

Electronic Supplementary Information

A Buried Glutamate in the Cross- β Core Renders β -endorphin Fibrils Reversible

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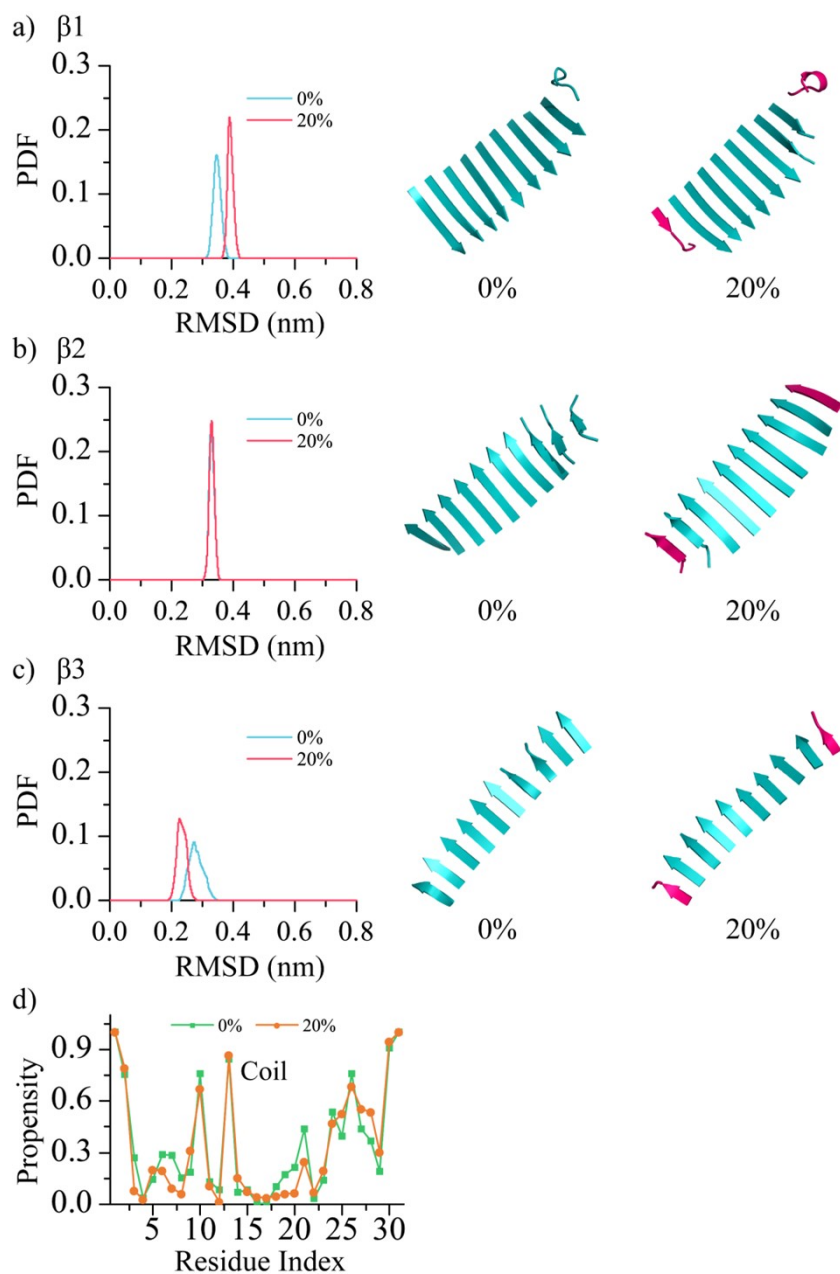


Fig. S1. The structure analysis with the Glu8 deprotonation ratio of 0% and 20%. The probability distribution as a function of RMSD of $\beta 1$ a), $\beta 2$ b) and $\beta 3$ c) regions. And the final snapshots of the three β -sheet regions in every molecular system. d) The probability of each residue to form random coil in the two systems are also shown on the right.

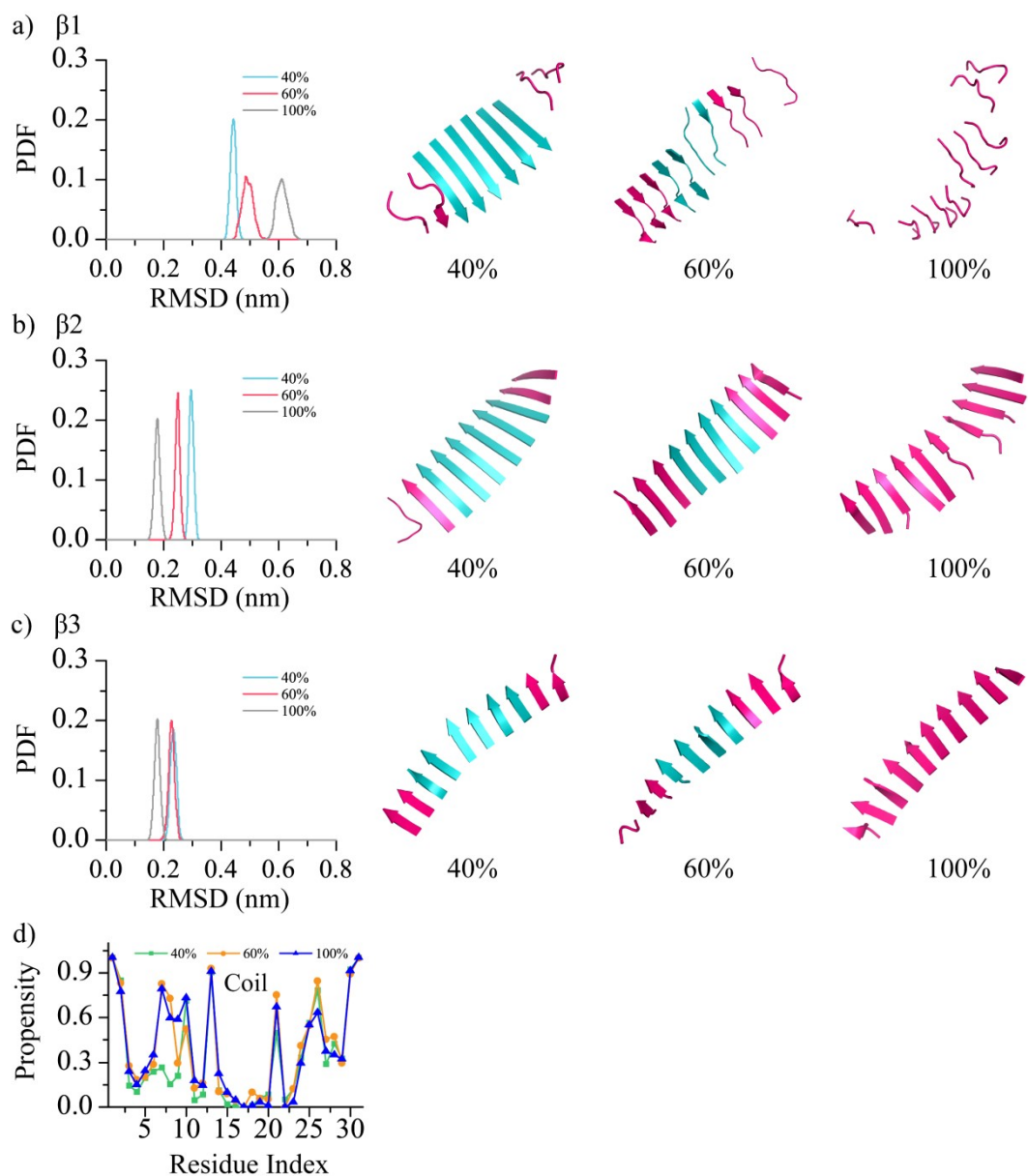


Fig. S2. The structure analysis with the Glu8 deprotonation ratio of 40%, 60% and 100%. The probability distribution as a function of RMSD of β_1 a), β_2 b) and β_3 c) regions. And the final snapshots of the three β -sheet regions in every molecular system. d) The probability of each residue to form random coil in the two systems are also shown on the right.

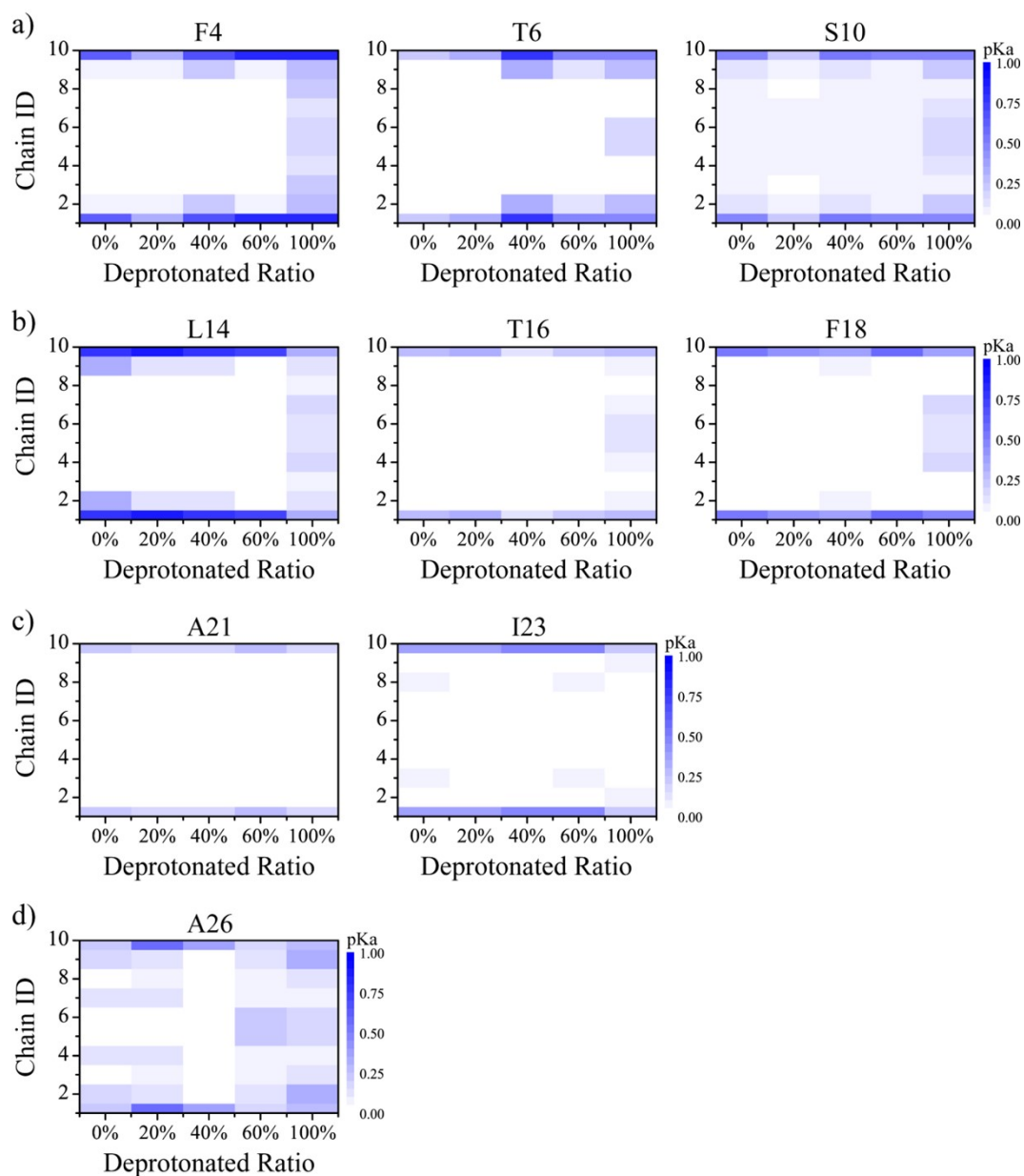


Fig. S3. The solvent-accessible surface area analysis for each residue from the hydrophobic and hydrophilic pores in each molecular system. The average solvent-accessible surface area of F4, T6, S10 amino acids from β -1 a), L14, T16, F18 amino acids from β -2, A21 b), I23 amino acids from β -3 c) and A26 from C-terminal region d) of β -endorphin fibril during last the 200 ns for each system.