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Effects of Proline Substitution/Inclusion on the Nanostructure of Self-assembling β -Sheet Forming Peptide – Supporting Information

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Table S1. Detailed information of performed molecular dynamics simulations.

		<i>Number of peptides</i>	<i>Number of H₂O molecules</i>	<i>Simulation box size [nm]</i>	<i>Simulation length [ns]</i>
<i>pre-assembled</i>	F8 single ladder	6	9347	7.6 × 6.7 × 5.7	500
	F8 double ladder	12	11521	7.8 × 6.7 × 6.9	500
	FP single ladder	6	12628	8.3 × 7.4 × 6.4	100
<i>self-assembly</i>	KPE	50	30002	10 × 10 × 10	100
	EPK	50	29957	10 × 10 × 10	100

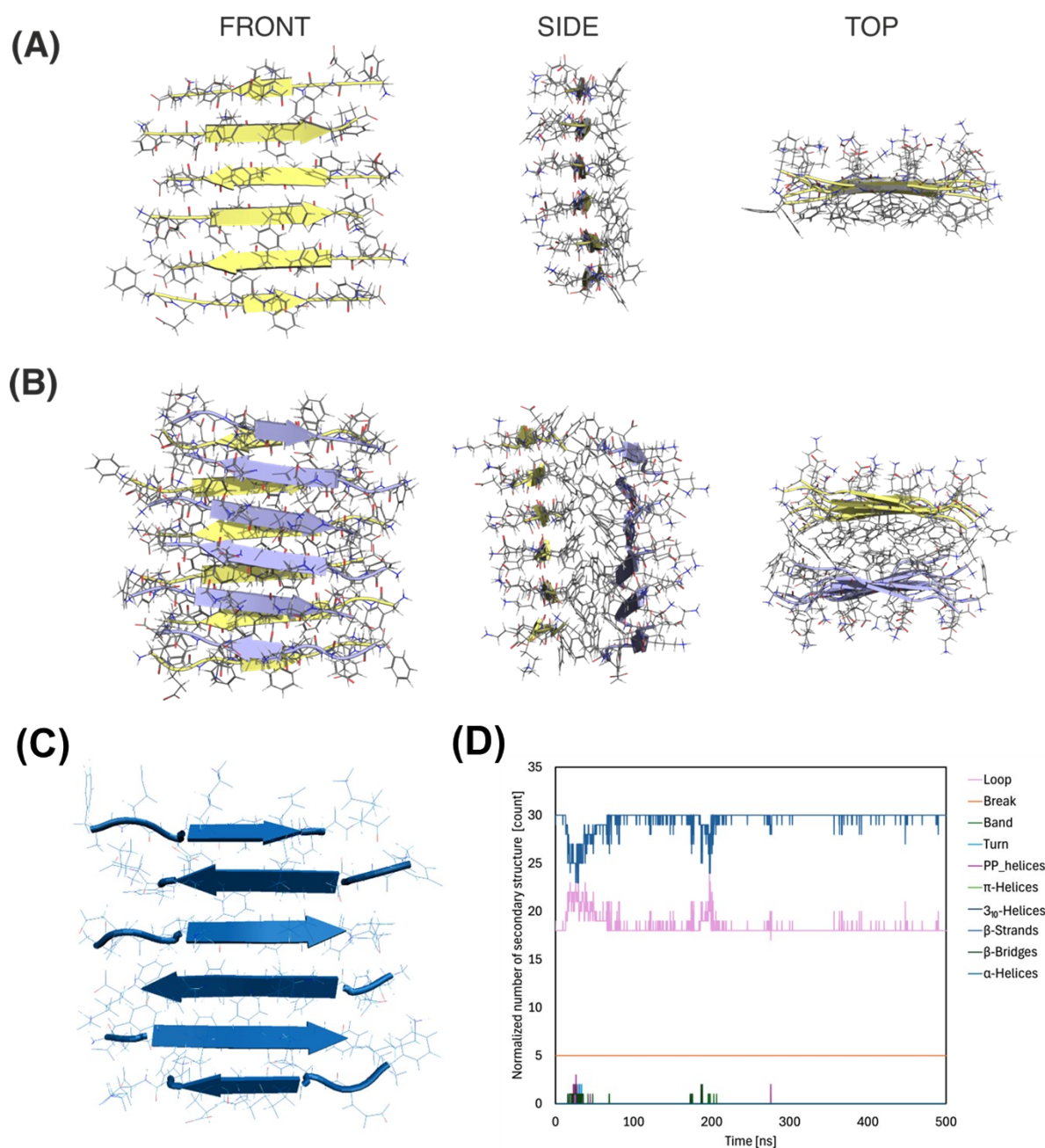


Figure S1. Final structures of F8 peptides (front, side, and top view) pre-assembled in single ladder (A) and double ladder (B). (C) Final snapshot of structure of F8 parental peptide sequence and (D) normalized secondary structural motifs as a function of time depicting a clear propensity of pre-assembled ladder conformation to form antiparallel stacking model.

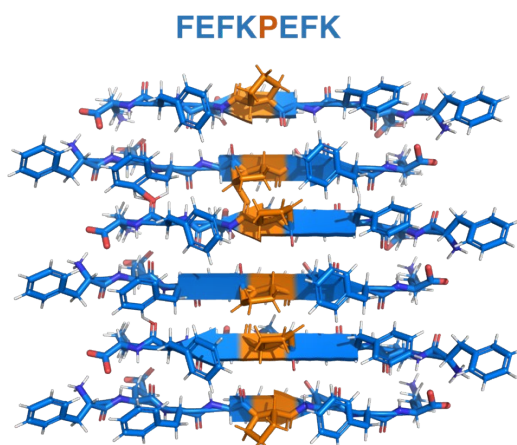


Figure S2. The initial structure of FP variant constructed as single amino acid replacement of phenylalanine to proline in the form of β -sheet ladder from parental F8 peptide.

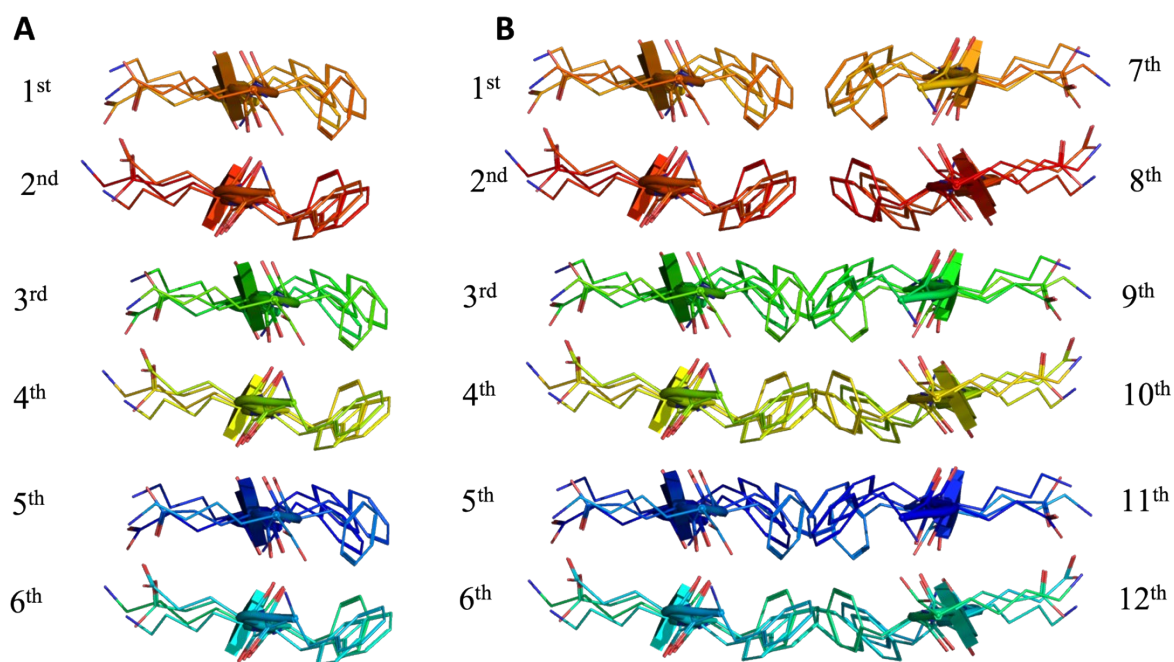


Figure S3. Numbering of single ladder (A) and double ladder (B) forms of F8 variant.

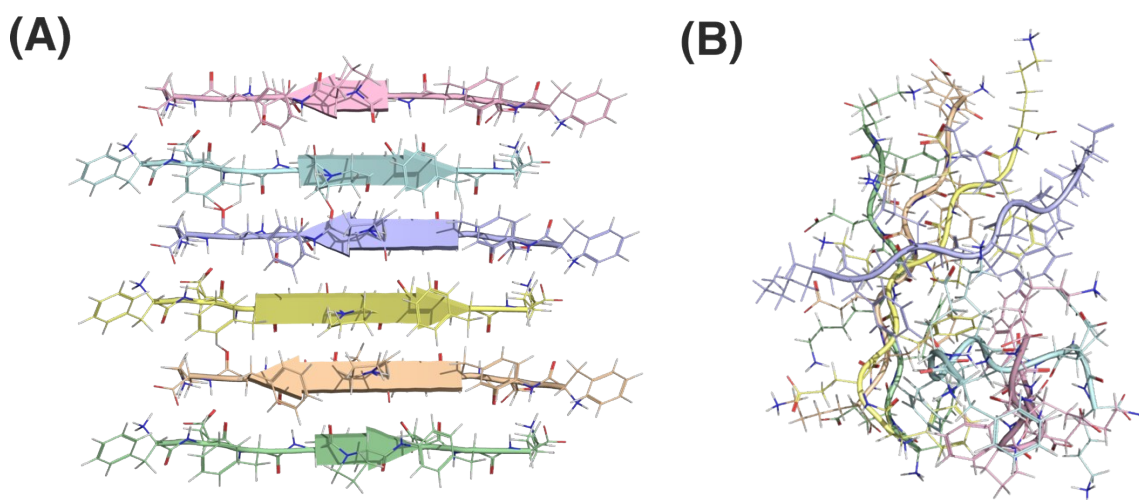


Figure S4. The starting structure **(A)** and final snapshot **(B)** of FP variant after 100 ns.

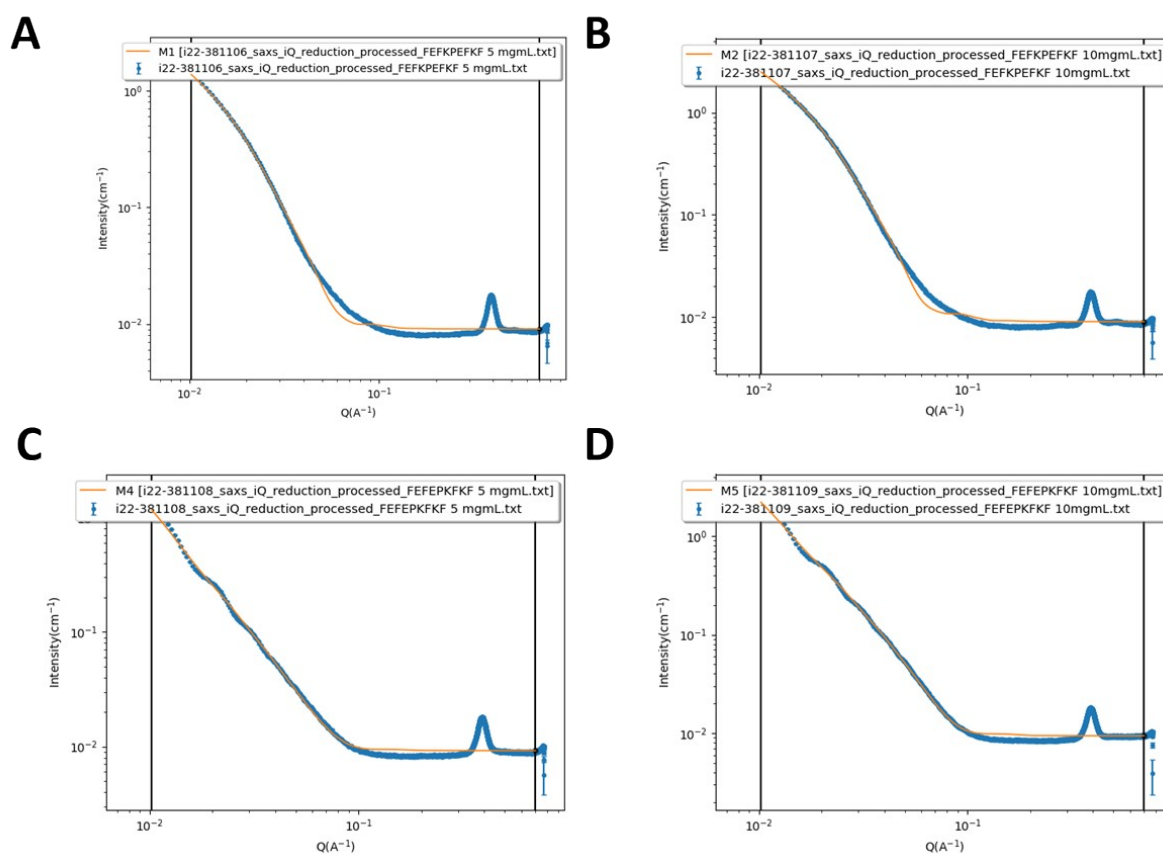


Figure S5. SasView fittings of SAXS patterns obtained for: **(A)** 5 mg mL⁻¹ KPE, **(B)** 10 mg mL⁻¹ KPE, **(C)** 5 mg mL⁻¹ EPK, **(D)** 10 mg mL⁻¹ EPK. Orange lines show the elliptical cylinder fitting and blue lines depict original data.