17)	-0.0212(18)
C47	0.030(2)	0.040(2)	0.0262(19)	0.0014(16)	-0.0081(15)	-0.0192(17)
C48	0.031(2)	0.028(2)	0.034(2)	0.0044(16)	0.0019(16)	-0.0137(16)
N49	0.017(3)	0.083(7)	0.051(5)	0.010(5)	-0.009(3)	-0.026(4)
C50	0.054(7)	0.049(6)	0.068(8)	0.010(6)	-0.020(6)	-0.032(5)
C51	0.048(8)	0.095(13)	0.115(15)	-0.042(11)	0.009(8)	-0.013(8)
C52	0.070(5)	0.083(6)	0.084(6)	-0.021(4)	-0.014(4)	-0.037(4)
O53	0.044(4)	0.109(7)	0.117(8)	-0.003(6)	-0.034(5)	-0.034(5)
N54	0.022(3)	0.039(4)	0.053(5)	-0.032(4)	-0.001(3)	0.009(3)
C55	0.075(7)	0.073(7)	0.121(9)	-0.063(7)	0.045(7)	-0.040(6)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C57	0.071(5)	0.065(5)	0.072(5)	-0.030(4)	-0.010(4)	-0.001(4)
C56	0.040(5)	0.047(5)	0.122(8)	-0.063(6)	-0.004(5)	0.006(4)
O58	0.150(10)	0.124(9)	0.203(11)	-0.076(8)	0.037(8)	-0.057(8)
N59	0.115(11)	0.054(6)	0.039(5)	-0.006(5)	-0.025(6)	-0.011(7)
C60	0.045(6)	0.134(14)	0.031(5)	-0.028(7)	-0.005(5)	-0.012(8)
C62	0.054(7)	0.064(7)	0.033(5)	-0.006(5)	-0.007(5)	-0.017(6)
C61	0.150(17)	0.112(14)	0.109(14)	-0.034(12)	-0.017(13)	-0.010(13)
O63	0.081(8)	0.109(10)	0.083(8)	-0.026(8)	-0.019(7)	-0.011(7)
O10W	0.015(5)	0.053(7)	0.019(5)	-0.013(5)	0.006(4)	-0.011(5)
O11W	0.010(5)	0.057(8)	0.040(7)	0.001(6)	-0.007(5)	-0.001(5)
C65B	0.079(4)	0.065(4)	0.072(4)	-0.027(4)	-0.009(4)	-0.023(4)
O68B	0.081(4)	0.050(4)	0.062(4)	-0.040(3)	-0.005(3)	-0.023(3)
C66B	0.076(5)	0.069(5)	0.078(5)	-0.028(4)	-0.010(5)	-0.020(5)
C67B	0.078(3)	0.067(3)	0.072(3)	-0.030(2)	-0.009(2)	-0.019(2)
N64B	0.078(3)	0.068(3)	0.074(3)	-0.028(2)	-0.008(2)	-0.020(2)
C65A	0.073(5)	0.049(5)	0.056(5)	-0.039(4)	-0.006(4)	-0.017(4)
C67A	0.078(3)	0.067(3)	0.073(3)	-0.029(2)	-0.008(2)	-0.019(2)
N64A	0.077(3)	0.064(3)	0.071(3)	-0.030(2)	-0.009(2)	-0.020(2)
C66A	0.082(5)	0.068(5)	0.074(5)	-0.028(4)	-0.013(5)	-0.020(5)
O68A	0.081(4)	0.077(4)	0.083(4)	-0.024(4)	-0.009(4)	-0.017(4)

Table S7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for Tb-MOF.

	x/a	y/b	z/c	U(eq)
H2	-0.0783	0.3102	0.0633	0.306
H9A	-0.1594	0.3156	-0.0374	0.05

	x/a	y/b	z/c	U(eq)
H9B	-0.1432	0.2331	-0.0388	0.05
H3	0.1878	0.0784	0.1711	0.052
H4	0.3003	0.0328	0.2680	0.048
H6	0.1556	0.2861	0.2891	0.105
H7	0.0414	0.3294	0.1948	0.128
H11	0.5223	-0.0487	0.2998	0.045
H12	0.6665	-0.0759	0.1999	0.043
H14	0.7141	0.1836	0.1363	0.046
H15	0.5603	0.2142	0.2296	0.044
H20	0.5954	0.0614	0.5357	0.034
H21	0.7708	0.0794	0.5589	0.039
H22	0.7763	0.2222	0.5609	0.037
H23	0.6058	0.3491	0.5382	0.03
H28	0.1614	0.1537	0.5709	0.038
H29	-0.0094	0.2456	0.6208	0.045
H30	-0.0035	0.3912	0.6170	0.04
H31	0.1716	0.4462	0.5632	0.03
H36	0.3574	0.7796	0.2968	0.034
H37	0.2724	0.9066	0.1988	0.033
H39	0.0870	0.7488	0.1725	0.034
H40	0.1756	0.6210	0.2687	0.03
H43	0.4856	0.6334	0.1913	0.043
H44	0.6127	0.7192	0.0989	0.045
H46	0.7945	0.7041	0.2552	0.043
H47	0.6614	0.6254	0.3485	0.039
H50A	-0.1139	0.0479	0.2438	0.089

	x/a	y/b	z/c	U(eq)
H50B	0.0193	-0.0140	0.2626	0.089
H50C	-0.0966	-0.0560	0.3031	0.089
H51A	-0.1873	0.1591	0.2872	0.134
H51B	-0.2187	0.1280	0.3759	0.134
H51C	-0.1012	0.1679	0.3349	0.134
H52	-0.0445	0.0342	0.4326	0.091
H55A	-0.1742	0.3487	0.3850	0.129
H55B	-0.0552	0.2846	0.4235	0.129
H55C	-0.1423	0.3671	0.4516	0.129
H57	-0.0950	0.4764	0.2591	0.085
H56A	0.0917	0.4568	0.3438	0.096
H56B	0.0207	0.4331	0.4267	0.096
H56C	0.1079	0.3506	0.3986	0.096
H60A	-0.5895	0.1868	0.0512	0.109
H60B	-0.5870	0.2229	0.1157	0.109
H60C	-0.6678	0.2888	0.0501	0.109
H62	-0.3228	0.2571	-0.0393	0.063
H61A	-0.5329	0.3871	0.0473	0.196
H61B	-0.3915	0.3347	0.0453	0.196
H61C	-0.4476	0.3970	-0.0308	0.196
H10A	0.5327	1.0257	-0.1193	0.05
H10B	0.4906	0.9807	-0.0305	0.05
H11B	0.4447	0.9771	-0.0384	0.05
H11A	0.4891	0.9943	0.0158	0.05
H65A	0.5469	0.4724	0.1218	0.105
H65B	0.4782	0.3980	0.1843	0.105

	x/a	y/b	z/c	U(eq)
H65C	0.4855	0.4869	0.1995	0.105
H66A	0.8220	0.3438	0.1929	0.109
H66B	0.7643	0.3555	0.1228	0.109
H66C	0.7747	0.4457	0.1347	0.109
H67B	0.6660	0.3130	0.3129	0.084
H65D	0.3146	0.3970	0.2845	0.079
H65E	0.4091	0.3030	0.3248	0.079
H65F	0.3889	0.3952	0.3437	0.079
H67A	0.5974	0.3456	0.3094	0.085
H66D	0.3316	0.4602	0.2030	0.109
H66E	0.4231	0.5259	0.1794	0.109
H66F	0.4497	0.4469	0.1435	0.109

Table S8. Sample and crystal data for Er-MOF.

Identification code	D8_4262_B2_8	
Chemical formula	$C_{54}H_{43}ErN_2O_{12}S_4$	
Formula weight	1207.40 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.051 x 0.064 x 0.081 mm	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.6009(10) Å	α = 66.704(3)°
	b = 16.1085(14) Å	β = 76.136(3)°
	c = 19.5975(17) Å	γ = 72.168(3)°
Volume	3172.5(5) $Å^3$	

Z	2
Density (calculated)	1.264 g/cm^3
Absorption coefficient	1.507 mm^{-1}
F(000)	1218

Table S9. Data collection and structure refinement for Er-MOF.

Theta range for data collection	2.06 to 28.31°	
Index ranges	-15<=h<=15, -21<=k<=21, -26<=l<=26	
Reflections collected	111398	
Independent reflections	15744 [R(int) = 0.0278]	
Coverage of independent reflections	99.6%	
Absorption correction	Multi-Scan	
Max. and min. transmission	1.0000 and 0.9313	
Structure solution technique	direct methods	
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2016/6 (Sheldrick, 2016)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	15744 / 295 / 808	
Goodness-of-fit on F^2	1.096	
Final R indices	15000 data; I>2σ(I)	R1 = 0.0466, wR2 = 0.1464
	all data	R1 = 0.0488, wR2 = 0.1492
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0887P)^2+11.5197P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	2.233 and -1.274 eÅ^{-3}	
R.M.S. deviation from mean	0.165 eÅ^{-3}	

Table S10. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for Er-MOF.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Er1	0.05505(2)	0.11134(2)	0.99630(2)	0.01982(7)
S1	0.24372(10)	0.14790(8)	0.43145(7)	0.0322(2)
S2	0.50979(9)	0.09388(7)	0.41115(6)	0.02583(19)
S3	0.26599(8)	0.53341(6)	0.42392(5)	0.02090(17)
S4	0.53314(8)	0.47745(7)	0.41191(6)	0.02376(19)
O1	0.0531(5)	0.1824(5)	0.0743(3)	0.0732(17)
O2	0.9200(7)	0.2732(7)	0.1171(5)	0.118(3)
O3	0.8053(3)	0.9735(2)	0.07288(16)	0.0292(6)
O4	0.8890(3)	0.0769(3)	0.08192(19)	0.0361(7)
O5	0.0634(3)	0.9079(3)	0.07015(17)	0.0424(9)
O6	0.1608(3)	0.9923(2)	0.09024(19)	0.0400(8)
O7	0.7590(3)	0.8289(2)	0.04364(19)	0.0354(7)
O8	0.9008(3)	0.7699(3)	0.1175(3)	0.0650(16)
O9W	0.8923(6)	0.2539(4)	0.9824(4)	0.0748(15)
C1	0.0238(8)	0.2183(7)	0.1179(6)	0.083(3)
C2	0.0967(7)	0.2005(7)	0.1767(6)	0.084(3)
C3	0.1799(5)	0.1181(5)	0.1948(4)	0.0519(16)
C4	0.2480(5)	0.0917(4)	0.2528(3)	0.0420(12)
C5	0.2371(4)	0.1522(4)	0.2899(3)	0.0393(11)
C6	0.1508(7)	0.2348(6)	0.2724(5)	0.074(2)
C7	0.0804(8)	0.2589(7)	0.2167(6)	0.088(3)
C8	0.3159(4)	0.1303(3)	0.3460(3)	0.0294(8)

	x/a	y/b	z/c	U(eq)
C9	0.4379(4)	0.1033(3)	0.3383(2)	0.0256(8)
C10	0.5256(4)	0.0855(3)	0.2734(2)	0.0241(7)
C11	0.5577(4)	0.9992(3)	0.2656(3)	0.0341(10)
C12	0.6464(4)	0.9829(3)	0.2070(3)	0.0326(9)
C13	0.7060(4)	0.0513(3)	0.1587(2)	0.0258(8)
C14	0.6757(5)	0.1366(3)	0.1675(3)	0.0359(10)
C15	0.5839(5)	0.1544(3)	0.2240(3)	0.0345(10)
C16	0.8085(4)	0.0324(3)	0.0990(2)	0.0271(8)
C17	0.3777(4)	0.1472(3)	0.4591(2)	0.0241(7)
C18	0.3802(4)	0.1879(3)	0.5068(2)	0.0223(7)
C19	0.4950(4)	0.1944(3)	0.5217(2)	0.0224(7)
C20	0.5990(4)	0.1205(3)	0.5348(2)	0.0268(8)
C21	0.7047(4)	0.1317(3)	0.5479(2)	0.0304(9)
C22	0.7085(4)	0.2162(3)	0.5488(2)	0.0296(8)
C23	0.6059(4)	0.2908(3)	0.5362(2)	0.0241(7)
C24	0.4990(3)	0.2807(3)	0.5221(2)	0.0205(7)
C25	0.3888(3)	0.3575(3)	0.5049(2)	0.0192(6)
C26	0.2726(3)	0.3287(3)	0.5374(2)	0.0195(7)
C27	0.2683(4)	0.2411(3)	0.5396(2)	0.0224(7)
C28	0.1620(4)	0.2092(3)	0.5719(3)	0.0293(8)
C29	0.0602(4)	0.2626(3)	0.6020(3)	0.0339(9)
C30	0.0645(4)	0.3490(3)	0.6004(3)	0.0287(8)
C31	0.1698(4)	0.3821(3)	0.5677(2)	0.0226(7)
C32	0.3949(3)	0.4443(2)	0.4564(2)	0.0192(6)
C33	0.3473(3)	0.6012(3)	0.3441(2)	0.0208(7)
C34	0.4702(3)	0.5755(3)	0.3388(2)	0.0216(7)

	x/a	y/b	z/c	U(eq)
C35	0.2780(3)	0.6840(3)	0.2906(2)	0.0205(7)
C36	0.3015(4)	0.7710(3)	0.2725(2)	0.0255(8)
C37	0.2504(4)	0.8465(3)	0.2147(2)	0.0258(8)
C38	0.1739(3)	0.8371(3)	0.1743(2)	0.0228(7)
C39	0.1433(4)	0.7523(3)	0.1954(2)	0.0248(7)
C40	0.1954(3)	0.6757(3)	0.2535(2)	0.0227(7)
C41	0.1294(4)	0.9178(3)	0.1070(2)	0.0303(9)
C42	0.5565(4)	0.6229(3)	0.2789(2)	0.0237(7)
C43	0.5398(4)	0.6543(3)	0.2036(2)	0.0312(9)
C44	0.6182(4)	0.7046(3)	0.1476(3)	0.0340(9)
C45	0.7151(4)	0.7209(3)	0.1665(3)	0.0312(9)
C46	0.7348(4)	0.6868(3)	0.2404(3)	0.0371(11)
C47	0.6558(4)	0.6393(3)	0.2966(3)	0.0318(9)
C48	0.7971(4)	0.7760(3)	0.1057(3)	0.0375(11)
N49	0.9140(7)	0.0471(7)	0.3413(5)	0.046(2)
C50	0.9273(11)	0.0057(7)	0.2836(6)	0.044(3)
C51	0.8365(11)	0.1365(12)	0.3335(9)	0.063(4)
C52	0.9636(12)	0.0070(9)	0.4032(8)	0.059(3)
O53	0.0215(8)	0.9246(8)	0.4229(7)	0.074(3)
N54	0.9578(5)	0.4116(5)	0.3544(4)	0.0242(14)
C55	0.8717(12)	0.3592(10)	0.3857(10)	0.066(4)
C57	0.9700(10)	0.4715(7)	0.2847(7)	0.045(2)
C56	0.0444(10)	0.4055(7)	0.3998(7)	0.046(2)
O58	0.0467(11)	0.5164(7)	0.2597(8)	0.083(3)
N59	0.5172(14)	0.2834(7)	0.0165(5)	0.064(3)
C60	0.4127(13)	0.2453(13)	0.0625(7)	0.068(4)

	x/a	y/b	z/c	U(eq)
C62	0.6067(10)	0.2362(7)	0.9804(5)	0.041(2)
C61	0.547(2)	0.3664(16)	0.0185(14)	0.105(7)
O63	0.5963(9)	0.1647(7)	0.9779(5)	0.057(2)
O10W	0.5333(8)	0.0102(6)	0.9328(5)	0.0106(15)
O11W	0.4332(9)	0.0075(7)	0.9928(6)	0.021(2)
C65B	0.562(3)	0.4645(19)	0.1491(10)	0.066(4)
O68B	0.3903(17)	0.3683(13)	0.3046(9)	0.055(3)
C66B	0.695533	0.382122	0.26015	0.065(4)
C67B	0.47401	0.379886	0.250361	0.053(2)
N64B	0.58719	0.408154	0.223593	0.058(2)
C65A	0.348454	0.380761	0.296206	0.046(3)
C67A	0.5624(18)	0.3417(16)	0.3025(13)	0.051(2)
N64A	0.4727(14)	0.3946(12)	0.2604(9)	0.046(2)
C66A	0.485(3)	0.4532(17)	0.1857(11)	0.054(3)
O68A	0.6586(19)	0.3585(15)	0.2699(13)	0.070(3)
O12W	0.8418(19)	0.4228(11)	0.8762(10)	0.058(4)
O13W	0.921(2)	0.4153(13)	0.9138(13)	0.067(5)

Table S11. Bond lengths (Å) for Er-MOF.

Er1-O1	2.237(4)	Er1-O5	2.262(4)
Er1-O4	2.281(3)	Er1-O3	2.321(3)
Er1-O6	2.328(3)	Er1-O8	2.361(4)
Er1-O9W	2.451(5)	Er1-O7	2.461(3)
Er1-C48	2.761(4)	Er1-H9B	2.4272(2)
S1-C17	1.760(4)	S1-C8	1.772(4)
S2-C9	1.754(4)	S2-C17	1.764(4)

S3-C33	1.760(4)	S3-C32	1.766(4)
S4-C34	1.757(4)	S4-C32	1.761(4)
O1-C1	1.144(9)	O2-C1	1.257(11)
O2-H2	0.84	O3-C16	1.256(6)
O4-C16	1.253(6)	O5-C41	1.251(6)
O6-C41	1.257(6)	O7-C48	1.268(6)
O8-C48	1.246(6)	O9W-H9A	0.969(5)
O9W-H9B	0.905(6)	C1-C2	1.477(9)
C2-C3	1.350(9)	C2-C7	1.392(9)
C3-C4	1.393(8)	C3-H3	0.95
C4-C5	1.391(6)	C4-H4	0.95
C5-C6	1.369(8)	C5-C8	1.467(7)
C6-C7	1.381(9)	C6-H6	0.95
C7-H7	0.95	C8-C9	1.337(6)
C9-C10	1.491(5)	C10-C11	1.384(6)
C10-C15	1.387(6)	C11-C12	1.397(6)
C11-H11	0.95	C12-C13	1.384(6)
C12-H12	0.95	C13-C14	1.379(6)
C13-C16	1.506(5)	C14-C15	1.393(6)
C14-H14	0.95	C15-H15	0.95
C17-C18	1.346(6)	C18-C19	1.472(6)
C18-C27	1.480(5)	C19-C20	1.402(5)
C19-C24	1.408(5)	C20-C21	1.388(6)
C20-H20	0.95	C21-C22	1.382(6)
C21-H21	0.95	C22-C23	1.398(6)
C22-H22	0.95	C23-C24	1.401(5)
C23-H23	0.95	C24-C25	1.478(5)

C25-C32	1.357(5)	C25-C26	1.475(5)
C26-C31	1.397(5)	C26-C27	1.410(5)
C27-C28	1.393(5)	C28-C29	1.388(6)
C28-H28	0.95	C29-C30	1.395(6)
C29-H29	0.95	C30-C31	1.392(6)
C30-H30	0.95	C31-H31	0.95
C33-C34	1.348(5)	C33-C35	1.472(5)
C34-C42	1.470(5)	C35-C40	1.397(5)
C35-C36	1.399(5)	C36-C37	1.381(5)
C36-H36	0.95	C37-C38	1.396(5)
C37-H37	0.95	C38-C39	1.393(6)
C38-C41	1.502(5)	C39-C40	1.395(5)
C39-H39	0.95	C40-H40	0.95
C42-C43	1.399(6)	C42-C47	1.402(5)
C43-C44	1.399(6)	C43-H43	0.95
C44-C45	1.388(6)	C44-H44	0.95
C45-C46	1.380(7)	C45-C48	1.500(6)
C46-C47	1.385(6)	C46-H46	0.95
C47-H47	0.95	N49-C52	1.308(15)
N49-C51	1.416(19)	N49-C50	1.481(16)
C50-H50A	0.98	C50-H50B	0.98
C50-H50C	0.98	C51-H51A	0.98
C51-H51B	0.98	C51-H51C	0.98
C52-O53	1.239(14)	C52-H52	0.95
N54-C57	1.329(14)	N54-C55	1.378(13)
N54-C56	1.452(12)	C55-H55A	0.98
C55-H55B	0.98	C55-H55C	0.98

C57-O58	1.208(13)	C57-H57	0.95
C56-H56A	0.98	C56-H56B	0.98
C56-H56C	0.98	N59-C62	1.321(17)
N59-C60	1.47(2)	N59-C61	1.50(3)
C60-H60A	0.98	C60-H60B	0.98
C60-H60C	0.98	C62-O63	1.215(12)
C62-H62	0.95	C61-H61A	0.98
C61-H61B	0.98	C61-H61C	0.98
O10W-H10A	0.952(8)	O10W-H10B	0.831(9)
O11W-H11B	0.889(12)	O11W-H11A	0.806(10)
C65B-N64B	1.426(17)	C65B-H65A	0.98
C65B-H65B	0.98	C65B-H65C	0.98
O68B-C67B	1.251(14)	C66B-N64B	1.46287(11)
C66B-H66A	0.98	C66B-H66B	0.98
C66B-H66C	0.98	C67B-N64B	1.43305(13)
C67B-H67B	0.95	C65A-N64A	1.486(15)
C65A-H65D	0.98	C65A-H65E	0.98
C65A-H65F	0.98	C67A-O68A	1.197(18)
C67A-N64A	1.342(17)	C67A-H67A	0.95
N64A-C66A	1.395(17)	C66A-H66D	0.98
C66A-H66E	0.98	C66A-H66F	0.98
O12W-H12A	0.86(2)	O12W-H12B	0.854(19)
O13W-H13A	0.91(2)	O13W-H13B	0.99(2)

Table S12. Bond angles (°) for Er-MOF.

O1-Er1-O5	143.51(19)	O1-Er1-O4	78.56(15)
O5-Er1-O4	76.79(12)	O1-Er1-O3	139.32(17)

O5-Er1-O3	76.85(12)	O4-Er1-O3	130.51(12)
O1-Er1-O6	77.3(2)	O5-Er1-O6	125.07(15)
O4-Er1-O6	82.66(13)	O3-Er1-O6	79.37(12)
O1-Er1-O8	97.8(2)	O5-Er1-O8	83.36(16)
O4-Er1-O8	138.15(13)	O3-Er1-O8	78.18(16)
O6-Er1-O8	137.82(12)	O1-Er1-O9W	66.9(2)
O5-Er1-O9W	79.82(18)	O4-Er1-O9W	70.98(18)
O3-Er1-O9W	141.85(17)	O6-Er1-O9W	138.66(18)
O8-Er1-O9W	69.45(19)	O1-Er1-O7	72.80(14)
O5-Er1-O7	131.19(12)	O4-Er1-O7	150.74(12)
O3-Er1-O7	72.50(12)	O6-Er1-O7	85.29(12)
O8-Er1-O7	53.99(12)	O9W-Er1-O7	102.34(17)
O1-Er1-C48	86.26(18)	O5-Er1-C48	106.83(15)
O4-Er1-C48	156.40(15)	O3-Er1-C48	72.13(14)
O6-Er1-C48	111.67(13)	O8-Er1-C48	26.73(14)
O9W-Er1-C48	86.51(18)	O7-Er1-C48	27.33(13)
O1-Er1-H9B	84.90(17)	O5-Er1-H9B	59.76(10)
O4-Er1-H9B	61.72(10)	O3-Er1-H9B	131.50(8)
O6-Er1-H9B	142.76(9)	O8-Er1-H9B	76.44(9)
O9W-Er1-H9B	21.37(15)	O7-Er1-H9B	120.33(8)
C48-Er1-H9B	99.29(9)	C17-S1-C8	95.6(2)
C9-S2-C17	95.9(2)	C33-S3-C32	95.90(17)
C34-S4-C32	96.15(17)	C1-O1-Er1	163.9(6)
C1-O2-H2	109.5	C16-O3-Er1	135.3(3)
C16-O4-Er1	142.3(3)	C41-O5-Er1	179.5(4)
C41-O6-Er1	110.7(3)	C48-O7-Er1	89.7(3)
C48-O8-Er1	94.8(3)	Er1-O9W-H9A	163.7(5)

Er1-O9W-H9B	77.8(3)	H9A-O9W-H9B	103.3(6)
O1-C1-O2	116.9(8)	O1-C1-C2	124.5(8)
O2-C1-C2	118.6(7)	C3-C2-C7	119.0(6)
C3-C2-C1	115.8(6)	C7-C2-C1	125.0(7)
C2-C3-C4	120.6(5)	C2-C3-H3	119.7
C4-C3-H3	119.7	C5-C4-C3	120.4(5)
C5-C4-H4	119.8	C3-C4-H4	119.8
C6-C5-C4	118.5(5)	C6-C5-C8	119.6(4)
C4-C5-C8	121.8(5)	C5-C6-C7	120.4(6)
C5-C6-H6	119.8	C7-C6-H6	119.8
C6-C7-C2	120.8(7)	C6-C7-H7	119.6
C2-C7-H7	119.6	C9-C8-C5	126.9(4)
C9-C8-S1	115.9(3)	C5-C8-S1	117.0(3)
C8-C9-C10	129.4(4)	C8-C9-S2	117.1(3)
C10-C9-S2	113.3(3)	C11-C10-C15	119.6(4)
C11-C10-C9	121.3(4)	C15-C10-C9	118.8(4)
C10-C11-C12	119.9(4)	C10-C11-H11	120.1
C12-C11-H11	120.1	C13-C12-C11	120.3(4)
C13-C12-H12	119.9	C11-C12-H12	119.9
C14-C13-C12	119.8(4)	C14-C13-C16	119.2(4)
C12-C13-C16	120.9(4)	C13-C14-C15	120.1(4)
C13-C14-H14	120.0	C15-C14-H14	120.0
C10-C15-C14	120.3(4)	C10-C15-H15	119.8
C14-C15-H15	119.8	O4-C16-O3	127.3(4)
O4-C16-C13	115.4(4)	O3-C16-C13	117.3(4)
C18-C17-S1	124.6(3)	C18-C17-S2	123.8(3)
S1-C17-S2	111.5(2)	C17-C18-C19	122.5(4)

C17-C18-C27	122.5(4)	C19-C18-C27	114.4(3)
C20-C19-C24	119.0(4)	C20-C19-C18	123.8(4)
C24-C19-C18	117.2(3)	C21-C20-C19	120.8(4)
C21-C20-H20	119.6	C19-C20-H20	119.6
C22-C21-C20	120.2(4)	C22-C21-H21	119.9
C20-C21-H21	119.9	C21-C22-C23	120.1(4)
C21-C22-H22	120.0	C23-C22-H22	120.0
C22-C23-C24	120.3(4)	C22-C23-H23	119.8
C24-C23-H23	119.8	C23-C24-C19	119.6(3)
C23-C24-C25	123.5(3)	C19-C24-C25	116.9(3)
C32-C25-C26	123.0(3)	C32-C25-C24	122.3(3)
C26-C25-C24	114.2(3)	C31-C26-C27	119.2(3)
C31-C26-C25	123.4(3)	C27-C26-C25	117.3(3)
C28-C27-C26	119.6(4)	C28-C27-C18	123.7(4)
C26-C27-C18	116.6(3)	C29-C28-C27	120.8(4)
C29-C28-H28	119.6	C27-C28-H28	119.6
C28-C29-C30	119.7(4)	C28-C29-H29	120.2
C30-C29-H29	120.2	C31-C30-C29	120.1(4)
C31-C30-H30	119.9	C29-C30-H30	119.9
C30-C31-C26	120.5(4)	C30-C31-H31	119.8
C26-C31-H31	119.8	C25-C32-S4	123.6(3)
C25-C32-S3	123.9(3)	S4-C32-S3	112.3(2)
C34-C33-C35	124.5(3)	C34-C33-S3	116.7(3)
C35-C33-S3	118.6(3)	C33-C34-C42	126.4(3)
C33-C34-S4	116.7(3)	C42-C34-S4	116.8(3)
C40-C35-C36	119.5(3)	C40-C35-C33	120.6(3)
C36-C35-C33	119.7(3)	C37-C36-C35	120.1(4)

C37-C36-H36	119.9	C35-C36-H36	119.9
C36-C37-C38	120.4(4)	C36-C37-H37	119.8
C38-C37-H37	119.8	C39-C38-C37	119.7(3)
C39-C38-C41	121.0(4)	C37-C38-C41	119.3(4)
C38-C39-C40	119.9(3)	C38-C39-H39	120.0
C40-C39-H39	120.0	C39-C40-C35	120.0(4)
C39-C40-H40	120.0	C35-C40-H40	120.0
O5-C41-O6	123.1(4)	O5-C41-C38	118.8(4)
O6-C41-C38	118.2(4)	C43-C42-C47	118.8(4)
C43-C42-C34	120.9(4)	C47-C42-C34	120.3(4)
C44-C43-C42	120.2(4)	C44-C43-H43	119.9
C42-C43-H43	119.9	C45-C44-C43	119.9(4)
C45-C44-H44	120.0	C43-C44-H44	120.0
C46-C45-C44	120.0(4)	C46-C45-C48	120.8(4)
C44-C45-C48	119.1(4)	C45-C46-C47	120.6(4)
C45-C46-H46	119.7	C47-C46-H46	119.7
C46-C47-C42	120.4(4)	C46-C47-H47	119.8
C42-C47-H47	119.8	O8-C48-O7	121.2(4)
O8-C48-C45	119.4(4)	O7-C48-C45	119.4(4)
O8-C48-Er1	58.4(2)	O7-C48-Er1	63.0(2)
C45-C48-Er1	173.7(4)	C52-N49-C51	114.0(13)
C52-N49-C50	126.2(11)	C51-N49-C50	119.7(9)
N49-C50-H50A	109.5	N49-C50-H50B	109.5
H50A-C50-H50B	109.5	N49-C50-H50C	109.5
H50A-C50-H50C	109.5	H50B-C50-H50C	109.5
N49-C51-H51A	109.5	N49-C51-H51B	109.5
H51A-C51-H51B	109.5	N49-C51-H51C	109.5

H51A-C51-H51C	109.5	H51B-C51-H51C	109.5
O53-C52-N49	122.0(14)	O53-C52-H52	119.0
N49-C52-H52	119.0	C57-N54-C55	126.5(11)
C57-N54-C56	113.8(9)	C55-N54-C56	119.7(11)
N54-C55-H55A	109.5	N54-C55-H55B	109.5
H55A-C55-H55B	109.5	N54-C55-H55C	109.5
H55A-C55-H55C	109.5	H55B-C55-H55C	109.5
O58-C57-N54	124.3(12)	O58-C57-H57	117.9
N54-C57-H57	117.9	N54-C56-H56A	109.5
N54-C56-H56B	109.5	H56A-C56-H56B	109.5
N54-C56-H56C	109.5	H56A-C56-H56C	109.5
H56B-C56-H56C	109.5	C62-N59-C60	121.5(11)
C62-N59-C61	113.0(15)	C60-N59-C61	124.2(14)
N59-C60-H60A	109.5	N59-C60-H60B	109.5
H60A-C60-H60B	109.5	N59-C60-H60C	109.5
H60A-C60-H60C	109.5	H60B-C60-H60C	109.5
O63-C62-N59	119.6(11)	O63-C62-H62	120.2
N59-C62-H62	120.2	N59-C61-H61A	109.5
N59-C61-H61B	109.5	H61A-C61-H61B	109.5
N59-C61-H61C	109.5	H61A-C61-H61C	109.5
H61B-C61-H61C	109.5	H10A-O10W-H10B	129.6(10)
H11B-O11W-H11A	115.5(12)	N64B-C65B-H65A	109.5
N64B-C65B-H65B	109.5	H65A-C65B-H65B	109.5
N64B-C65B-H65C	109.5	H65A-C65B-H65C	109.5
H65B-C65B-H65C	109.5	N64B-C66B-H66A	109.5
N64B-C66B-H66B	109.5	H66A-C66B-H66B	109.5

N64B-C66B-H66C	109.5	H66A-C66B-H66C	109.5		
H66B-C66B-H66C	109.5	O68B-C67B-N64B	143.5(9)		
O68B-C67B-H67B	108.2	N64B-C67B-H67B	108.2		
C65B-N64B-C67B	97.1(12)	C65B-N64B-C66B	131.9(12)		
C67B-N64B-C66B	130.936(4)	N64A-C65A-H65D	109.5		
N64A-C65A-H65E	109.5	H65D-C65A-H65E	109.5		
N64A-C65A-H65F	109.5	H65D-C65A-H65F	109.5		
H65E-C65A-H65F	109.5	O68A-C67A-N64A	111.(2)		
O68A-C67A-H67A	124.7	N64A-C67A-H67A	124.7		
C67A-N64A-C66A	127.4(19)	C67A-N64A-C65A	115.1(15)		
C66A-N64A-C65A	117.2(17)	N64A-C66A-H66D	109.5		
N64A-C66A-H66E	109.5	H66D-C66A-H66E	109.5		
N64A-C66A-H66F	109.5	H66D-C66A-H66F	109.5		
H66E-C66A-H66F	109.5	H12A-O12W-H12B	108.(2)		
H13A-O13W-H13B	111.(3)				

Table S13. Anisotropic atomic displacement parameters (Å^2) for Er-MOF.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Er1	0.02165(10)	0.02083(10)	0.01591(9)	-0.00433(6)	0.00193(6)	-0.00978(6)
S1	0.0222(4)	0.0417(6)	0.0432(6)	-0.0300(5)	0.0104(4)	-0.0131(4)
S2	0.0229(4)	0.0290(5)	0.0241(4)	-0.0128(4)	0.0021(3)	-0.0034(4)
S3	0.0165(4)	0.0189(4)	0.0226(4)	-0.0008(3)	-0.0042(3)	-0.0050(3)
S4	0.0163(4)	0.0217(4)	0.0258(4)	0.0021(3)	-0.0048(3)	-0.0066(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.084(3)	0.128(5)	0.056(3)	-0.068(3)	0.028(2)	-0.073(3)
O2	0.099(5)	0.151(6)	0.106(5)	-0.059(5)	-0.054(4)	0.017(4)
O3	0.0255(14)	0.0374(16)	0.0205(13)	-0.0111(12)	0.0026(11)	-0.0049(12)
O4	0.0254(15)	0.054(2)	0.0296(16)	-0.0166(15)	0.0088(12)	-0.0164(14)
O5	0.0244(15)	0.072(3)	0.0169(14)	-0.0056(15)	-0.0091(11)	-0.0013(15)
O6	0.0374(18)	0.0324(17)	0.0266(16)	0.0064(13)	-0.0027(13)	0.0003(14)
O7	0.0383(17)	0.0343(16)	0.0297(16)	-0.0018(13)	0.0004(13)	-0.0196(14)
O8	0.0235(16)	0.052(2)	0.072(3)	0.039(2)	-0.0160(17)	-0.0180(16)
O9W	0.078(4)	0.052(3)	0.087(4)	-0.022(3)	-0.018(3)	-0.003(3)
C1	0.064(4)	0.114(6)	0.093(5)	-0.069(5)	-0.037(4)	0.015(4)
C2	0.058(4)	0.110(6)	0.124(7)	-0.099(6)	-0.053(5)	0.034(4)
C3	0.033(2)	0.072(4)	0.081(4)	-0.063(4)	-0.007(3)	-0.007(2)
C4	0.034(2)	0.050(3)	0.060(3)	-0.040(3)	0.001(2)	-0.011(2)
C5	0.024(2)	0.052(3)	0.059(3)	-0.041(3)	-0.006(2)	-0.0029(19)
C6	0.066(4)	0.081(4)	0.103(5)	-0.075(4)	-0.048(4)	0.031(3)
C7	0.087(5)	0.093(5)	0.106(6)	-0.077(5)	-0.060(4)	0.041(4)
C8	0.0244(19)	0.036(2)	0.035(2)	-0.0239(18)	0.0050(16)	-0.0093(16)
C9	0.0232(18)	0.0292(19)	0.0258(19)	-0.0142(16)	0.0035(14)	-0.0072(15)
C10	0.0197(16)	0.0299(19)	0.0229(17)	-0.0122(15)	0.0018(14)	-0.0057(14)
C11	0.035(2)	0.032(2)	0.033(2)	-0.0160(18)	0.0136(18)	-0.0147(18)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C12	0.034(2)	0.031(2)	0.032(2)	-0.0170(18)	0.0087(17)	-0.0080(17)
C13	0.0200(17)	0.036(2)	0.0206(17)	-0.0109(16)	0.0008(14)	-0.0065(15)
C14	0.041(2)	0.033(2)	0.030(2)	-0.0115(18)	0.0116(19)	-0.0161(19)
C15	0.039(2)	0.029(2)	0.034(2)	-0.0139(18)	0.0085(19)	-0.0119(18)
C16	0.0213(17)	0.038(2)	0.0176(17)	-0.0094(16)	0.0014(14)	-0.0040(15)
C17	0.0218(17)	0.0236(17)	0.0261(18)	-0.0112(15)	0.0063(14)	-0.0083(14)
C18	0.0240(17)	0.0174(16)	0.0221(17)	-0.0059(13)	0.0033(14)	-0.0064(13)
C19	0.0248(18)	0.0206(17)	0.0179(16)	-0.0051(13)	0.0013(13)	-0.0056(14)
C20	0.032(2)	0.0202(17)	0.0239(18)	-0.0067(14)	-0.0028(15)	-0.0015(15)
C21	0.031(2)	0.0255(19)	0.029(2)	-0.0089(16)	-0.0095(16)	0.0040(16)
C22	0.0264(19)	0.031(2)	0.028(2)	-0.0066(16)	-0.0102(16)	-0.0023(16)
C23	0.0253(18)	0.0213(17)	0.0228(17)	-0.0047(14)	-0.0060(14)	-0.0034(14)
C24	0.0213(16)	0.0197(16)	0.0168(15)	-0.0037(13)	-0.0015(13)	-0.0042(13)
C25	0.0186(16)	0.0187(16)	0.0197(16)	-0.0057(13)	-0.0024(13)	-0.0049(13)
C26	0.0203(16)	0.0205(16)	0.0162(15)	-0.0046(13)	0.0010(12)	-0.0078(13)
C27	0.0254(18)	0.0210(17)	0.0195(16)	-0.0076(13)	0.0044(14)	-0.0084(14)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C28	0.031(2)	0.0254(19)	0.032(2)	-0.0128(16)	0.0091(16)	-0.0142(16)
C29	0.028(2)	0.034(2)	0.039(2)	-0.0170(19)	0.0125(18)	-0.0154(17)
C30	0.0247(19)	0.029(2)	0.032(2)	-0.0157(17)	0.0072(16)	-0.0084(15)
C31	0.0228(17)	0.0219(17)	0.0220(17)	-0.0077(14)	0.0004(14)	-0.0061(14)
C32	0.0161(15)	0.0188(16)	0.0208(16)	-0.0036(13)	-0.0038(12)	-0.0049(12)
C33	0.0211(16)	0.0198(16)	0.0196(16)	-0.0007(13)	-0.0068(13)	-0.0074(13)
C34	0.0212(17)	0.0201(16)	0.0207(17)	-0.0001(13)	-0.0058(13)	-0.0083(13)
C35	0.0183(15)	0.0221(17)	0.0177(16)	-0.0021(13)	-0.0045(13)	-0.0050(13)
C36	0.0290(19)	0.0222(18)	0.0250(18)	-0.0025(15)	-0.0120(15)	-0.0069(15)
C37	0.0300(19)	0.0221(17)	0.0232(18)	-0.0023(14)	-0.0090(15)	-0.0065(15)
C38	0.0200(16)	0.0273(18)	0.0154(15)	-0.0030(14)	-0.0037(13)	-0.0027(14)
C39	0.0196(16)	0.035(2)	0.0190(17)	-0.0056(15)	-0.0063(13)	-0.0080(15)
C40	0.0197(16)	0.0269(18)	0.0207(17)	-0.0044(14)	-0.0038(13)	-0.0089(14)
C41	0.0222(18)	0.038(2)	0.0163(17)	-0.0011(16)	-0.0024(14)	0.0020(16)
C42	0.0196(16)	0.0233(17)	0.0242(18)	-0.0013(14)	-0.0032(14)	-0.0087(14)
C43	0.030(2)	0.039(2)	0.025(2)	-0.0042(17)	-0.0031(16)	-0.0194(18)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C44	0.033(2)	0.038(2)	0.026(2)	0.0009(17)	-0.0025(17)	-0.0181(19)
C45	0.0222(18)	0.0256(19)	0.033(2)	0.0041(16)	-0.0011(16)	-0.0096(15)
C46	0.026(2)	0.035(2)	0.042(3)	0.0073(19)	-0.0117(18)	-0.0166(18)
C47	0.0268(19)	0.033(2)	0.031(2)	0.0044(17)	-0.0108(16)	-0.0151(17)
C48	0.0222(19)	0.027(2)	0.044(3)	0.0084(18)	-0.0010(18)	-0.0087(16)
N49	0.020(3)	0.068(6)	0.041(4)	0.012(4)	-0.014(3)	-0.030(4)
C50	0.051(6)	0.039(5)	0.042(5)	0.011(4)	-0.026(5)	-0.030(5)
C51	0.029(5)	0.097(11)	0.072(9)	-0.042(8)	0.010(5)	-0.021(6)
C52	0.052(5)	0.070(5)	0.060(5)	-0.011(4)	-0.020(4)	-0.027(4)
O53	0.040(4)	0.087(6)	0.081(6)	0.004(5)	-0.027(4)	-0.028(4)
N54	0.008(2)	0.021(3)	0.048(4)	-0.025(3)	-0.001(2)	0.006(2)
C55	0.037(5)	0.057(6)	0.101(8)	-0.036(6)	0.024(5)	-0.022(5)
C57	0.044(4)	0.037(4)	0.055(4)	-0.024(3)	-0.015(3)	0.004(3)
C56	0.041(5)	0.028(4)	0.075(6)	-0.032(4)	-0.028(5)	0.017(3)
O58	0.090(7)	0.046(5)	0.115(8)	-0.027(5)	0.009(6)	-0.037(5)
N59	0.121(11)	0.039(5)	0.027(4)	-0.003(4)	-0.024(6)	-0.014(6)
C60	0.053(7)	0.114(13)	0.037(6)	-0.039(7)	-0.009(5)	-0.002(8)
C62	0.046(5)	0.052(6)	0.022(4)	-0.005(4)	-0.008(4)	-0.017(5)
C61	0.114(11)	0.090(9)	0.104(10)	-0.038(8)	-0.003(8)	-0.018(8)
O63	0.050(5)	0.061(6)	0.055(5)	-0.012(4)	-0.015(4)	-0.012(4)
O10W	0.006(3)	0.017(3)	0.005(3)	-0.002(2)	0.000(2)	0.000(2)
O11W	0.010(4)	0.023(5)	0.019(5)	0.003(4)	-0.004(4)	0.000(4)
C65B	0.069(5)	0.061(5)	0.066(5)	-0.023(4)	-0.007(5)	-0.012(5)
O68B	0.067(4)	0.049(4)	0.055(4)	-0.027(3)	-0.006(4)	-0.012(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C66B	0.068(5)	0.060(5)	0.065(5)	-0.023(4)	-0.004(4)	-0.015(4)
C67B	0.059(3)	0.049(3)	0.055(3)	-0.024(2)	-0.006(2)	-0.013(2)
N64B	0.063(3)	0.053(3)	0.059(3)	-0.024(2)	-0.005(2)	-0.012(2)
C65A	0.053(5)	0.047(4)	0.051(4)	-0.025(4)	-0.012(4)	-0.014(4)
C67A	0.060(3)	0.049(3)	0.054(3)	-0.026(2)	-0.008(2)	-0.014(2)
N64A	0.058(3)	0.043(3)	0.052(3)	-0.029(2)	-0.008(2)	-0.016(2)
C66A	0.061(4)	0.049(4)	0.055(4)	-0.023(4)	-0.004(4)	-0.015(4)
O68A	0.074(5)	0.062(4)	0.068(4)	-0.024(4)	-0.006(4)	-0.012(4)
O12W	0.081(11)	0.025(6)	0.052(9)	0.004(6)	-0.032(8)	0.000(7)
O13W	0.080(12)	0.048(9)	0.078(11)	-0.034(8)	-0.033(10)	0.010(8)

Table S14. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for Er-MOF.

	x/a	y/b	z/c	U(eq)
H2	-0.1107	0.2792	0.0802	0.177
H9A	-0.1594	0.3156	-0.0374	0.09
H9B	-0.1432	0.2173	-0.0268	0.09
H3	0.1920	0.0779	0.1677	0.062
H4	0.3022	0.0319	0.2672	0.05
H6	0.1394	0.2757	0.2987	0.089
H7	0.0201	0.3159	0.2056	0.106
H11	0.5196	-0.0487	0.3000	0.041
H12	0.6658	-0.0753	0.2004	0.039
H14	0.7174	0.1833	0.1349	0.043
H15	0.5612	0.2140	0.2286	0.041
H20	0.5970	0.0620	0.5347	0.032

	x/a	y/b	z/c	U(eq)
H21	0.7747	0.0811	0.5562	0.037
H22	0.7810	0.2235	0.5580	0.036
H23	0.6087	0.3487	0.5372	0.029
H28	0.1591	0.1503	0.5732	0.035
H29	-0.0120	0.2404	0.6236	0.041
H30	-0.0045	0.3853	0.6216	0.034
H31	0.1716	0.4414	0.5660	0.027
H36	0.3527	0.7781	0.3001	0.031
H37	0.2673	0.9052	0.2023	0.031
H39	0.0870	0.7467	0.1703	0.03
H40	0.1748	0.6178	0.2678	0.027
H43	0.4751	0.6414	0.1905	0.037
H44	0.6050	0.7276	0.0966	0.041
H46	0.8031	0.6960	0.2528	0.044
H47	0.6689	0.6177	0.3474	0.038
H50A	-0.1193	0.0505	0.2429	0.065
H50B	0.0138	-0.0101	0.2635	0.065
H50C	-0.1039	-0.0508	0.3063	0.065
H51A	-0.1972	0.1621	0.2860	0.095
H51B	-0.2304	0.1316	0.3752	0.095
H51C	-0.1165	0.1775	0.3338	0.095
H52	-0.0451	0.0421	0.4341	0.071
H55A	-0.1166	0.3209	0.4379	0.099
H55B	-0.2103	0.4005	0.3842	0.099
H55C	-0.1190	0.3187	0.3573	0.099
H57	-0.0851	0.4796	0.2525	0.054

	x/a	y/b	z/c	U(eq)
H56A	0.0302	0.3604	0.4502	0.069
H56B	0.1278	0.3855	0.3766	0.069
H56C	0.0336	0.4667	0.4031	0.069
H60A	-0.6437	0.2902	0.0846	0.101
H60B	-0.6298	0.2331	0.0311	0.101
H60C	-0.5582	0.1871	0.1026	0.101
H62	-0.3213	0.2580	-0.0434	0.049
H61A	-0.5222	0.3986	0.0458	0.158
H61B	-0.3805	0.3461	0.0438	0.158
H61C	-0.4362	0.4088	-0.0328	0.158
H10A	0.5327	1.0257	-0.1193	0.013
H10B	0.4906	0.9807	-0.0305	0.013
H11B	0.4446	0.9770	-0.0384	0.025
H11A	0.4891	0.9943	0.0158	0.025
H65A	0.6323	0.4912	0.1206	0.099
H65B	0.5486	0.4263	0.1248	0.099
H65C	0.4894	0.5147	0.1506	0.099
H66A	0.6800	0.3420	0.3125	0.097
H66B	0.7651	0.3486	0.2340	0.097
H66C	0.7141	0.4383	0.2585	0.097
H67B	0.4557	0.3641	0.2130	0.063
H65D	0.2891	0.4220	0.2617	0.069
H65E	0.3472	0.3159	0.3081	0.069
H65F	0.3270	0.3953	0.3424	0.069
H67A	0.5511	0.2970	0.3513	0.062
H66D	0.4038	0.4831	0.1695	0.081

	x/a	y/b	z/c	U(eq)
H66E	0.5253	0.5010	0.1806	0.081
H66F	0.5340	0.4168	0.1543	0.081
H12A	-0.0819	0.4221	-0.1340	0.069
H12B	-0.1681	0.3783	-0.1334	0.069
H13A	-0.0819	0.4221	-0.1340	0.08
H13B	0.0001	0.4236	-0.0822	0.08

Table S15. Sample and crystal data for Eu-MOF.

Identification code	Q_0981_Monica_137Eu	
Chemical formula	$C_{54}H_{43.50}EuN_2O_{12.25}S_4$	
Formula weight	1196.61 g/mol	
Temperature	163(2) K	
Wavelength	0.71073 Å	
Crystal size	0.170 x 0.180 x 0.220 mm	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.6915(6) Å	α = 66.8521(13)°
	b = 16.0431(8) Å	β = 76.8187(14)°
	c = 19.7816(10) Å	γ = 71.4086(14)°
Volume	3211.1(3) $Å^3$	
Z	2	
Density (calculated)	1.238 g/cm^3	
Absorption coefficient	1.159 mm^{-1}	
F(000)	1213	

Table S16. Data collection and structure refinement for Eu-MOF.

Theta range for data collection	3.08 to 28.34°	
Index ranges	-15<=h<=15, -21<=k<=21, -26<=l<=26	
Reflections collected	105127	
Independent reflections	15974 [R(int) = 0.0321]	
Max. and min. transmission	1.0000 and 0.9409	
Structure solution technique	direct methods	
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2016/6 (Sheldrick, 2016)	
Function minimized	$\Sigma\ w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	15974 / 381 / 808	
Goodness-of-fit on F^2	1.119	
Final R indices	14485 data; $I>2\sigma(I)$	R1 = 0.0508, wR2 = 0.1518
	all data	R1 = 0.0564, wR2 = 0.1564
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0831P)^2+12.9517P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	2.856 and -1.624 eÅ^{-3}	
R.M.S. deviation from mean	0.165 eÅ^{-3}	

Table S17. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for Eu-MOF.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Eu1	0.04693(2)	0.11614(2)	0.99149(2)	0.01677(7)

	x/a	y/b	z/c	U(eq)
S1	0.24648(10)	0.15303(10)	0.42582(7)	0.0317(3)
S2	0.51078(9)	0.09379(8)	0.40941(6)	0.0250(2)
S3	0.26904(9)	0.54007(7)	0.41877(6)	0.0226(2)
S4	0.53400(9)	0.47934(7)	0.41112(6)	0.0219(2)
O1	0.0394(4)	0.1908(4)	0.0755(3)	0.0529(11)
O2	0.9465(12)	0.3126(9)	0.0981(7)	0.183(4)
O3	0.7990(3)	0.9789(2)	0.07099(18)	0.0299(7)
O4	0.8701(3)	0.0908(3)	0.0743(2)	0.0393(9)
O5	0.0589(3)	0.9266(2)	0.07236(16)	0.0273(6)
O6	0.1701(3)	0.0031(2)	0.08846(19)	0.0336(7)
O7	0.7748(4)	0.8143(3)	0.04954(19)	0.0427(9)
O8	0.8939(4)	0.7794(3)	0.1330(2)	0.0587(14)
O9W	0.8870(6)	0.2637(4)	0.9564(3)	0.0811(19)
C1	0.0257(8)	0.2356(7)	0.1106(6)	0.083(3)
C2	0.0974(7)	0.2102(6)	0.1721(5)	0.070(2)
C3	0.1782(5)	0.1252(4)	0.1916(3)	0.0412(12)
C4	0.2483(5)	0.0980(4)	0.2486(3)	0.0390(11)
C5	0.2386(4)	0.1572(4)	0.2859(3)	0.0356(11)
C6	0.1569(8)	0.2443(6)	0.2652(5)	0.085(3)
C7	0.0912(10)	0.2728(8)	0.2067(6)	0.090(3)
C8	0.3180(4)	0.1333(4)	0.3428(3)	0.0283(9)
C9	0.4394(4)	0.1045(3)	0.3364(2)	0.0265(8)
C10	0.5254(4)	0.0867(3)	0.2724(2)	0.0247(8)
C11	0.5639(5)	0.9992(4)	0.2650(3)	0.0388(12)
C12	0.6500(5)	0.9849(4)	0.2060(3)	0.0371(11)
C13	0.6998(4)	0.0562(3)	0.1564(2)	0.0254(8)

	x/a	y/b	z/c	U(eq)
C14	0.6629(6)	0.1429(4)	0.1642(3)	0.0450(14)
C15	0.5756(6)	0.1585(4)	0.2219(3)	0.0425(13)
C16	0.7983(4)	0.0403(3)	0.0950(3)	0.0272(9)
C17	0.3795(4)	0.1496(3)	0.4551(2)	0.0222(8)
C18	0.3816(4)	0.1908(3)	0.5024(2)	0.0202(7)
C19	0.4952(4)	0.1962(3)	0.5193(2)	0.0199(7)
C20	0.5973(4)	0.1200(3)	0.5345(3)	0.0276(9)
C21	0.7019(4)	0.1295(3)	0.5500(3)	0.0317(10)
C22	0.7046(4)	0.2144(3)	0.5511(3)	0.0297(9)
C23	0.6042(4)	0.2908(3)	0.5355(2)	0.0235(8)
C24	0.4992(4)	0.2828(3)	0.5190(2)	0.0189(7)
C25	0.3902(3)	0.3614(3)	0.5000(2)	0.0179(7)
C26	0.2741(4)	0.3347(3)	0.5302(2)	0.0195(7)
C27	0.2705(4)	0.2465(3)	0.5332(2)	0.0222(8)
C28	0.1649(4)	0.2158(3)	0.5642(3)	0.0302(10)
C29	0.0636(5)	0.2715(4)	0.5924(3)	0.0390(12)
C30	0.0663(4)	0.3583(4)	0.5893(3)	0.0342(10)
C31	0.1710(4)	0.3899(3)	0.5584(2)	0.0242(8)
C32	0.3966(3)	0.4481(3)	0.4525(2)	0.0181(7)
C33	0.3510(4)	0.6083(3)	0.3425(2)	0.0220(8)
C34	0.4717(4)	0.5805(3)	0.3392(2)	0.0210(7)
C35	0.2826(4)	0.6931(3)	0.2892(2)	0.0226(8)
C36	0.3118(4)	0.7781(3)	0.2687(2)	0.0283(9)
C37	0.2605(4)	0.8554(3)	0.2113(2)	0.0277(9)
C38	0.1774(4)	0.8491(3)	0.1741(2)	0.0224(8)
C39	0.1410(4)	0.7668(3)	0.1978(2)	0.0271(9)

	x/a	y/b	z/c	U(eq)
C40	0.1930(4)	0.6886(3)	0.2553(2)	0.0262(8)
C41	0.1327(4)	0.9312(3)	0.1076(2)	0.0239(8)
C42	0.5592(4)	0.6274(3)	0.2820(2)	0.0226(8)
C43	0.5518(5)	0.6497(4)	0.2072(3)	0.0343(11)
C44	0.6283(5)	0.6992(4)	0.1537(3)	0.0377(12)
C45	0.7172(4)	0.7222(3)	0.1738(2)	0.0272(9)
C46	0.7282(4)	0.6963(4)	0.2479(3)	0.0319(10)
C47	0.6494(4)	0.6496(3)	0.3018(2)	0.0300(9)
C48	0.8016(4)	0.7741(3)	0.1152(3)	0.0304(9)
N49	0.9186(12)	0.0347(11)	0.3417(9)	0.077(3)
C50	0.9354(16)	0.9980(13)	0.2892(12)	0.085(4)
C51	0.8465(18)	0.1258(16)	0.3358(13)	0.099(5)
C52	0.9622(15)	0.9975(12)	0.4089(12)	0.081(3)
O53	0.0200(11)	0.9134(10)	0.4266(8)	0.091(3)
N54	0.9508(12)	0.3979(9)	0.3668(7)	0.063(2)
C55	0.9086(15)	0.3398(12)	0.4206(9)	0.069(3)
C57	0.8840(15)	0.4389(11)	0.2978(10)	0.069(3)
C56	0.0500(12)	0.4250(10)	0.3657(9)	0.059(3)
O58	0.9558(16)	0.4860(12)	0.2540(9)	0.133(4)
N59	0.5017(19)	0.2725(16)	0.0128(10)	0.117(4)
C60	0.405(2)	0.2366(18)	0.0565(11)	0.102(5)
C62	0.613(3)	0.2487(19)	0.9706(13)	0.114(4)
C61	0.521(3)	0.349(2)	0.0203(16)	0.136(6)
O63	0.5928(17)	0.1743(15)	0.9736(9)	0.127(5)
O10W	0.5221(15)	0.0205(13)	0.9296(10)	0.048(4)
O11W	0.4303(14)	0.0120(16)	0.9909(12)	0.067(6)

	x/a	y/b	z/c	U(eq)
C65B	0.624(4)	0.455(3)	0.1450(11)	0.119(6)
O68B	0.413(3)	0.367(2)	0.3095(12)	0.101(5)
C66B	0.695533	0.382122	0.26015	0.118(5)
C67B	0.473989	0.379886	0.250361	0.113(5)
N64B	0.58719	0.408154	0.223593	0.114(4)
C65A	0.348454	0.380761	0.296206	0.109(5)
C67A	0.584(2)	0.355(3)	0.276(2)	0.112(5)
N64A	0.4656(18)	0.401(3)	0.2636(18)	0.112(4)
C66A	0.442(4)	0.464(3)	0.1880(17)	0.110(5)
O68A	0.675(3)	0.368(3)	0.2210(19)	0.118(5)
O12W	0.040(2)	0.4845(13)	0.9873(12)	0.064(5)
O13W	0.9736(12)	0.4321(9)	0.8103(9)	0.096(4)

Table S18. Bond lengths (Å) for Eu-MOF.

Eu1-O5	2.352(3)	Eu1-O4	2.365(3)
Eu1-O1	2.374(4)	Eu1-O3	2.411(3)
Eu1-O6	2.430(3)	Eu1-O9W	2.461(5)
Eu1-O8	2.463(4)	Eu1-O7	2.499(3)
Eu1-O5	2.798(3)	Eu1-C48	2.838(4)
Eu1-C41	2.980(4)	Eu1-Eu1	4.0815(4)
Eu1-H9B	2.3535(2)	S1-C17	1.757(4)
S1-C8	1.763(4)	S2-C9	1.753(5)
S2-C17	1.762(4)	S3-C33	1.762(4)
S3-C32	1.768(4)	S4-C32	1.758(4)
S4-C34	1.759(4)	O1-C1	1.135(8)
O2-C1	1.257(13)	O2-H2	0.84

O3-C16	1.246(6)	O4-C16	1.244(6)
O5-C41	1.260(5)	O6-C41	1.253(6)
O7-C48	1.264(6)	O8-C48	1.246(6)
O9W-H9A	0.891(6)	O9W-H9B	0.942(6)
C1-C2	1.486(9)	C2-C3	1.354(9)
C2-C7	1.399(12)	C3-C4	1.393(8)
C3-H3	0.95	C4-C5	1.379(6)
C4-H4	0.95	C5-C6	1.382(9)
C5-C8	1.478(7)	C6-C7	1.379(12)
C6-H6	0.95	C7-H7	0.95
C8-C9	1.338(6)	C9-C10	1.488(6)
C10-C11	1.386(6)	C10-C15	1.389(7)
C11-C12	1.400(6)	C11-H11	0.95
C12-C13	1.375(6)	C12-H12	0.95
C13-C14	1.377(7)	C13-C16	1.513(6)
C14-C15	1.392(7)	C14-H14	0.95
C15-H15	0.95	C17-C18	1.349(6)
C18-C19	1.477(5)	C18-C27	1.478(6)
C19-C20	1.397(6)	C19-C24	1.404(5)
C20-C21	1.392(7)	C20-H20	0.95
C21-C22	1.382(7)	C21-H21	0.95
C22-C23	1.387(6)	C22-H22	0.95
C23-C24	1.394(6)	C23-H23	0.95
C24-C25	1.475(5)	C25-C32	1.353(5)
C25-C26	1.477(5)	C26-C31	1.396(6)
C26-C27	1.407(5)	C27-C28	1.396(6)
C28-C29	1.389(7)	C28-H28	0.95

C29-C30	1.380(7)	C29-H29	0.95
C30-C31	1.392(6)	C30-H30	0.95
C31-H31	0.95	C33-C34	1.332(6)
C33-C35	1.472(5)	C34-C42	1.478(5)
C35-C36	1.392(6)	C35-C40	1.400(6)
C36-C37	1.383(6)	C36-H36	0.95
C37-C38	1.394(6)	C37-H37	0.95
C38-C39	1.388(6)	C38-C41	1.501(6)
C39-C40	1.395(6)	C39-H39	0.95
C40-H40	0.95	C42-C47	1.390(6)
C42-C43	1.396(6)	C43-C44	1.383(6)
C43-H43	0.95	C44-C45	1.387(7)
C44-H44	0.95	C45-C46	1.382(6)
C45-C48	1.501(6)	C46-C47	1.383(6)
C46-H46	0.95	C47-H47	0.95
N49-C50	1.33(3)	N49-C52	1.37(2)
N49-C51	1.41(3)	C50-H50A	0.98
C50-H50B	0.98	C50-H50C	0.98
C51-H51A	0.98	C51-H51B	0.98
C51-H51C	0.98	C52-O53	1.247(15)
C52-H52	0.95	N54-C55	1.23(2)
N54-C56	1.355(19)	N54-C57	1.53(2)
C55-H55A	0.98	C55-H55B	0.98
C55-H55C	0.98	C57-O58	1.259(16)
C57-H57	0.95	C56-H56A	0.98
C56-H56B	0.98	C56-H56C	0.98
N59-C61	1.388(19)	N59-C60	1.394(18)

N59-C62	1.40(3)	C60-H60A	0.98
C60-H60B	0.98	C60-H60C	0.98
C62-O63	1.266(17)	C62-H62	0.95
C61-H61A	0.98	C61-H61B	0.98
C61-H61C	0.98	O10W-H10A	0.920(18)
O10W-H10B	0.888(17)	O11W-H11B	0.91(3)
O11W-H11A	0.847(16)	C65B-N64B	1.467(17)
C65B-H65A	0.98	C65B-H65B	0.98
C65B-H65C	0.98	O68B-C67B	1.200(18)
C66B-N64B	1.46455(5)	C66B-H66A	0.98
C66B-H66B	0.98	C66B-H66C	0.98
C67B-N64B	1.45327(7)	C67B-H67B	0.95
C65A-N64A	1.456(17)	C65A-H65D	0.98
C65A-H65E	0.98	C65A-H65F	0.98
C67A-O68A	1.330(19)	C67A-N64A	1.372(18)
C67A-H67A	0.95	N64A-C66A	1.468(19)
C66A-H66D	0.98	C66A-H66E	0.98
C66A-H66F	0.98	O12W-H12A	0.96(2)
O12W-H12B	0.91(2)	O13W-H13A	1.032(16)
O13W-H13B	1.054(15)		

Table S19. Bond angles (°) for Eu-MOF.

O5-Eu1-O4	76.76(12)	O5-Eu1-O1	148.30(14)
O4-Eu1-O1	76.30(15)	O5-Eu1-O3	74.59(11)
O4-Eu1-O3	132.97(12)	O1-Eu1-O3	136.92(14)
O5-Eu1-O6	123.25(11)	O4-Eu1-O6	89.31(14)
O1-Eu1-O6	72.71(15)	O3-Eu1-O6	76.57(12)

O5-Eu1-O9W	82.18(19)	O4-Eu1-O9W	72.88(18)
O1-Eu1-O9W	74.2(2)	O3-Eu1-O9W	137.05(16)
O6-Eu1-O9W	145.28(18)	O5-Eu1-O8	83.84(14)
O4-Eu1-O8	139.76(14)	O1-Eu1-O8	106.73(19)
O3-Eu1-O8	72.20(16)	O6-Eu1-O8	130.47(13)
O9W-Eu1-O8	69.77(18)	O5-Eu1-O7	131.84(11)
O4-Eu1-O7	149.43(13)	O1-Eu1-O7	73.14(15)
O3-Eu1-O7	73.55(13)	O6-Eu1-O7	82.50(13)
O9W-Eu1-O7	97.7(2)	O8-Eu1-O7	52.41(13)
O5-Eu1-O5	75.51(10)	O4-Eu1-O5	66.52(12)
O1-Eu1-O5	108.16(14)	O3-Eu1-O5	70.66(11)
O6-Eu1-O5	48.99(10)	O9W-Eu1-O5	137.00(17)
O8-Eu1-O5	141.06(16)	O7-Eu1-O5	124.52(12)
O5-Eu1-C48	107.75(13)	O4-Eu1-C48	155.31(14)
O1-Eu1-C48	90.49(16)	O3-Eu1-C48	70.30(13)
O6-Eu1-C48	106.80(13)	O9W-Eu1-C48	83.56(18)
O8-Eu1-C48	25.98(14)	O7-Eu1-C48	26.44(13)
O5-Eu1-C48	138.11(12)	O5-Eu1-C41	100.15(12)
O4-Eu1-C41	75.76(13)	O1-Eu1-C41	89.08(15)
O3-Eu1-C41	73.60(12)	O6-Eu1-C41	24.15(11)
O9W-Eu1-C41	147.10(16)	O8-Eu1-C41	143.07(14)
O7-Eu1-C41	104.32(13)	O5-Eu1-C41	24.94(10)
C48-Eu1-C41	125.51(13)	O5-Eu1-Eu1	41.59(8)
O4-Eu1-Eu1	66.10(9)	O1-Eu1-Eu1	134.75(13)
O3-Eu1-Eu1	67.65(8)	O6-Eu1-Eu1	82.30(8)
O9W-Eu1-Eu1	115.03(18)	O8-Eu1-Eu1	118.12(13)
O7-Eu1-Eu1	140.62(10)	O5-Eu1-Eu1	33.91(6)

C48-Eu1-Eu1	133.33(10)	C41-Eu1-Eu1	58.66(8)
O5-Eu1-H9B	75.22(8)	O4-Eu1-H9B	50.74(10)
O1-Eu1-H9B	74.91(11)	O3-Eu1-H9B	146.50(8)
O6-Eu1-H9B	133.45(9)	O9W-Eu1-H9B	22.43(15)
O8-Eu1-H9B	90.47(11)	O7-Eu1-H9B	118.46(11)
O5-Eu1-H9B	114.88(6)	C48-Eu1-H9B	105.99(10)
C41-Eu1-H9B	126.22(8)	Eu1-Eu1-H9B	98.131(8)
C17-S1-C8	95.8(2)	C9-S2-C17	95.7(2)
C33-S3-C32	96.03(19)	C32-S4-C34	96.24(19)
C1-O1-Eu1	171.5(6)	C1-O2-H2	109.5
C16-O3-Eu1	134.3(3)	C16-O4-Eu1	141.0(3)
C41-O5-Eu1	166.6(3)	C41-O5-Eu1	85.6(3)
Eu1-O5-Eu1	104.50(10)	C41-O6-Eu1	103.4(3)
C48-O7-Eu1	91.9(3)	C48-O8-Eu1	94.0(3)
Eu1-O9W-H9A	128.9(5)	Eu1-O9W-H9B	72.3(3)
H9A-O9W-H9B	99.4(6)	O1-C1-O2	120.2(8)
O1-C1-C2	124.3(7)	O2-C1-C2	115.5(7)
C3-C2-C7	118.8(7)	C3-C2-C1	118.2(6)
C7-C2-C1	122.8(7)	C2-C3-C4	120.7(5)
C2-C3-H3	119.7	C4-C3-H3	119.7
C5-C4-C3	121.1(5)	C5-C4-H4	119.5
C3-C4-H4	119.5	C4-C5-C6	118.0(5)
C4-C5-C8	122.4(5)	C6-C5-C8	119.5(5)
C7-C6-C5	121.0(7)	C7-C6-H6	119.5
C5-C6-H6	119.5	C6-C7-C2	120.1(9)
C6-C7-H7	120.0	C2-C7-H7	120.0
C9-C8-C5	127.1(4)	C9-C8-S1	116.0(3)

C5-C8-S1	116.7(3)	C8-C9-C10	128.8(4)
C8-C9-S2	117.1(3)	C10-C9-S2	113.9(3)
C11-C10-C15	119.2(4)	C11-C10-C9	122.2(4)
C15-C10-C9	118.4(4)	C10-C11-C12	119.9(4)
C10-C11-H11	120.1	C12-C11-H11	120.1
C13-C12-C11	120.5(4)	C13-C12-H12	119.8
C11-C12-H12	119.8	C12-C13-C14	119.8(4)
C12-C13-C16	121.1(4)	C14-C13-C16	119.1(4)
C13-C14-C15	120.3(5)	C13-C14-H14	119.8
C15-C14-H14	119.8	C10-C15-C14	120.3(5)
C10-C15-H15	119.9	C14-C15-H15	119.9
O4-C16-O3	127.5(4)	O4-C16-C13	115.1(4)
O3-C16-C13	117.4(4)	C18-C17-S1	124.4(3)
C18-C17-S2	123.9(3)	S1-C17-S2	111.6(2)
C17-C18-C19	123.1(4)	C17-C18-C27	122.6(4)
C19-C18-C27	113.8(3)	C20-C19-C24	119.5(4)
C20-C19-C18	123.1(4)	C24-C19-C18	117.4(4)
C21-C20-C19	120.4(4)	C21-C20-H20	119.8
C19-C20-H20	119.8	C22-C21-C20	119.9(4)
C22-C21-H21	120.0	C20-C21-H21	120.0
C21-C22-C23	120.2(4)	C21-C22-H22	119.9
C23-C22-H22	119.9	C22-C23-C24	120.6(4)
C22-C23-H23	119.7	C24-C23-H23	119.7
C23-C24-C19	119.3(4)	C23-C24-C25	123.8(4)
C19-C24-C25	116.9(3)	C32-C25-C24	122.4(3)
C32-C25-C26	122.9(4)	C24-C25-C26	114.3(3)
C31-C26-C27	118.9(4)	C31-C26-C25	123.8(4)

C27-C26-C25	117.2(4)	C28-C27-C26	119.7(4)
C28-C27-C18	123.4(4)	C26-C27-C18	116.9(3)
C29-C28-C27	120.5(4)	C29-C28-H28	119.8
C27-C28-H28	119.8	C30-C29-C28	120.1(4)
C30-C29-H29	120.0	C28-C29-H29	120.0
C29-C30-C31	120.1(4)	C29-C30-H30	120.0
C31-C30-H30	120.0	C30-C31-C26	120.8(4)
C30-C31-H31	119.6	C26-C31-H31	119.6
C25-C32-S4	123.7(3)	C25-C32-S3	124.1(3)
S4-C32-S3	112.0(2)	C34-C33-C35	124.8(4)
C34-C33-S3	116.7(3)	C35-C33-S3	118.4(3)
C33-C34-C42	126.6(4)	C33-C34-S4	117.0(3)
C42-C34-S4	116.4(3)	C36-C35-C40	119.2(4)
C36-C35-C33	119.9(4)	C40-C35-C33	120.8(4)
C37-C36-C35	120.6(4)	C37-C36-H36	119.7
C35-C36-H36	119.7	C36-C37-C38	120.1(4)
C36-C37-H37	119.9	C38-C37-H37	119.9
C39-C38-C37	119.6(4)	C39-C38-C41	121.7(4)
C37-C38-C41	118.7(4)	C38-C39-C40	120.4(4)
C38-C39-H39	119.8	C40-C39-H39	119.8
C39-C40-C35	119.8(4)	C39-C40-H40	120.1
C35-C40-H40	120.1	O6-C41-O5	121.6(4)
O6-C41-C38	118.6(4)	O5-C41-C38	119.8(4)
O6-C41-Eu1	52.5(2)	O5-C41-Eu1	69.4(2)
C38-C41-Eu1	169.0(3)	C47-C42-C43	119.3(4)
C47-C42-C34	120.7(4)	C43-C42-C34	120.0(4)
C44-C43-C42	119.8(4)	C44-C43-H43	120.1

C42-C43-H43	120.1	C43-C44-C45	120.5(4)
C43-C44-H44	119.8	C45-C44-H44	119.8
C46-C45-C44	119.6(4)	C46-C45-C48	120.4(4)
C44-C45-C48	120.0(4)	C45-C46-C47	120.4(4)
C45-C46-H46	119.8	C47-C46-H46	119.8
C46-C47-C42	120.3(4)	C46-C47-H47	119.9
C42-C47-H47	119.9	O8-C48-O7	121.6(4)
O8-C48-C45	119.2(4)	O7-C48-C45	119.2(4)
O8-C48-Eu1	60.0(2)	O7-C48-Eu1	61.7(2)
C45-C48-Eu1	175.6(3)	C50-N49-C52	130.5(18)
C50-N49-C51	123.2(18)	C52-N49-C51	106.3(19)
N49-C50-H50A	109.5	N49-C50-H50B	109.5
H50A-C50-H50B	109.5	N49-C50-H50C	109.5
H50A-C50-H50C	109.5	H50B-C50-H50C	109.5
N49-C51-H51A	109.5	N49-C51-H51B	109.5
H51A-C51-H51B	109.5	N49-C51-H51C	109.5
H51A-C51-H51C	109.5	H51B-C51-H51C	109.5
O53-C52-N49	115.2(19)	O53-C52-H52	122.4
N49-C52-H52	122.4	C55-N54-C56	124.2(16)
C55-N54-C57	115.4(15)	C56-N54-C57	120.3(13)
N54-C55-H55A	109.5	N54-C55-H55B	109.5
H55A-C55-H55B	109.5	N54-C55-H55C	109.5
H55A-C55-H55C	109.5	H55B-C55-H55C	109.5
O58-C57-N54	98.2(15)	O58-C57-H57	130.9
N54-C57-H57	130.9	N54-C56-H56A	109.5
N54-C56-H56B	109.5	H56A-C56-H56B	109.5
N54-C56-H56C	109.5	H56A-C56-H56C	109.5

H56B-C56-H56C	109.5	C61-N59-C60	119.(2)
C61-N59-C62	97.(2)	C60-N59-C62	142.(2)
N59-C60-H60A	109.5	N59-C60-H60B	109.5
H60A-C60-H60B	109.5	N59-C60-H60C	109.5
H60A-C60-H60C	109.5	H60B-C60-H60C	109.5
O63-C62-N59	93.(2)	O63-C62-H62	133.7
N59-C62-H62	133.7	N59-C61-H61A	109.5
N59-C61-H61B	109.5	H61A-C61-H61B	109.5
N59-C61-H61C	109.5	H61A-C61-H61C	109.5
H61B-C61-H61C	109.5	H10A-O10W-H10B	130.(2)
H11B-O11W-H11A	110.(2)	N64B-C65B-H65A	109.5
N64B-C65B-H65B	109.5	H65A-C65B-H65B	109.5
N64B-C65B-H65C	109.5	H65A-C65B-H65C	109.5
H65B-C65B-H65C	109.5	N64B-C66B-H66A	109.5
N64B-C66B-H66B	109.5	H66A-C66B-H66B	109.5
N64B-C66B-H66C	109.5	H66A-C66B-H66C	109.5
H66B-C66B-H66C	109.5	O68B-C67B-N64B	131.2(15)
O68B-C67B-H67B	114.4	N64B-C67B-H67B	114.4
C67B-N64B-C66B	130.853(3)	C67B-N64B-C65B	123.0(15)
C66B-N64B-C65B	104.9(15)	N64A-C65A-H65D	109.5
N64A-C65A-H65E	109.5	H65D-C65A-H65E	109.5
N64A-C65A-H65F	109.5	H65D-C65A-H65F	109.5
H65E-C65A-H65F	109.5	O68A-C67A-N64A	121.(3)
O68A-C67A-H67A	119.3	N64A-C67A-H67A	119.3
C67A-N64A-C65A	135.(3)	C67A-N64A-C66A	117.(2)
C65A-N64A-C66A	102.(2)	N64A-C66A-H66D	109.5

N64A-C66A-H66E	109.5	H66D-C66A-H66E	109.5
N64A-C66A-H66F	109.5	H66D-C66A-H66F	109.5
H66E-C66A-H66F	109.5	H12A-O12W-H12B	125.(2)
H13A-O13W-H13B	119.1(15)		

Table S20. Anisotropic atomic displacement parameters (Å^2) for Eu-MOF.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Eu1	0.01788(10)	0.01817(11)	0.01358(10)	-0.00333(7)	-0.00135(7)	-0.00687(7)
S1	0.0210(5)	0.0520(7)	0.0369(6)	-0.0327(6)	0.0069(4)	-0.0140(5)
S2	0.0219(5)	0.0321(5)	0.0249(5)	-0.0165(4)	0.0021(4)	-0.0073(4)
S3	0.0162(4)	0.0229(5)	0.0230(5)	-0.0007(4)	-0.0045(3)	-0.0054(3)
S4	0.0165(4)	0.0213(4)	0.0228(5)	0.0006(4)	-0.0043(3)	-0.0073(3)
O1	0.053(2)	0.076(3)	0.055(3)	-0.050(2)	-0.007(2)	-0.012(2)
O2	0.208(8)	0.189(7)	0.193(7)	-0.108(6)	-0.121(6)	0.016(6)
O3	0.0250(15)	0.0411(18)	0.0305(16)	-0.0219(14)	0.0067(12)	-0.0125(13)
O4	0.0328(18)	0.044(2)	0.049(2)	-0.0282(18)	0.0215(16)	-0.0221(16)
O5	0.0241(15)	0.0403(18)	0.0174(13)	-0.0046(12)	-0.0084(11)	-0.0108(13)
O6	0.047(2)	0.0273(16)	0.0278(16)	-0.0005(13)	-0.0190(15)	-0.0119(14)
O7	0.063(3)	0.056(2)	0.0220(16)	-0.0060(16)	0.0001(16)	-0.045(2)
O8	0.034(2)	0.071(3)	0.044(2)	0.030(2)	-0.0162(17)	-0.033(2)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O9W	0.088(4)	0.043(3)	0.068(3)	-0.004(2)	-0.008(3)	0.022(3)
C1	0.079(5)	0.089(5)	0.101(6)	-0.068(5)	-0.055(4)	0.029(4)
C2	0.058(4)	0.079(5)	0.097(6)	-0.072(5)	-0.046(4)	0.027(4)
C3	0.043(3)	0.049(3)	0.048(3)	-0.034(3)	-0.009(2)	-0.009(2)
C4	0.043(3)	0.037(3)	0.047(3)	-0.028(2)	-0.010(2)	-0.002(2)
C5	0.028(2)	0.049(3)	0.043(3)	-0.033(2)	-0.006(2)	-0.004(2)
C6	0.090(5)	0.085(5)	0.109(6)	-0.081(5)	-0.056(4)	0.028(4)
C7	0.094(3)	0.090(3)	0.091(3)	-0.039(2)	-0.0183(19)	-0.0153(19)
C8	0.024(2)	0.041(2)	0.029(2)	-0.025(2)	0.0024(17)	-0.0085(18)
C9	0.025(2)	0.033(2)	0.026(2)	-0.0162(18)	0.0038(16)	-0.0104(17)
C10	0.0235(19)	0.032(2)	0.0220(19)	-0.0154(17)	0.0036(15)	-0.0081(16)
C11	0.045(3)	0.033(2)	0.039(3)	-0.020(2)	0.021(2)	-0.020(2)
C12	0.041(3)	0.030(2)	0.041(3)	-0.021(2)	0.018(2)	-0.015(2)
C13	0.0221(19)	0.033(2)	0.024(2)	-0.0154(17)	0.0047(15)	-0.0092(16)
C14	0.062(4)	0.035(3)	0.034(3)	-0.017(2)	0.022(3)	-0.021(3)
C15	0.057(3)	0.030(2)	0.037(3)	-0.020(2)	0.016(2)	-0.012(2)
C16	0.0219(19)	0.030(2)	0.027(2)	-0.0124(18)	0.0049(16)	-0.0060(16)
C17	0.0208(18)	0.0254(19)	0.0237(19)	-0.0125(16)	0.0042(15)	-0.0099(15)
C18	0.0221(18)	0.0208(18)	0.0198(18)	-0.0083(15)	0.0030(14)	-0.0102(15)
C19	0.0218(18)	0.0233(19)	0.0151(16)	-0.0055(14)	0.0006(14)	-0.0097(15)
C20	0.032(2)	0.0218(19)	0.029(2)	-0.0084(17)	-0.0047(17)	-0.0059(17)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C21	0.032(2)	0.025(2)	0.036(2)	-0.0088(18)	-0.0116(19)	-0.0010(17)
C22	0.029(2)	0.029(2)	0.030(2)	-0.0057(18)	-0.0116(18)	-0.0052(17)
C23	0.026(2)	0.0223(19)	0.0235(19)	-0.0064(15)	-0.0060(15)	-0.0073(16)
C24	0.0215(18)	0.0206(18)	0.0152(16)	-0.0055(14)	-0.0017(13)	-0.0074(14)
C25	0.0179(17)	0.0198(17)	0.0177(17)	-0.0065(14)	-0.0025(13)	-0.0068(14)
C26	0.0204(18)	0.0238(18)	0.0170(17)	-0.0073(14)	0.0000(14)	-0.0102(15)
C27	0.0243(19)	0.027(2)	0.0194(18)	-0.0119(16)	0.0043(15)	-0.0127(16)
C28	0.031(2)	0.033(2)	0.035(2)	-0.0186(19)	0.0103(18)	-0.0188(19)
C29	0.029(2)	0.053(3)	0.047(3)	-0.031(3)	0.017(2)	-0.025(2)
C30	0.025(2)	0.044(3)	0.043(3)	-0.028(2)	0.0098(19)	-0.014(2)
C31	0.024(2)	0.026(2)	0.026(2)	-0.0131(17)	0.0014(16)	-0.0087(16)
C32	0.0143(16)	0.0214(18)	0.0187(17)	-0.0061(14)	-0.0031(13)	-0.0053(14)
C33	0.0252(19)	0.0201(18)	0.0175(17)	0.0014(14)	-0.0068(15)	-0.0087(15)
C34	0.0233(19)	0.0212(18)	0.0157(17)	0.0001(14)	-0.0047(14)	-0.0086(15)
C35	0.0214(18)	0.0246(19)	0.0180(18)	-0.0019(15)	-0.0067(14)	-0.0049(15)
C36	0.035(2)	0.026(2)	0.027(2)	-0.0051(17)	-0.0174(18)	-0.0082(18)
C37	0.036(2)	0.0222(19)	0.027(2)	-0.0048(17)	-0.0166(18)	-0.0062(17)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C38	0.0218(18)	0.0255(19)	0.0186(18)	-0.0053(15)	-0.0075(14)	-0.0041(15)
C39	0.025(2)	0.034(2)	0.0206(19)	-0.0009(17)	-0.0089(16)	-0.0125(17)
C40	0.026(2)	0.029(2)	0.0223(19)	-0.0014(16)	-0.0061(16)	-0.0127(17)
C41	0.0236(19)	0.028(2)	0.0177(18)	-0.0062(16)	-0.0071(15)	-0.0022(16)
C42	0.0223(19)	0.0224(19)	0.0196(18)	-0.0016(15)	-0.0027(15)	-0.0082(15)
C43	0.042(3)	0.049(3)	0.021(2)	-0.0064(19)	-0.0012(18)	-0.032(2)
C44	0.051(3)	0.050(3)	0.020(2)	-0.004(2)	-0.001(2)	-0.034(3)
C45	0.028(2)	0.024(2)	0.025(2)	-0.0014(16)	-0.0008(16)	-0.0122(17)
C46	0.029(2)	0.038(2)	0.027(2)	0.0014(19)	-0.0084(18)	-0.0199(19)
C47	0.030(2)	0.039(2)	0.0201(19)	0.0008(18)	-0.0080(16)	-0.0177(19)
C48	0.031(2)	0.025(2)	0.029(2)	-0.0003(17)	0.0002(18)	-0.0132(18)
N49	0.049(4)	0.085(5)	0.094(5)	-0.010(4)	-0.011(4)	-0.037(4)
C50	0.063(6)	0.075(7)	0.108(8)	-0.004(7)	-0.008(7)	-0.042(6)
C51	0.061(7)	0.097(8)	0.111(8)	-0.013(7)	0.002(7)	-0.023(6)
C52	0.062(4)	0.086(4)	0.093(5)	-0.017(3)	-0.012(3)	-0.034(3)
O53	0.056(5)	0.099(6)	0.109(6)	-0.007(5)	-0.027(4)	-0.031(4)
N54	0.058(4)	0.058(4)	0.075(4)	-0.044(3)	0.005(3)	0.001(3)
C55	0.066(6)	0.066(6)	0.068(6)	-0.036(5)	0.013(5)	-0.006(5)
C57	0.064(4)	0.064(4)	0.077(4)	-0.036(3)	0.001(3)	-0.004(3)
C56	0.048(5)	0.056(5)	0.095(6)	-0.063(4)	-0.006(5)	0.001(4)
O58	0.121(6)	0.102(6)	0.131(7)	-0.034(5)	0.007(6)	0.007(5)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N59	0.112(7)	0.153(9)	0.075(5)	-0.035(6)	-0.029(5)	-0.012(7)
C60	0.096(9)	0.152(11)	0.060(7)	-0.039(8)	-0.018(7)	-0.024(9)
C62	0.109(7)	0.153(9)	0.072(6)	-0.037(7)	-0.032(5)	-0.011(7)
C61	0.132(8)	0.149(9)	0.104(7)	-0.032(7)	-0.022(6)	-0.017(7)
O63	0.110(8)	0.162(10)	0.077(6)	-0.028(7)	-0.024(6)	-0.002(8)
O10W	0.043(5)	0.054(5)	0.046(5)	-0.015(4)	-0.002(3)	-0.015(4)
O11W	0.017(6)	0.090(12)	0.068(11)	0.007(9)	-0.019(7)	-0.014(7)
C65B	0.124(7)	0.115(7)	0.121(7)	-0.046(5)	-0.016(5)	-0.027(5)
O68B	0.117(6)	0.101(6)	0.105(6)	-0.053(4)	-0.012(4)	-0.032(4)
C66B	0.122(6)	0.115(6)	0.119(6)	-0.044(4)	-0.015(4)	-0.028(4)
C67B	0.118(5)	0.111(5)	0.115(5)	-0.045(3)	-0.013(2)	-0.029(3)
N64B	0.118(5)	0.111(5)	0.116(5)	-0.044(3)	-0.013(2)	-0.029(2)
C65A	0.117(6)	0.107(6)	0.111(6)	-0.047(4)	-0.011(4)	-0.029(4)
C67A	0.118(5)	0.110(5)	0.115(5)	-0.045(3)	-0.014(2)	-0.030(2)
N64A	0.118(5)	0.110(5)	0.115(5)	-0.046(3)	-0.013(2)	-0.030(3)
C66A	0.120(6)	0.108(6)	0.113(6)	-0.047(4)	-0.015(4)	-0.032(4)
O68A	0.124(6)	0.113(6)	0.121(6)	-0.046(4)	-0.015(4)	-0.029(4)
O12W	0.099(15)	0.037(9)	0.057(11)	-0.018(7)	-0.012(10)	-0.014(9)
O13W	0.078(8)	0.068(7)	0.113(10)	-0.012(7)	-0.050(7)	0.019(6)

Table S21. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for Eu-MOF.

	x/a	y/b	z/c	U(eq)
H2	-0.0892	0.3219	0.0624	0.274
H9A	-0.1395	0.3078	-0.0229	0.097
H9B	-0.1495	0.2174	-0.0076	0.097

	x/a	y/b	z/c	U(eq)
H3	0.1872	0.0837	0.1662	0.049
H4	0.3038	0.0377	0.2620	0.047
H6	0.1458	0.2851	0.2916	0.101
H7	0.0416	0.3351	0.1900	0.108
H11	0.5319	-0.0509	0.3000	0.047
H12	0.6743	-0.0745	0.2000	0.045
H14	0.6972	0.1922	0.1300	0.054
H15	0.5502	0.2186	0.2266	0.051
H20	0.5953	0.0614	0.5342	0.033
H21	0.7713	0.0776	0.5598	0.038
H22	0.7754	0.2206	0.5626	0.036
H23	0.6070	0.3491	0.5360	0.028
H28	0.1623	0.1563	0.5660	0.036
H29	-0.0077	0.2499	0.6137	0.047
H30	-0.0032	0.3965	0.6084	0.041
H31	0.1722	0.4497	0.5564	0.029
H36	0.3675	0.7831	0.2943	0.034
H37	0.2819	0.9128	0.1973	0.033
H39	0.0804	0.7637	0.1747	0.033
H40	0.1676	0.6324	0.2715	0.031
H43	0.4944	0.6308	0.1930	0.041
H44	0.6199	0.7177	0.1028	0.045
H46	0.7901	0.7107	0.2618	0.038
H47	0.6571	0.6325	0.3526	0.036
H50A	-0.1091	0.0439	0.2478	0.128
H50B	0.0222	-0.0183	0.2717	0.128

	x/a	y/b	z/c	U(eq)
H50C	-0.0946	-0.0586	0.3095	0.128
H51A	-0.1531	0.1382	0.3804	0.148
H51B	-0.1206	0.1716	0.2923	0.148
H51C	-0.2370	0.1308	0.3304	0.148
H52	-0.0507	0.0331	0.4398	0.097
H55A	-0.1629	0.3318	0.4083	0.104
H55B	-0.0299	0.2797	0.4335	0.104
H55C	-0.1150	0.3618	0.4628	0.104
H57	-0.1889	0.4311	0.2905	0.083
H56A	0.0662	0.4716	0.3171	0.088
H56B	0.0353	0.4524	0.4042	0.088
H56C	0.1204	0.3703	0.3749	0.088
H60A	-0.5972	0.1828	0.0452	0.153
H60B	-0.5852	0.2165	0.1089	0.153
H60C	-0.6716	0.2852	0.0462	0.153
H62	-0.3216	0.2774	-0.0516	0.137
H61A	-0.4086	0.3667	-0.0137	0.203
H61B	-0.5513	0.4023	0.0085	0.203
H61C	-0.4650	0.3336	0.0713	0.203
H10A	0.5327	1.0257	-0.1193	0.058
H10B	0.4906	0.9807	-0.0305	0.058
H11B	0.4446	0.9770	-0.0384	0.08
H11A	0.4891	0.9943	0.0158	0.08
H65A	0.7032	0.4675	0.1393	0.178
H65B	0.6311	0.4139	0.1174	0.178
H65C	0.5636	0.5138	0.1256	0.178

	x/a	y/b	z/c	U(eq)
H66A	0.7557	0.4143	0.2259	0.177
H66B	0.6732	0.4005	0.3041	0.177
H66C	0.7301	0.3141	0.2750	0.177
H67B	0.4426	0.3695	0.2149	0.136
H65D	0.2836	0.4331	0.2714	0.163
H65E	0.3467	0.3234	0.2902	0.163
H65F	0.3361	0.3719	0.3490	0.163
H67A	0.6020	0.3138	0.3239	0.134
H66D	0.3547	0.4926	0.1868	0.165
H66E	0.4846	0.5138	0.1723	0.165
H66F	0.4716	0.4284	0.1544	0.165
H12A	0.1061	0.4717	0.0144	0.077
H12B	-0.0398	0.5022	0.0032	0.077
H13A	-0.1033	0.4216	-0.1530	0.115
H13B	0.0313	0.4638	-0.1798	0.115