

Supporting Information

Dissecting the contributions of β -hairpin tyrosine pair to the folding and stability of long-lived human γ D-crystallins

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PS 1: RMSDs (C α) for the wild-type at 310 K.

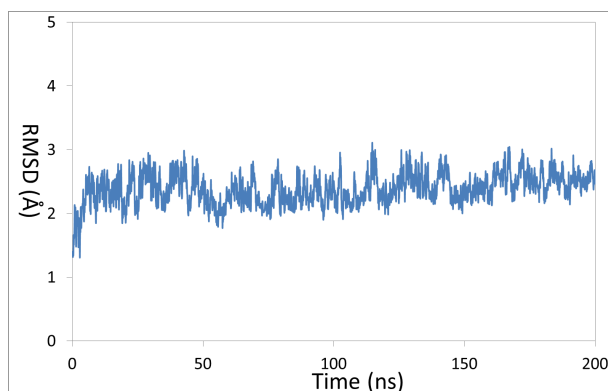


Fig. S1. The time evolution of RMSDs (C α) for the wild-type system at 310 K in pure water as control runs.

PS 2: Solvent accessible surface (SAS) area of M43, L44, and L132 residues as a function of simulation time.

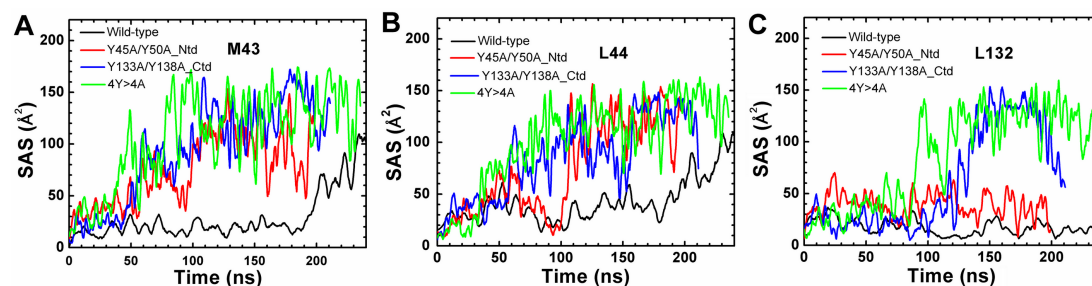


Fig. S2. The time evolution of solvent accessible surface (SAS) area of key residues M43 (A), L44 (B), and L132 (C), respectively, for both the wild-type (black), Y45A/Y50A_N-td (red), Y133A/Y138A_C-td (blue), and 4Y>4A (green) mutants.

PS 3: Snapshots of the wild-type and Try-to-Ala pair(s) mutants during their respective representative unfolding trajectories.

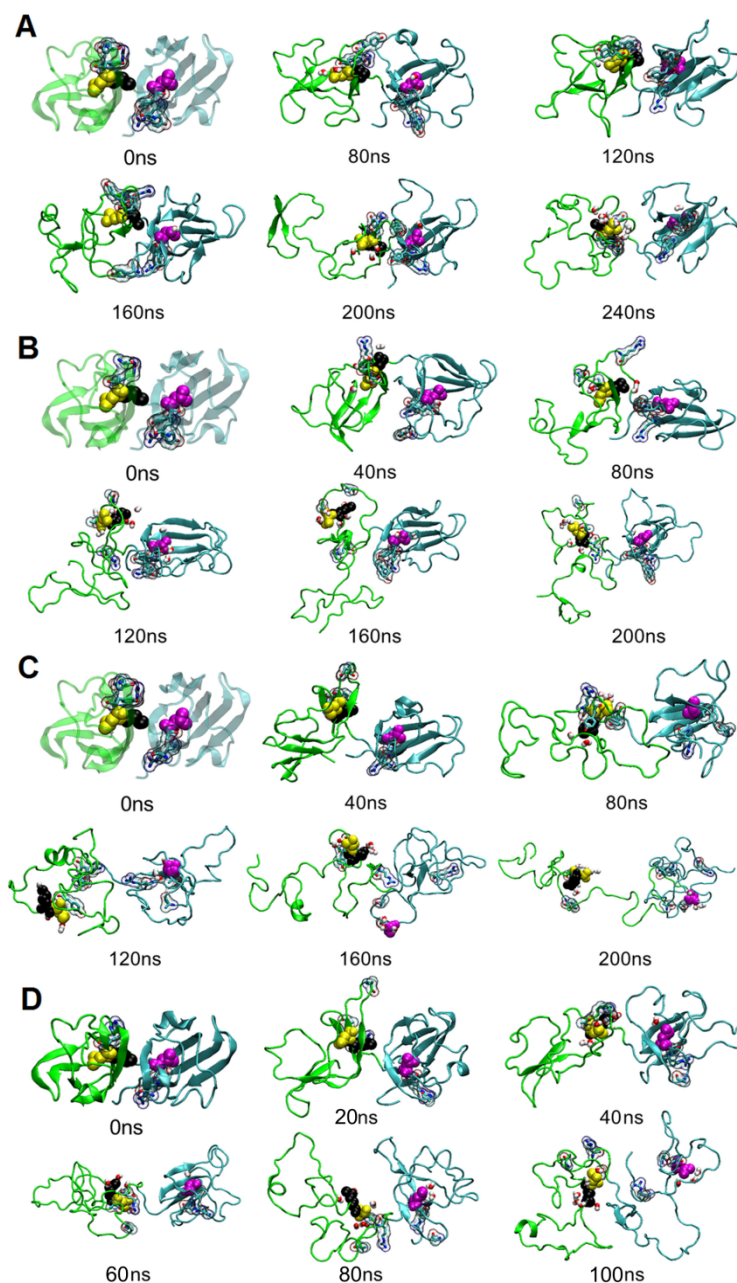


Fig. S3. Snapshots of the wild-type (A), Y45A/Y50A_N-td (B), Y133A/Y138A_C-td (C), and 4Y>4A mutant (D) proteins during their respective representative trajectories. N-td is shown in green, C-td in cyan. Water molecules are shown with bold bond, and residues M43 shown in black, L44 in yellow, and L132 in magenta. Residues Y45/A45, Y50/A50, R79, Y133/A133, Y138/A138, and R167 are shown with transparent surfaces.