Electronic Supplementary Information for Dalton Transactions

SUPPLEMENTARY MATERIAL

Table S1 Refinement and quality of refined models. The Ramachandran analysis[1] was determined by Rampage[2].

	E498D	**E498T**	**E498L**
No. of protein atoms	4122	4119	4150
No. of solvent atoms	495	518	645
No. of hetero atoms	4	4	4
Final R-factor	0.177	0.177	0.175
Final free R-factor	0.206	0.215	0.194
Mean B values (Å^2)			
: protein	26.04	24.25	17.65
: solvent	36.91	32.94	30.69
: overall	27.25	25.26	19.47
Estimated overall coordinate uncertainty (Å) ‡	0.088	0.089	0.049
Distance deviations †			
Bond distances (Å)	0.007	0.009	0.007
Bond angles (^{o})	1.036	1.145	1.064
Planar groups (Å)	0.003	0.004	0.003
Chiral volume deviation (Å^3)	0.068	0.077	0.071
Quality of Models*			
Ramachandran analysis %			
Favourable	97.2	97.8	97.2
Allowed	2.8	2.2	2.8
Disallowed	0.0	0.0	0.0

‡ based on maximum likelihood.
† rms deviations from standard values

1 C. Ramakrishnan and G.N. Ramachan, *Biophys. J.,* 1965, **5**, 909-933.
2 S.C. Lovell, I.W. Davis, W.B. Adrendall, de P.I.W. Bakker, J.M. Word, M.G. Prisant, J.S. Richardson, and D.C. Richardson, *Proteins-Structure Function and Genetics.*, 2003, **50**, 437-450.

Table S2 Copper content, molar absorptivity, and reduction potentials for CotA proteins

CotA	Copper content	E^o	$\varepsilon_{330\ nm}$	$\varepsilon_{330\ nm}$	$\varepsilon_{609\ nm}$	$\varepsilon_{609\ nm}$
	g atoms Cu/mol CotA	*mV*	as-isolated $mM^{-1}.cm^{-1}$	oxidized $mM^{-1}.cm^{-1}$	as isolated $mM^{-1}.cm^{-1}$	oxidized $mM^{-1}.cm^{-1}$
Wild type	4.2 ± 0.1	525	3.4 ± 0.1	4.4 ± 0.8	3.8 ± 0.3	3.9 ± 0.4
E498D	3.7 ± 0.2	525	1.0 ± 0.02	3.1 ± 0.3	1.3 ± 0.02	1.6 ± 0.1
E498T	3.7 ± 0.1	521	1.8 ± 0.2	3.3 ± 0.9	3.2 ± 0.7	3.4 ± 0.7
E498L	3.7 ± 0.2	516	1.6 ± 0.1	3.7 ± 0.2	0.8 ± 0.1	3.4 ± 0.1

Table S3 Occupancies of copper sites in the crystal structures

CotA / Copper Site	Wild type	E498T	E498L	E498D
Type 1	1.0	1.0	1.0	0.7
Type 2	1.0	0.8	0.3	1.0
Type 3 (x2)	1.0	0.8	0.8	1.0