Supporting Information

Structural basis for the heterotropic and homotropic interactions of giant hemoglobin

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Ca²⁺, A1

Ca²⁺, A2

Ca²⁺, B1

Ca²⁺, B2

Mg²⁺, A1

Mg²⁺, A2

Mg²⁺, B1

Mg²⁺, B2

Figure S1. The $2F_o-F_c$ electron density maps (cyan: contoured at 1.2σ) and the ligand-omitted F_o-F_c maps (magenta: contoured at 3.5σ) around the ligand sites at all four subunits in both Ca- and Mg-oxyHb.

Figure S2. A comparison of the heme geometry of all four subunits in both Ca- and Mg-oxyHb (white) with that in met(A1-oxy)Hb (blue). The models were superimposed by fitting of all of the atoms of proximal histidines.