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Supporting information for article:

The structure of a deoxygenated 400 kDa haemoglobin reveals ternary and quaternary structural changes of giant haemoglobins

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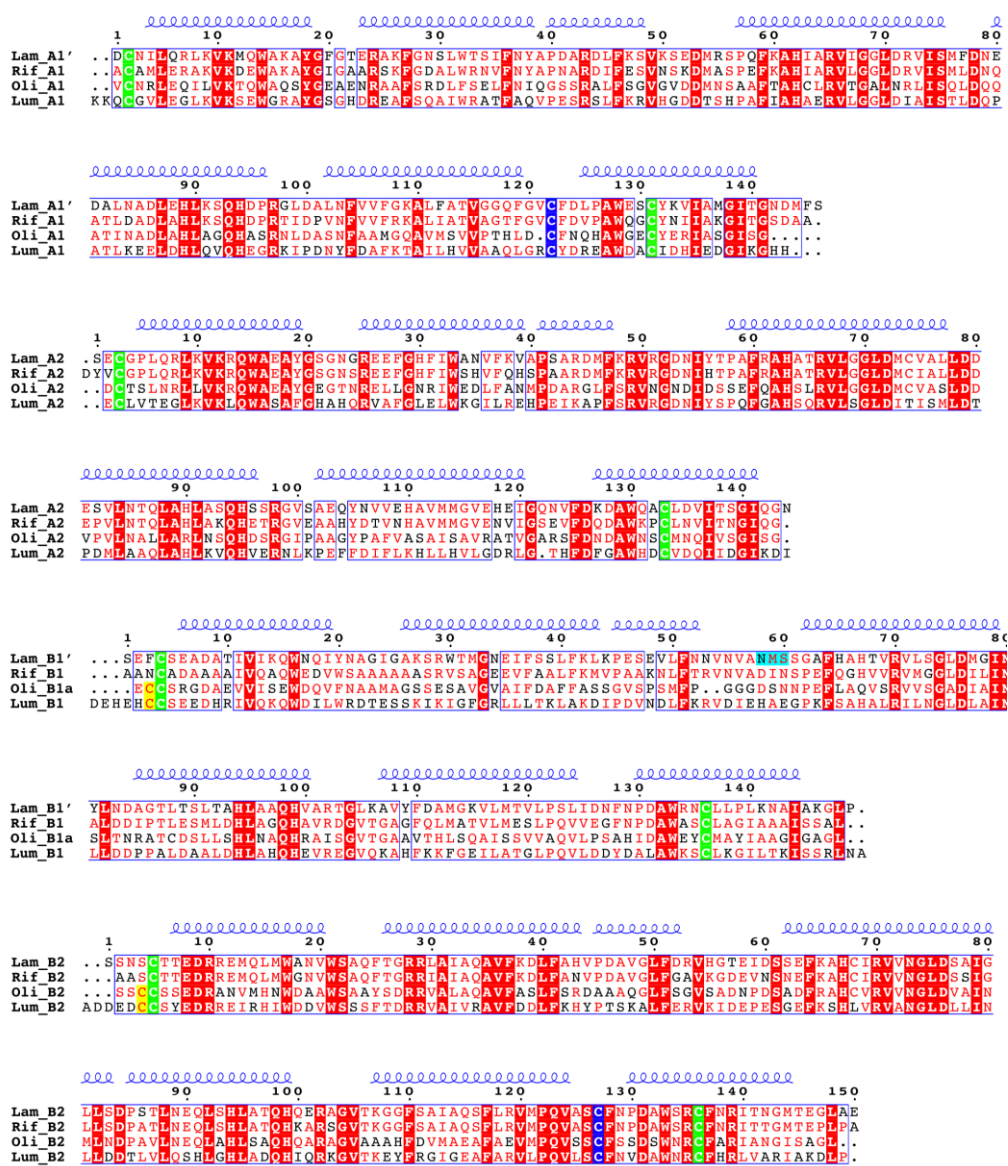


Figure S1 Alignments of the amino acid sequences of *Lamellibrachia* V2Hb (Lam) with *Riftia* C1 (Rif), *Oligobranchia* Hb (Oli), and *Lumbricus* Hb (Lum). The secondary structures based on oxy V2Hb structure are indicated above the sequences. The conserved Cys residues concerned with the inter- and intra-subunit disulfide-bonds are indicated as blue and green backgrounds. Another inter-subunit disulfide bond between the N-terminus of the B1 and B2 subunits (Yellow background) is not conserved in *Lamellibrachia* V2Hb and *Riftia* C1. The consensus sequence of the glycosylation site at Asn58 of the B1 subunit is shown as cyan background. The figure was prepared with the program ESPript (Gouet, P., Courcelle, E., Stuart, D.I. and Metoz, F. (1999). ESPript: multiple sequence alignments in PostScript. *Bioinformatics*. 15 305-8)

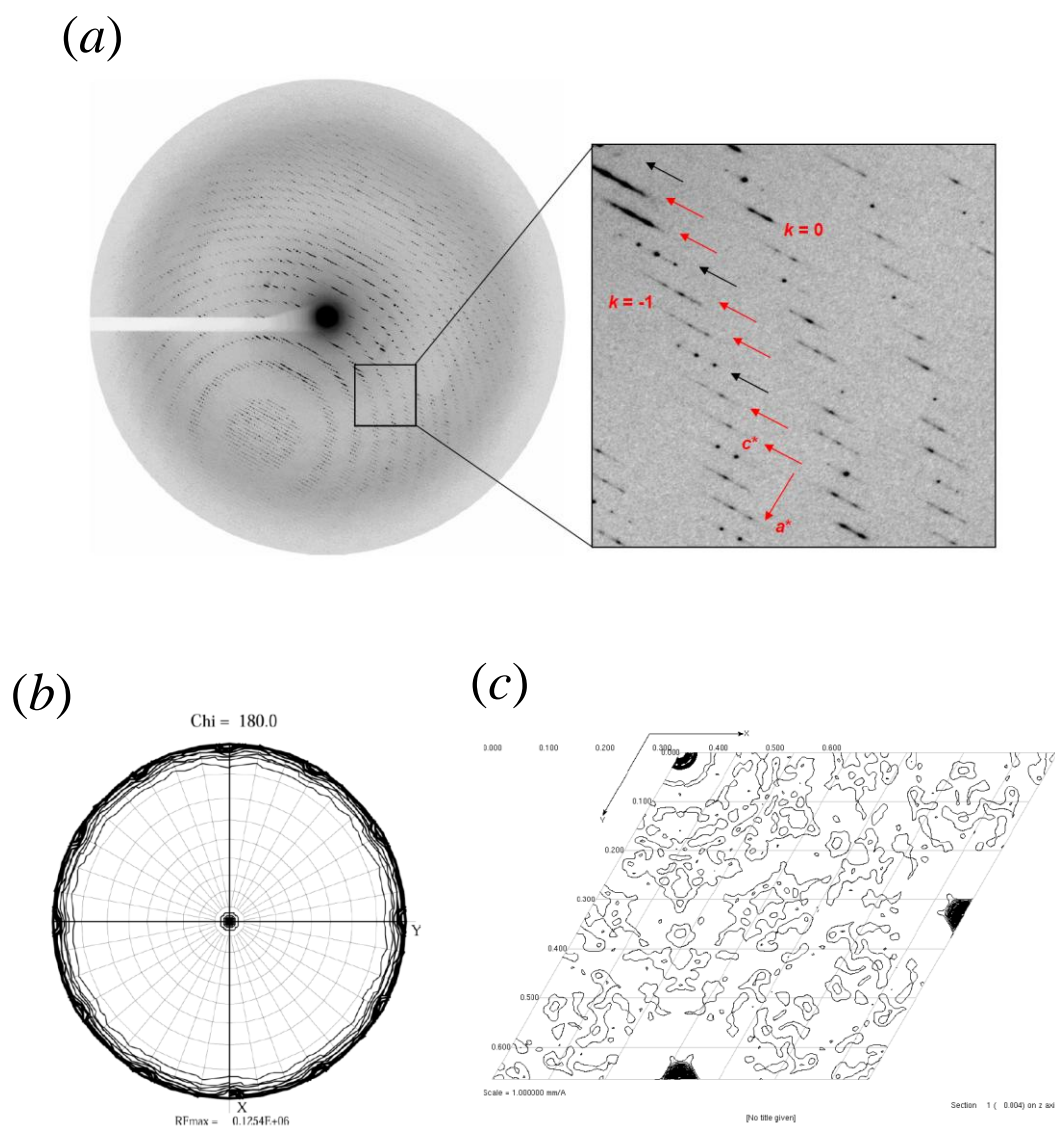


Figure S2 (a) Diffraction pattern of the crystal obtained under higher salt condition. Diffuse reflections (red arrows) and sharp reflections (black arrows) are periodically observed. (b) $\chi = 180^\circ$ section of the self-rotation function. (c) $w = 0$ section of the native Patterson map.

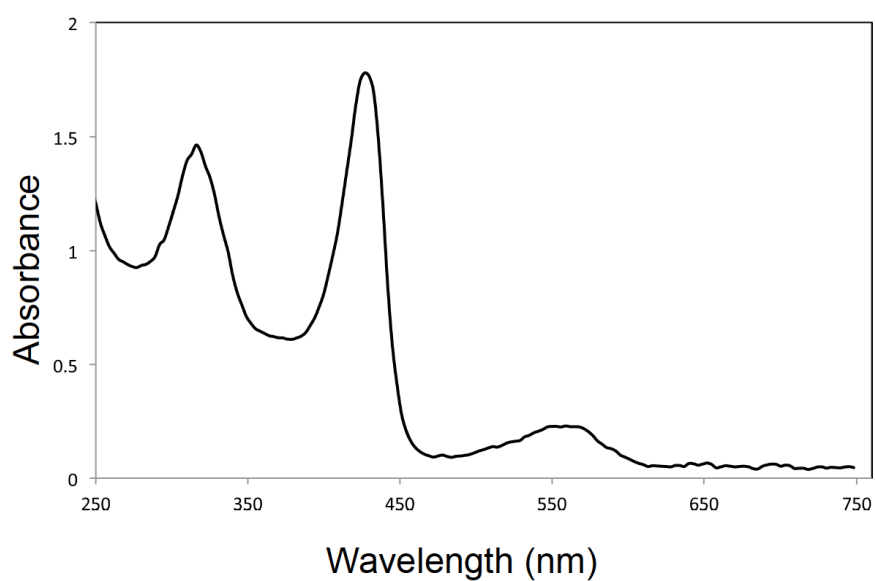


Figure S3 Absorption spectra of the V2Hb solution mixed with the solution containing sodium hydrosulfite.

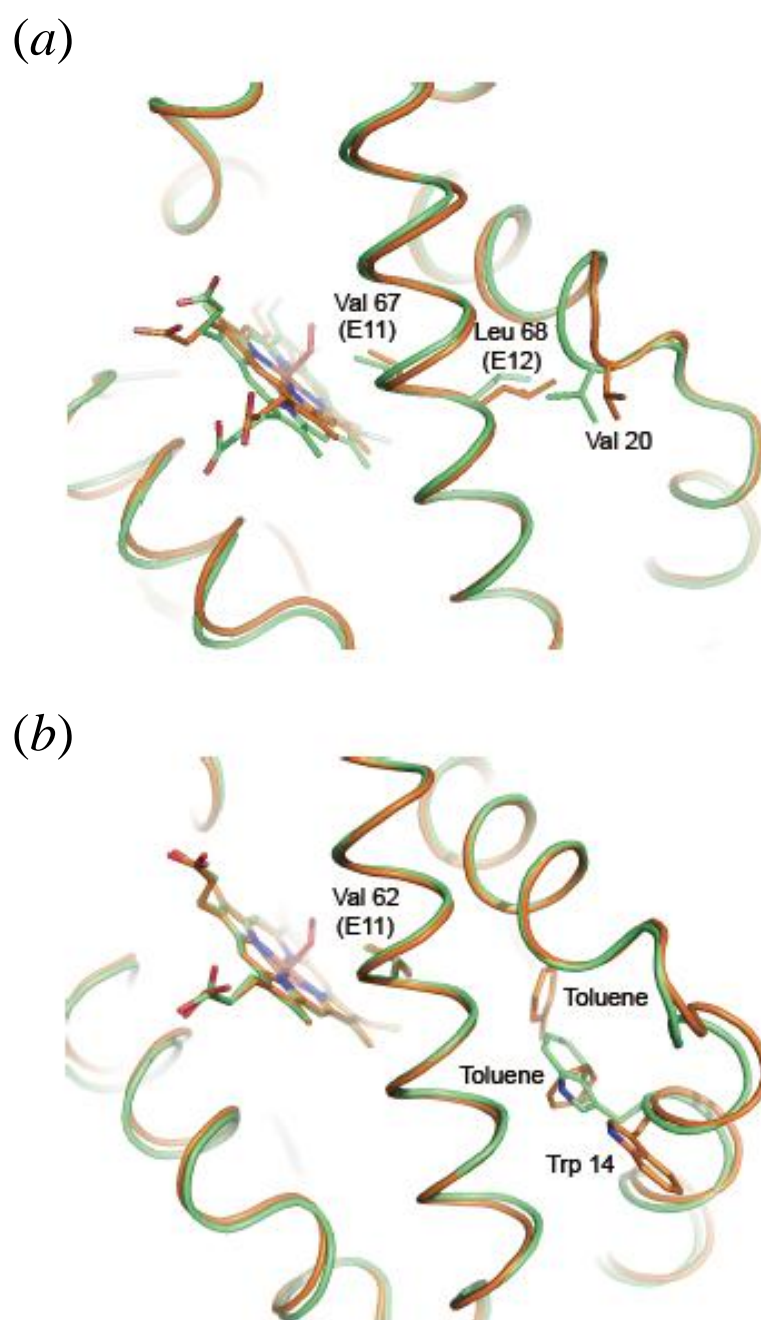


Figure S4 Close-up views around the E helices and AB loops of the oxy (orange: 2DN1) and deoxy (green: 2DN2) forms of the beta subunits of human hemoglobin (*a*) and those of the alpha subunits (*b*).

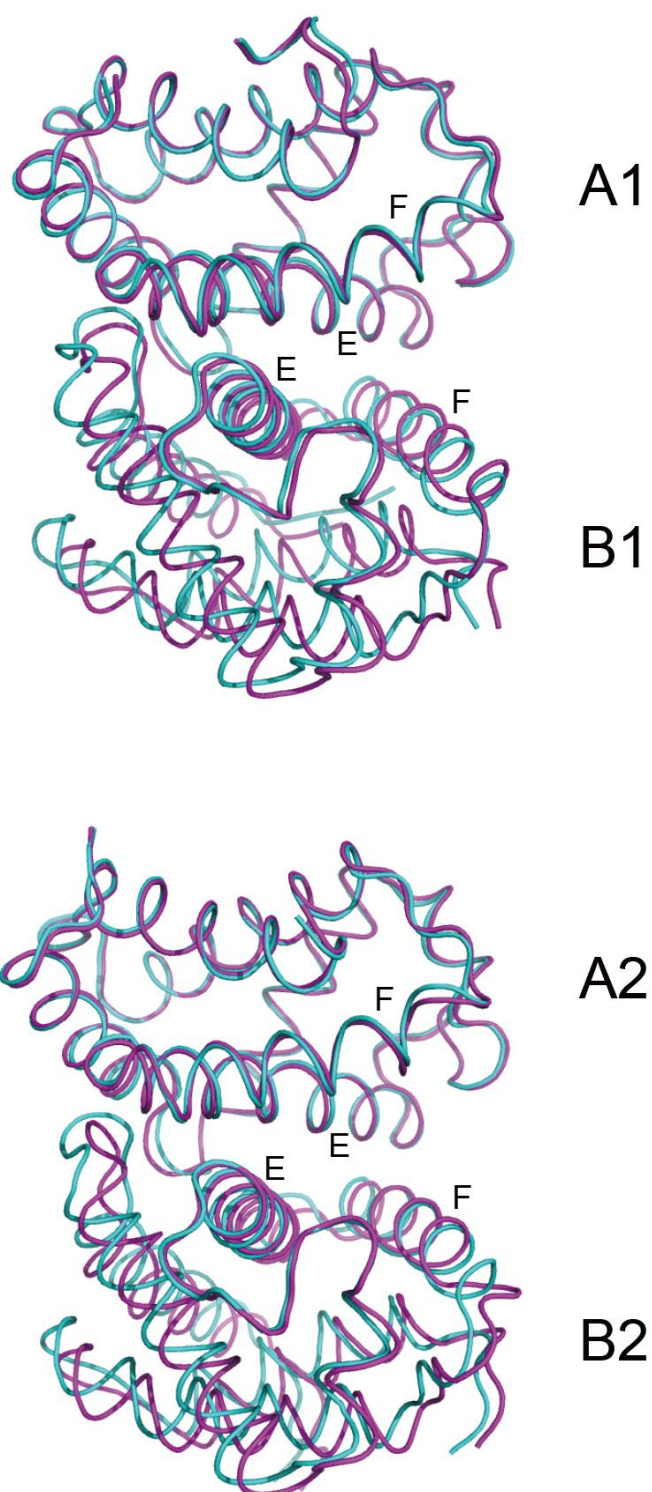


Figure S5 Comparisons of the A1B1 (upper) and A2B2 (lower) dimer structures of the oxy (magenta) and deoxy (cyan) forms of V2Hb. The E and F helices of each subunit are indicated.