

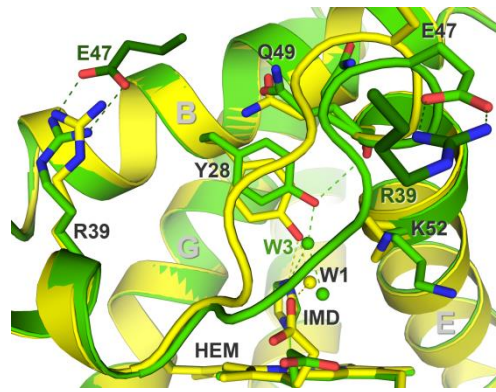
Supplementary information

Open and His–Lys Hexacoordinated Closed Structures of a Globin with Swapped Proximal and Distal Sites

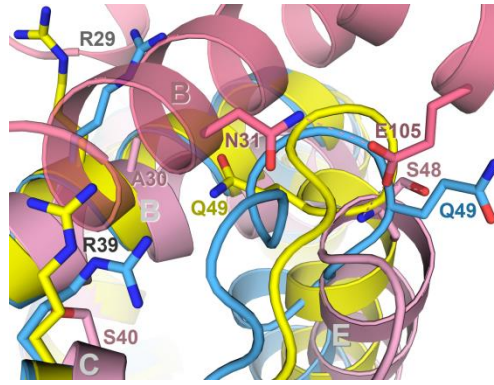
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Supplementary Figure S1 | Conformational changes in subunit B* of the open form. Because of interactions with Arg39(C5) and Glu47 from a neighbouring asymmetric unit (dark green), absent in subunit A* (yellow), a different conformation of loop CE is observed in subunit B* (green) of the open form. A slight movement of helix E is also observed, allowing Tyr28(B10) in the distal site to move to an upward position similar to that of the closed form, and W3 to move in.



Supplementary Figure S2 | Absence of HGbI dimerization in *N*-HGbRL. In both the open (yellow) and closed (blue) forms of *N*-HGbRL, the lengthened loop CE and several residue replacements, such as the bulky Arg29(B11) and Arg39(C5), have disrupted the dimeric interface present in HGbI (pink; second subunit in dark pink).