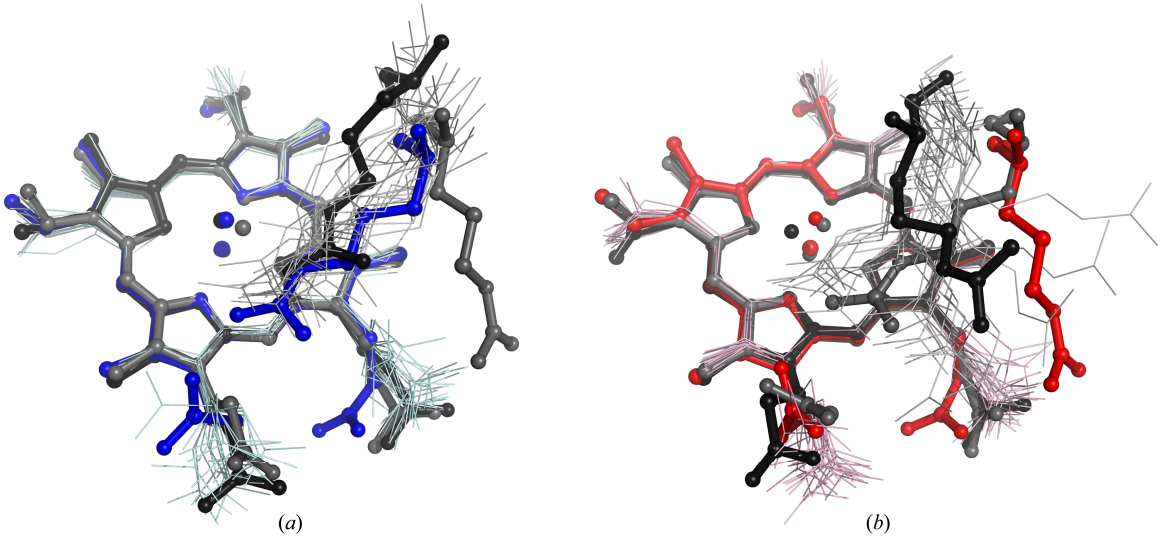
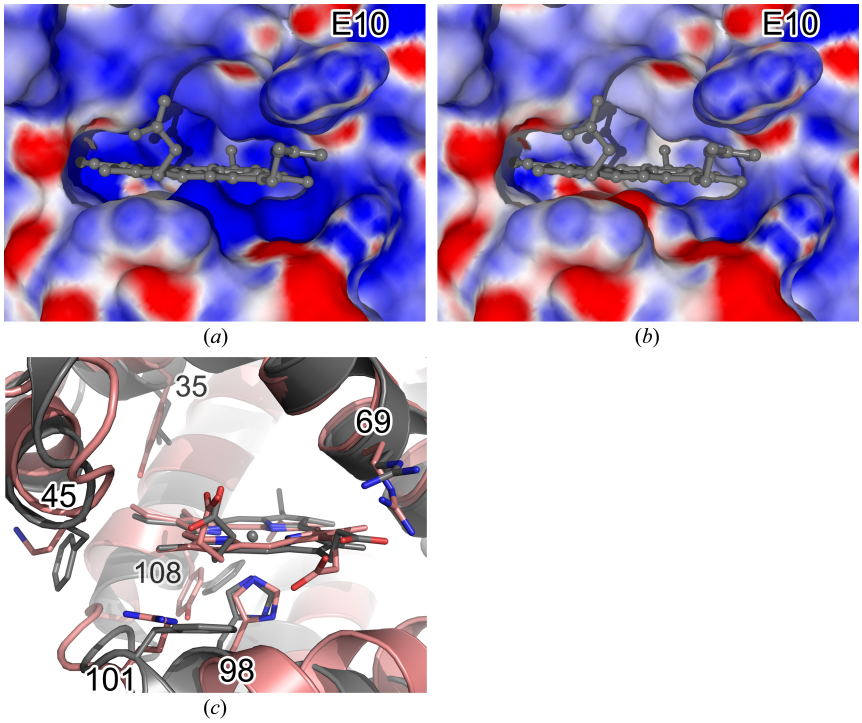
Supplementary Figures



Supplementary Figure 1. Superimposed snapshots taken every 1 ns during a 25-ns simulation using the Arg swing-out form binding the Cl^- ion and the Arg swing-in form binding the water are shown in (*a*) and (*b*), respectively. The starting and ending structures of the simulation are shown as grey and black sticks, respectively. Line models represent the middle structures during the simulations. Crystallographic structures of Hb V at pH 4.6 under 500 *mM* NaCl and no salt are coloured blue in (*a*) and red in (*b*), respectively. These structures were superimposed based on haem N atoms.



Supplementary Figure 2. Electrostatic surface of the haem pocket of *A. limacina* Mb at pH 4.6 (*a*) and pH 7.0 (*b*). Red surfaces indicate negative potential, and blue positive (±15 kT/e). Electrostatic surface at each pH was computed with the Arg-E10 swing-out form, imidazole-binding Mb (PDB entry 4mba; Conti *et al*., 1993). To compare the haem region, superposition of *P. akamusi* Hb V (pink) and *A. limacina* Mb (gray) was shown in (c). Although the distal Arg-E10 (69) and the proximal His-F8 (98) were common between these two globins, the positions corresponding to other polar residues in Hb V, Try35, Lys45, Arg101, and Try108, were occupied by non-polar residues, Leu, Phe, Phe and Phe, respectively, in *A. limacina* Mb.