

Table S2. Comparison of ligand geometry to previous ba_3 structures

Distance (Å)	Current Structure	1XME	1EHK
NE of His384A to Fe of heme- a_3	2.2	2.5	3.3
Cu _B to Fe of heme- a_3	4.9	4.4	4.4
Bridging ion* to Fe of heme- a_3	2.39	2.4	2.3
Bridging ion* to Cu _B	2.25	2.1	2.3
CU1 of Cu _A to Fe of heme- b	19.2	19.2	19.0
CU1 of Cu _A to Fe of heme- a_3	21.8	21.7	21.8
CU1 of Cu _A to Cu _B	21.5	21.6	21.6
Fe of heme- b to Fe of heme- a_3	13.7	13.9	13.9
OH of Tyr237A to Fe of heme- a_3	5.7	5.8	5.6
Axial ligands His72A/NE2 and His386A/NE2 to heme- b	2.1	2.2	2.2
Separation of Cu _A atoms	2.6	2.5	2.6

*Bridging ion is a peroxide in the current structure and a water molecule in 1XME and 1EHK