Supporting Information

Crystallographic Characterization of the Nitric Oxide Derivative of *R*-State Human Hemoglobin

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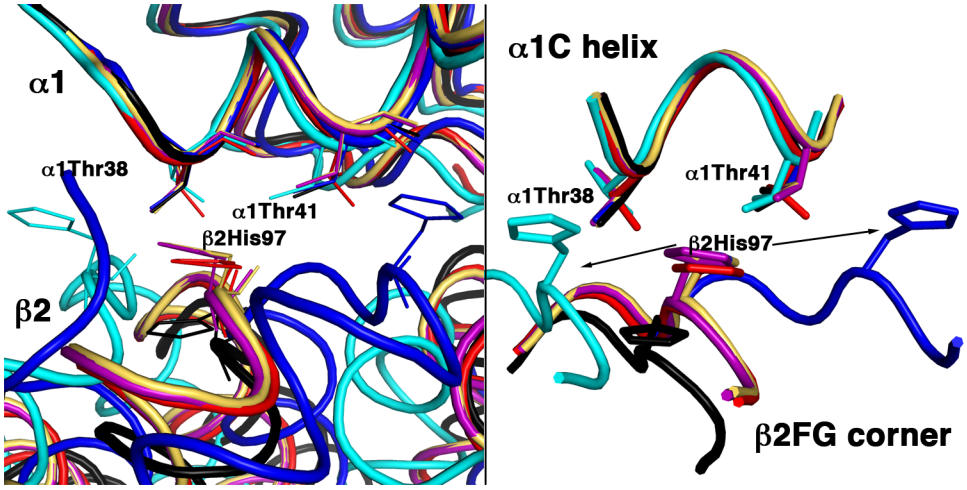

Figure S1. The α1β2 interface of representative Hb structures. (**left**) The α1β1 subunits were superimposed using a *T*-state deoxy Hb structure as the reference (PDB accession code: 1B86, 2.5 Å resolution; shown in blue) [1]. This generates the same positions of the α1 C helices, but clearly shows different positions of the β2 FG corners for different quaternary structures. The *R*-state Hb(CO) (PDB accession code: 1AJ9, 2.2 Å resolution) is shown in red [2]; the R2-state Hb(CO) (PDB accession code: 1BBB, 1.7 Å resolution) is shown in black ;[3] the R3-state Hb(CO) (PDB accession code: 1YZI, 2.07 Å resolution) is shown in cyan [4]; the aquometHb (PDB accession code: 3P5Q, 2.0 Å resolution) is shown in yellow [5]; and the Hb(NO) (PDB accession code: 4N8T, 1.9 Å resolution; this work) is shown in magenta. (**right**) Highlights of key residues (α1Thr38, α1Thr41 and β2His97) at this α1β2 interface. This analysis shows that the Hb(NO) and the aquometHb structures are in the R state.

References:

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[2] G.B. Vasquez, X. Ji, C. Fronticelli, G.L. Gilliland, Human Carboxyhemoglobin at 2.2 Å Resolution: Structure and Solvent Comparisons of R-state, R2-state and T-state Hemoglobins, Acta Cryst. D54 (1998) 355-366.

[3] M.M. Silva, P.H. Rogers, A. Arnone, A Third Quartenary Structure of Human Hemoglobin A at 1.7 Å Resolution, J. Biol. Chem. 267 (1992) 17248-17256.

[4] M.K. Safo, D.J. Abraham, The Enigma of the Liganded Hemoglobin End State: A Novel Quaternary Structure of Human Carbonmonoxy Hemoglobin, Biochemistry 44 (2005) 8347-8359.

[5] J. Yi, L.M. Thomas, G.B. Richter-Addo, Crystal Structure of Human *R*-State Aquomethemoglobin at 2.0 Å Resolution, Acta Cryst. F 67 (2011) 647-651.