SUPPLEMENTARY MATERIAL

Crystal Structures of Manganese- and Cobalt-substituted Myoglobin in Complex with NO and Nitrite Reveal Unusual Ligand Conformations

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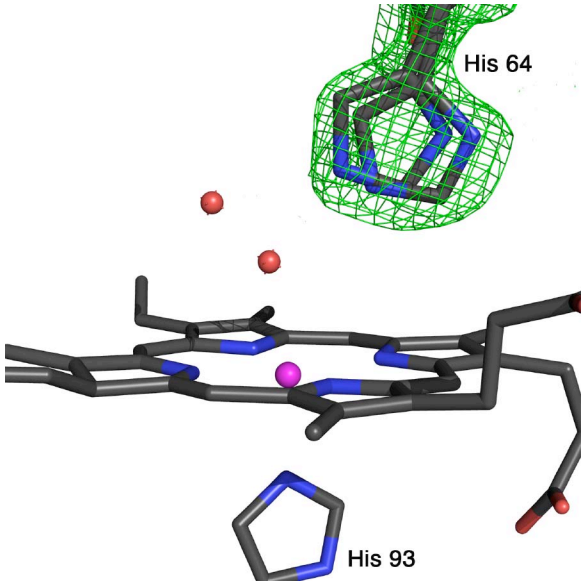

Fig. S1. Final model of the Mn-heme environment in $Mn^{III}Mb(H_2O)$, and the $2F_o$-F_c electron density map, contoured at 1σ, associated with the two conformations of the distal His64 residue.

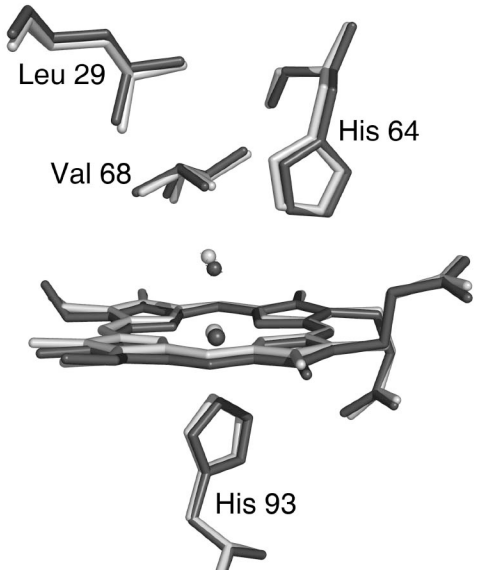

Fig. S2. A superposition of the heme environments in the crystal structures of hh $Co^{III}Mb(H_2O)$ (this work, shown in light grey) and sw $Co^{III}Mb(H_2O)$ (pdb code 1YOH [69], shown in dark grey) using a global Cα structural alignment.

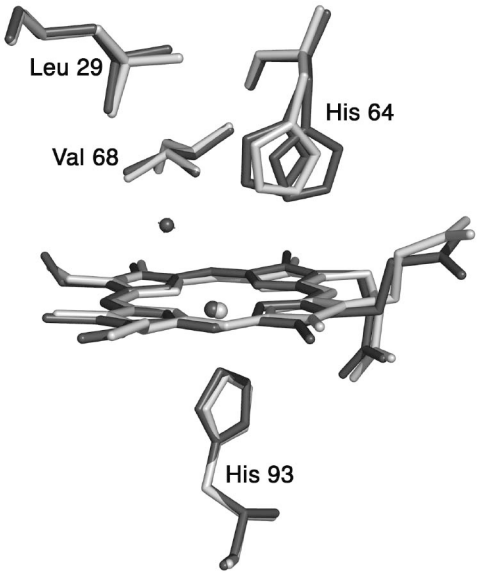

Fig. S3. A superposition of the heme environments in the crystal structures of hh $Mn^{II}Mb$ (this work, shown in light grey) and hh $Fe^{II}Mb$ (pdb code 1A6N [90], shown in dark grey) using a global Cα structural alignment. The distal pocket water in hh $Fe^{II}Mb$ is located 3.53 Å from Fe, and is 2.76 Å from the inward conformation of the distal His64 residue; the outer conformation overlaps with that of *aquomet*Mb.