Supporting Material

Solid-state NMR evidence for β-hairpin structure within MAX8 designer peptide nanofibers

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Keywords: Self-assembly; molecular structure

NMR evidence of MAX8 β-hairpin structure

FIGURE S1 A 2D ^{13}C-^{13}C fpRFDR NMR spectrum for Sample A with horizontal slices at peak frequencies of V3 C_α (green), T12 C_β (red), and K17 C_α (blue) signals.

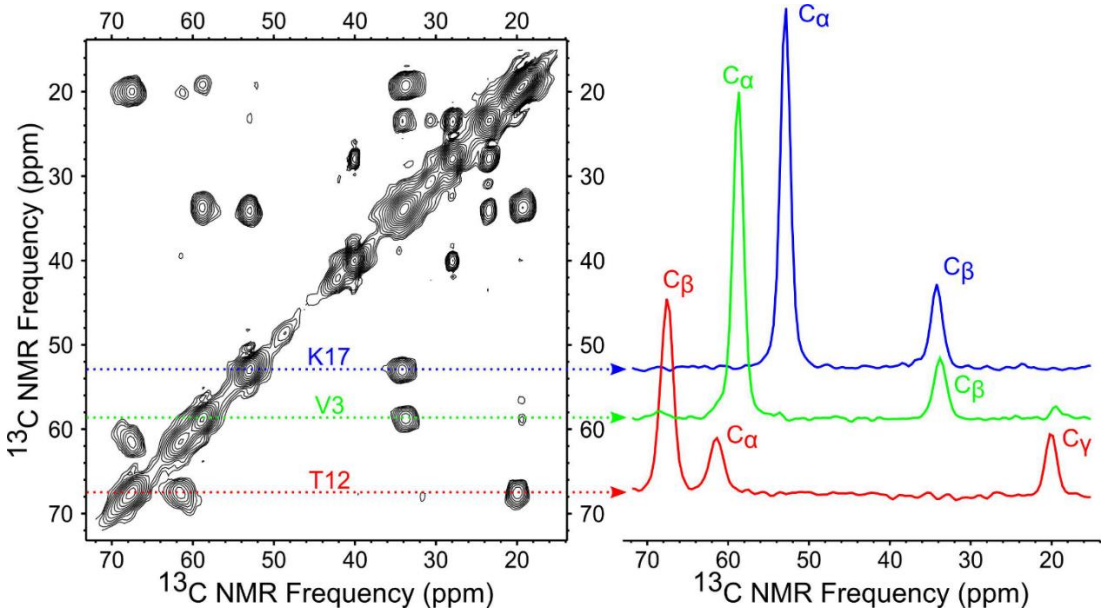

TABLE S1 Backbone torsion angles, ϕ and ψ, predicted using TALOS software and measured chemical shifts for V3 and K17 residues (bold). Agreement between CPMAS spectra from Samples A and B in Fig. 3 indicates little variation in chemical shift between different V and K residues.

Residue	**ϕ**	**ψ**
K2, K4, K6, K8, **K17**, K19	-122.6± 16.8	143.9 ± 11.5
V3, V5, V7, V18	-128.5 ± 8.6	136.5 ± 14.8
V9	-113.8 ± 23.4	133.3 ± 28.5
K13	-130.3 ± 19.9	146.4 ± 17.0
V14	-127.7 ± 14.4	142.3 ± 17.9
V16	-122.5 ± 8.8	137.0 ± 16.0

FIGURE S2 PITHIRDS-CT NMR data for Sample D and a V36 ^{13}C CO labeled Aβ(1-42) fibril sample. Solid curves show simulated behaviors for 8 evenly spaced ^{13}C nuclei in linear geometries (nearest neighbor distances indicated for each curve).

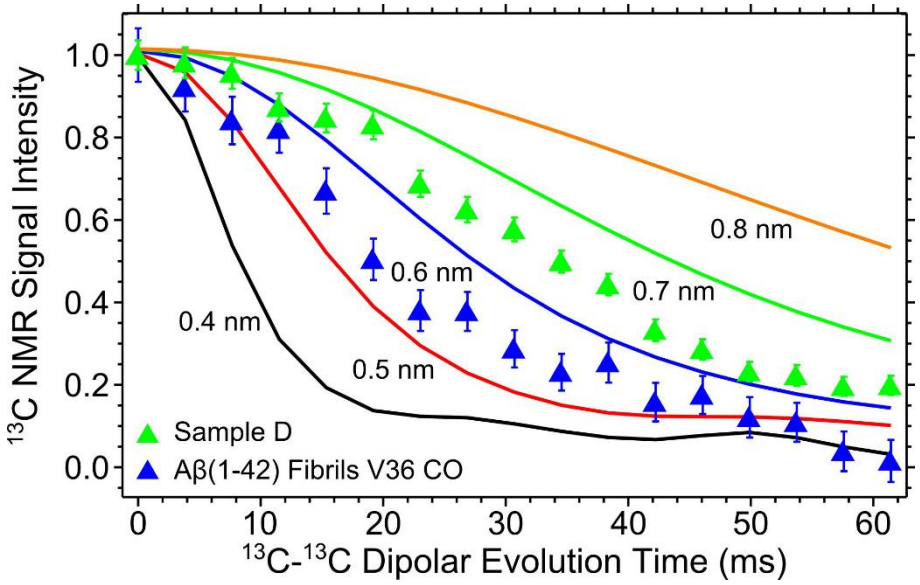

FIGURE S3 An all-atom model of a single MAX8 β-hairpin. The hydrophobic residues (P and V) are drawn in green, the positively charged residues (K) are drawn in blue, the negatively charged residue (E) is drawn in red, and the polar residue (T) is drawn in magenta. The peptide backbone is represented as a ribbon.

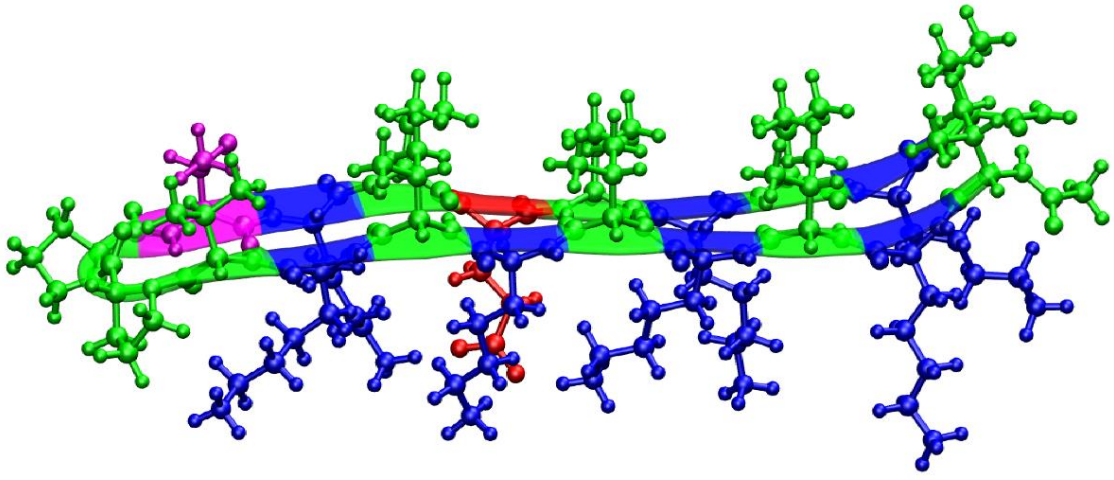

FIGURE S4 PITHIRDS-CT NMR data for Sample E and solid curves showing simulated behavior for pairs of ^{13}C nuclei separated by the indicated distances. The dashed curve shows how the prediction for a 0.5 nm inter-nuclear distance is expected to change upon 33% incorporation of MAX8 molecules which do not exhibit ^{13}C-^{13}C dipolar couplings.