

Supplementary Material

Cooperative Protein Structural Dynamics of Homodimeric Hemoglobin Linked to Water Cluster at Subunit Interface revealed by Time-Resolved X-ray Solution Scattering

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Supplementary Figure

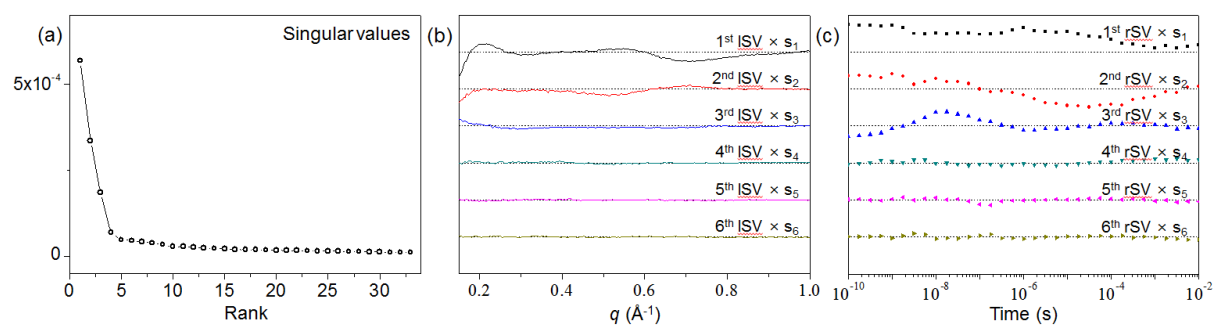


Figure S1. (a) Singular values obtained from time-resolved difference X-ray solution scattering data for HbI T72V mutant are shown. (b) The first six left singular vectors multiplied by singular values are shown. (c) The first six right singular vectors multiplied by singular values are shown. Judging from the amplitudes of singular values, which reflect the contributions of left and right singular vectors on the entire time-resolved difference X-ray solution scattering data, the first three singular vectors were used for our kinetic analysis.

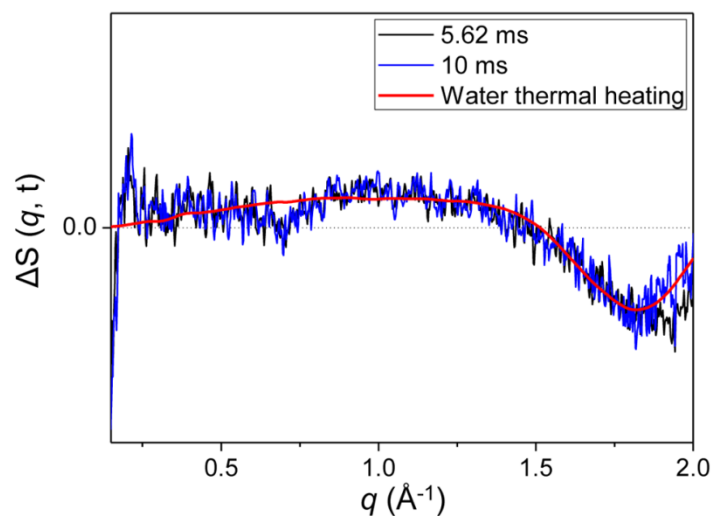


Figure S2. Difference X-ray scattering intensities in a wide-angle region ($q > 1.0 \text{ \AA}^{-1}$) at 5.62 ms and 10 ms can be well represented by a sum of scattering intensity changes of bulk water due to the temperature change at a constant density ($(\partial S(q)/\partial T)_\rho$) and the density change at a constant temperature ($(\partial S(q)/\partial \rho)_T$). This thermal heating signal was subtracted from the raw time-resolved difference scattering curves so that heat-free time-resolved difference scattering curves were obtained for the subsequent kinetic and structural analyses.