Supporting Information for:

The cation diffusion facilitator protein MamM's cytoplasmic domain exhibits metal-type dependent binding modes and discriminates against Mn^{2+}

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List of the material included:

Table S1: Crystallization of MamM CTD with different metals.

Protein name	**MamM CTD Cu^{2+}-bound**	**MamM CTD Cd^{2+}-bound**	**MamM CTD Ni^{2+}-bound**
PDB ID	6GP6	6GMT	6GMV
Crystallization conditions	0.2 M NaCl, 0.1 M TRIS pH 8.7, 25% PEG 3350	0.2 M Li_2SO_4, 0.1 M BIS-TRIS pH 5.7, 25% PEG 3350	0.2 M $(NH_4)_2SO_4$, 0.1 M BIS-TRIS pH 5.5, 25% PEG 3350
Cryo protectant	50% PEG 3350	-	-
Protein concentration (mg mL^{-1})	10	10	10
Crystallization type	Vapor diffusion (sitting drop)		
Data collection	ESRF – ID30A3	ESRF – ID30A3	ESRF – ID23-1
Detector	Eiger X 4M	Eiger X 4M	Pilatus 6M

Table S2: Data collection and refinement statistics of MamM CTD with different metals.

Protein name	**MamM CTD Cu^{2+}-bound** [a]	**MamM CTD Cd^{2+}-bound**	**MamM CTD Ni^{2+}-bound**
PDB ID	6GP6	6GMT	6GMV
Data collection	ESRF – ID30A3	ESRF – ID30A3	ESRF – ID23-1
Space group	P 2 2_1 2_1	C 2 2 2_1	C 2 2 2_1
Cell dimensions			
a, b, c (Å)	28.93, 73.75, 89.41	36.53, 94.25, 53.32	37.34, 94.48, 53.69
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 90, 90
Resolution (Å)	2.14-44.71 (2.14-2.20) [b]	1.59-47.12 (1.59-1.61)	1.59-47.24 (1.59-1.62)
Rsym or Rmerge	0.106 (1.863)	0.027 (1.046)	0.059 (2.376)
I/σI	8.5 (1.0)	20.6 (1.2)	24.3 (1.4)
$CC_{1/2}$	0.996 (0.436)	1.000 (0.445)	1.000 (0.769)
Completeness (%)	99.6 (96.9)	98.2 (97.9)	99.9 (97.4)
Redundancy	5.8 (5.8)	3.9 (4.0)	19.4 (19.1)
Wavelength (Å)	0.96771	0.96771	0.977999
No. unique reflections	11127 (864)	12566 (597)	13052 (616)
Refinement			
Resolution (Å)	2.15-44.71 (2.15-2.46)	1.59-47.12 (1.59-1.63)	1.59-47.24 (1.59-1.64)
Rwork/Rfree	22.01/27.51 (25.6/34.5)	18.68/23.93 (40.0/39.9)	18.82/22.18 (33.9/38.5)
No. atoms			
Protein	A-796, B-714	637	664
Ligand/ion	7	16	15
Water	21	53	64
B-factors			
Protein	A-40.12, B-47.18	34.95	35.94
Ligand/ion	Cu^{2+}-76.95, βME-50.81	Cd^{2+}-43.55, SO_4-38.82, βME-60.39	Ni^{2+}-68.24, SO_4-38.59, βME-73.73
Water	41.44	42.77	44.10
RMSD			

Bond lengths (Å)	0.009	0.028	0.031
Bond angles (°)	1.076	2.620	2.595
Ramachandran statistics [c]	P: 181 (97.31%), A: 2 (1.08%), O: 3 (1.61%)	P: 76 (98.70%), A: 1 (1.30%), O: 0 (0%)	P: 71 (98.61%), A: 1 (1.39%), O: 0 (0%)
Missing residues	A: 211, 315-318 B: 302-318	211-212, 293-318	211, 293-318

Values in parentheses are for the highest resolution shell.

One crystal was used per dataset.

Datasets were collected at 100K.

[a] Collection statistics are given after the Aimless scaling; data were further processed with UCLA-DOE-LAB Diffraction Anisotropy Server (http://services.int.mbi.ucla.edu/anisoscale/).

[b] Best resolution is given for b axis (best resolution is 2.3 Å and 2.6 Å for a and c axes, respectively, after anisotropic data reduction).

[c] P- Preferred region, A- Allowed region, and O- outliers.

Table S3: Crystallographic software used for structure solution of MamM CTD with different metals.

Protein name	**MamM CTD Cu^{2+}-bound** [a]	**MamM CTD Cd^{2+}-bound**	**MamM CTD Ni^{2+}-bound**
PDB ID	6GP6	6GMT	6GMV
Data reduction	XDS (37)		
Data scaling	Aimless (38) [a]	Aimless	Aimless
Structure solution method	Molecular replacement – using MamM CTD wildtype structure (PDB ID: 3W5X)		
Phasing	Phaser MR (39)		
Refinement	Phenix (40)	Refmac5 (41)	Refmac5

Manual refinement was performed using Coot version 0.8.9 (42).

Aimless, Phaser MR and Refmac5 were used through the CCP4i package (43).

[a] After Aimless scaling, data were further processed with UCLA-DOE-LAB Diffraction Anisotropy Server.

Table S4: Dihedral angles and distances between selected residues in all CDFs' CTD structures.

	Distance (Å)			Dihedral angle (°)	
Protein form	R240-R240	G276-G276	V242-V242	R240-P256-P256-R240	V242-V260-V260-V242
MamM apo (3W5X)	25.78	45.40	30.03	48.759	-47.116
MamM apo (3W5Y)	22.86	44.31	27.34	43.240	-41.640
MamM Cu^{2+}-bound (6GP6)	21.47	39.57	19.39	28.533	-34.863
MamM Cd^{2+}-bound (6GMT)	26.18	45.11	29.23	48.110	-48.105
MamM Ni^{2+}-bound (6GMV)	26.34	45.51	30.01	50.176	-47.742
	R234-R234	Q270-Q270	A236-A236	R234-G250-G250-R234	A236-V254-V254-A236
CzrB apo (3BYP)	28.13	45.54	30.96	51.849	-51.592
CzrB bound (3BYR)	12.22	37.60	13.16	21.354	-14.796
	R237-R237	R273-R273	S239-S239	R237-D253-D253-R237	S239-L257-L257-S239
EcYiiP bound (3H90)	14.26	36.86	13.89	23.880	-16.838
	R239-R239	A275-A275	A241-A241	R239-G255-G255-R239	A241-L259-L259-A241
SoYiiP bound (5VRF)	15.28	39.11	15.19	23.801	-17.963
	R238-R238	A274-A274	V240-V240	R238-A254-A254-R238	V240-V258-V258-V240
MamB apo (5HO5)	19.44	39.79	17.10	28.135	-30.799
MamB bound (5HO1)	19.10	38.93	18.25	26.612	-32.822

All distances and dihedral angles were measured between the residues' C_α from both monomers, using UCSF Chimera package, version 1.12 (34).

All the residues in each column are found in the same location in all the proteins.