Dissecting the structural determinants for the difference in mechanical stability of silk and amyloid beta-sheet stacks

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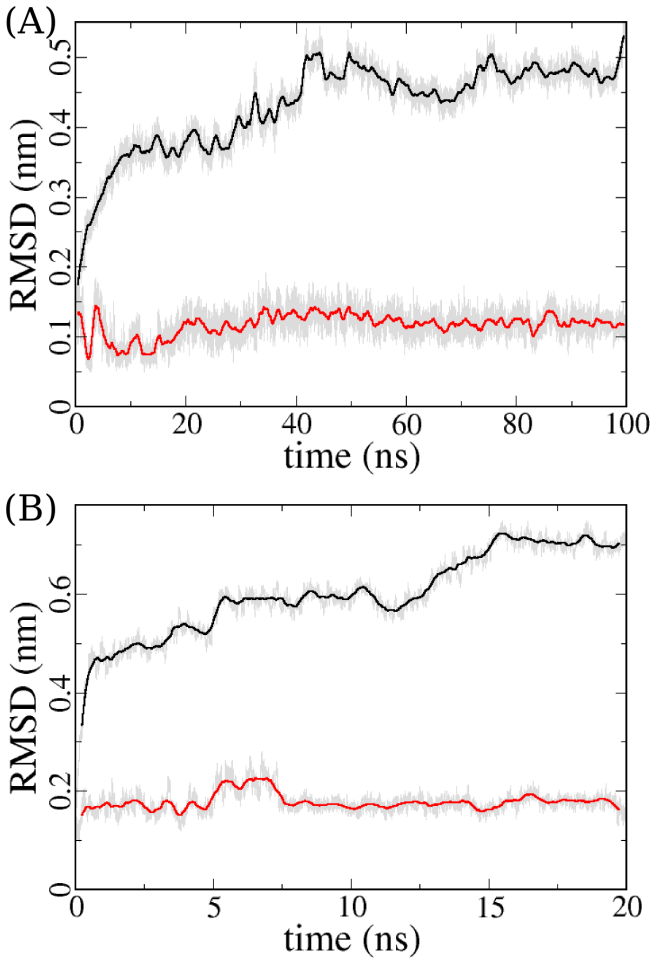
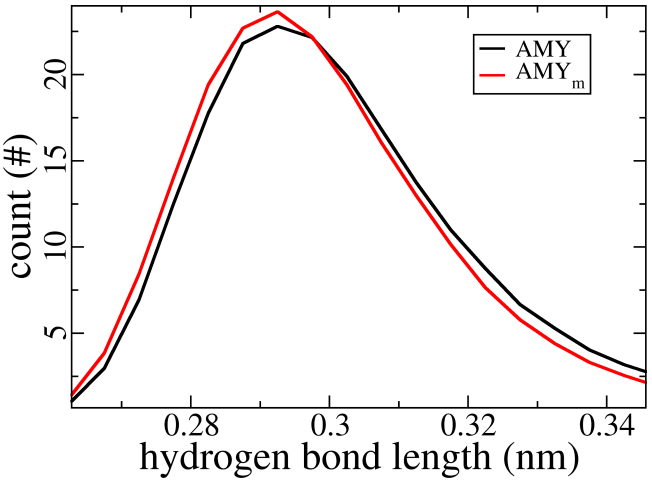
Supplements



Supplementary Figure S1 Structural stability of AMY β-stacks measured by the root-mean-square deviation (RMSD). (A) RMSD of AMY during 100 ns of equilibrium MD simulations. The increase in RMSD up to 0.5 nm (black curve) of all heavy atoms of the structure can be attributed to the fluctuation of the outer layers in the β-stacks. The inner layer β-sheet, which is exposed to pulling force in subsequent FPMD simulations, shows a low RMSD of 0.1 nm (red curve) and thus high structural stability. (B) RMSD of AMY with all residues mutated to alanine during 20 ns equilibrium MD simulations. While the RMSD of all heavy atoms reaches ~0.7 nm, the central β-sheet layer shows a relatively stable RMSD below 0.2 nm.



Supplementary Figure S2 Hydrogen bond length in the inner layer β-sheet of AMY (black) and AMY_m (red). Shorter hydrogen bonds are found in AMY_m, as indicated by the minor and yet significant shift of the length distribution.

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