Supplemental Table 1. Summary of Zn^{2+} EXAFS fitting analysis for all M3M4 samples using single-scattering model. Data fit over a k range of 1 to 13.5 $Å^{-1}$. Best fit simulation parameters are partitioned between independent ligand scattering environments in the nearest neighbor and long range interactions.

Sample	Fit[b]	Nearest-Neighbor Ligand Environment[a]				Long-Range Ligand Environment[a]				F'[g]
		Atom[c]	R(Å)[d]	C.N.[e]	σ^{2}[f]	Atom[c]	R(Å)[d]	C.N.[e]	σ^{2}[f]	
Wild-type + 0.5 Zn^{2+}	1	O/N	2.01	2.5	5.4					1.55
	2	O/N	1.99	2.5	5.4					0.525
		S	2.28	1.5	5.1					
	3	O/N	1.99	2.5	4.9	C	3.04	4.5	6.2	0.12
		S	2.28	1.5	5.2	C	3.26	5.0	5.7	
						C	3.46	5.5	3.7	
						C	3.75	7.0	5.0	
						C	4.00	11.0	4.7	
Wild-type + 1 Zn^{2+}	1	O/N	2.01	3.0	4.6					1.90
	2	O/N	1.99	3.0	4.0					1.41
		S	2.28	1.0	4.3					
	3	O/N	1.99	3.0	5.1	C	3.06	5.0	4.0	0.71
		S	2.27	1.0	5.2	C	3.28	6.5	4.5	
						C	3.46	5.0	4.6	
						C	3.99	3.5	4.9	
						C	4.43	4.0	1.3	
						C	4.62	4.0	1.8	
Wild-type + 2 Zn^{2+}	1	O/N	1.99	3.5	4.8					0.54
	2	O/N	1.99	3.5	4.8	C	3.02	1.0	0.3	0.41
	3	O/N	1.99	3.5	4.8	C	3.02	1.0	3.8	0.23
						C	3.41	12.0	4.1	
						C	3.71	4.0	4.1	
						C	3.94	2.5	3.8	
						C	4.10	7.5	4.7	
C436A/ H438A/ H441A	1	O/N	1.98	4.0	4.6					0.84
	2	O/N	1.98	4.0	4.7	C	3.01	2.5	5.1	0.73
	3	O/N	1.98	4.0	4.7	C	3.01	2.5	4.8	0.33
						C	3.76	6.0	1.3	
						C	3.91	6.0	0.3	
						C	4.03	8.0	0.2	
H443A/ H446A/ H448A	1	O/N	2.01	3.0	5.3					1.62
	2	O/N	1.99	3.0	4.8					0.71
		S	2.28	1.5	5.0					
	3	O/N	1.98	3.0	5.0	C	3.06	2.5	3.3	0.19
		S	2.27	1.5	5.3	C	3.34	5.0	1.3	
						C	3.90	6.0	1.1	
						C	4.06	2.0	2.1	

[a] Independent metal-ligand scattering environments at R < 3.0 Å
[b] Independent metal-ligand scattering environments at R > 3.0 Å
[c] Scattering atoms: S (Sulfur), C (carbon), O (oxygen), N (nitrogen)
[d] Average metal-ligand bond length
[e] Average metal-ligand coordination number
[f] Average Debye-Waller factor in $Å^2 \times 10^3$
[g] Number of degrees of freedom weighted mean square deviation between data and fit