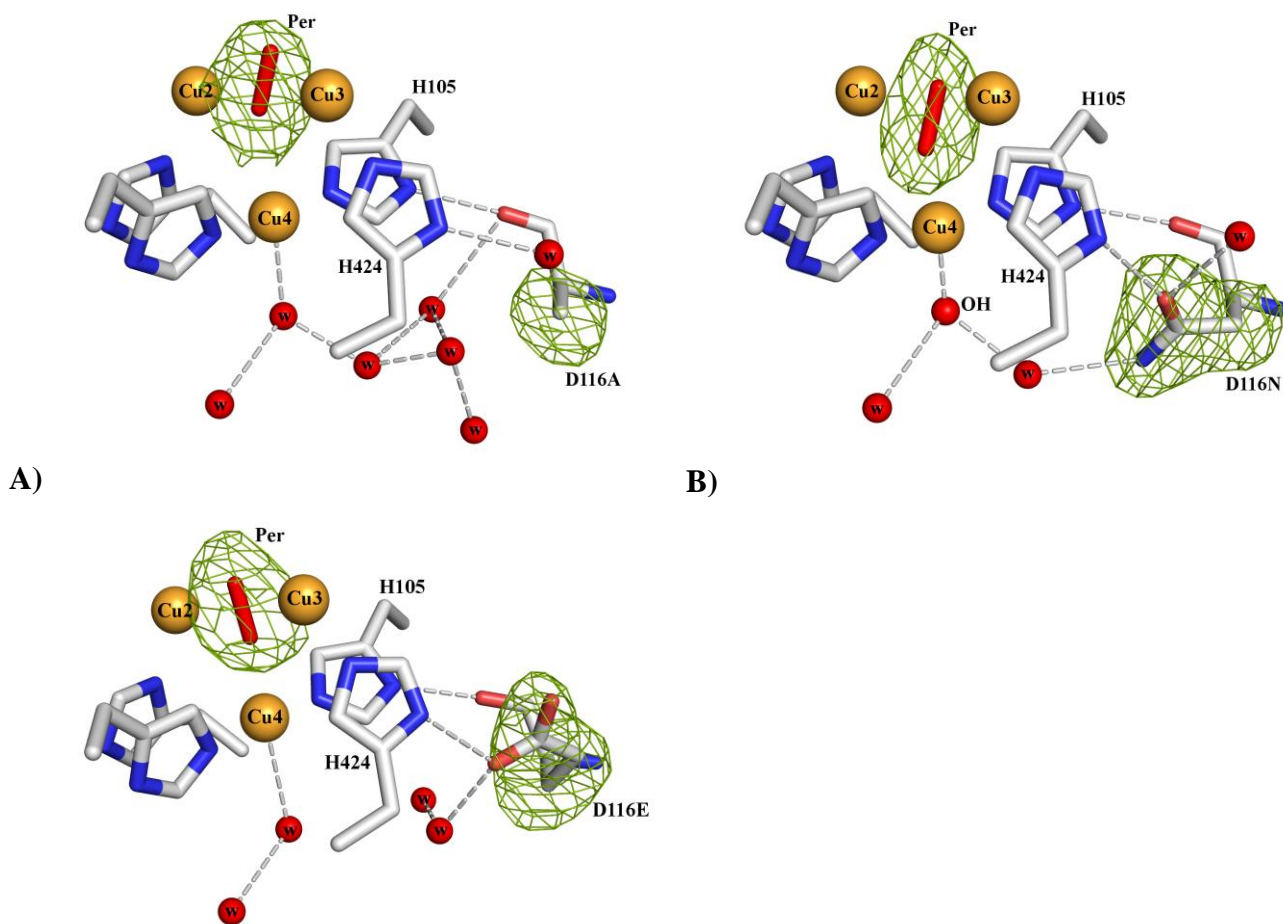


SUPPLEMENTARY MATERIAL

Table S1. Copper-copper and copper-solvent ligand distances (Å) at the trinuclear site for the native CotA laccase and its mutants D116A, D116N and D116E.

	CotA laccase			
	Native	D116A	D116N	D116E
Cu2-Cu3	4.73	4.58	4.63	4.74
Cu2-Cu4	3.99	4.01	4.17	3.97
Cu3-Cu4	3.66	3.61	3.74	3.61
Cu2-O1	2.57	2.90	2.76	2.56
Cu2-O2	2.59	2.32	2.88	2.61
Cu3-O1	2.31	2.11	1.88	2.31
Cu3-O2	2.29	2.32	2.42	2.45
Cu4-O2	2.42	2.68	1.95	2.10
Cu4-O	2.98	2.55	2.12	3.06



C)
Figure S1. Close view of the CotA trinuclear cluster at the dioxygen binding site. $|F_o| - |F_c|$ difference-Fourier omit map for the peroxide species placed in between both type T3 Cu ions and for the D116 residue side chain in (A) D116A, (B) D116N and (C) D116E. Contour level is 4.0σ . The peroxide species is shown as a red stick.