Supporting Material

Antimicrobial Protegrin-1 (PG-1) Forms Amyloid-like Fibrils with Rapid Kinetics Suggesting a Functional Link

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Running title: Antimicrobial PG-1 forms fibrils

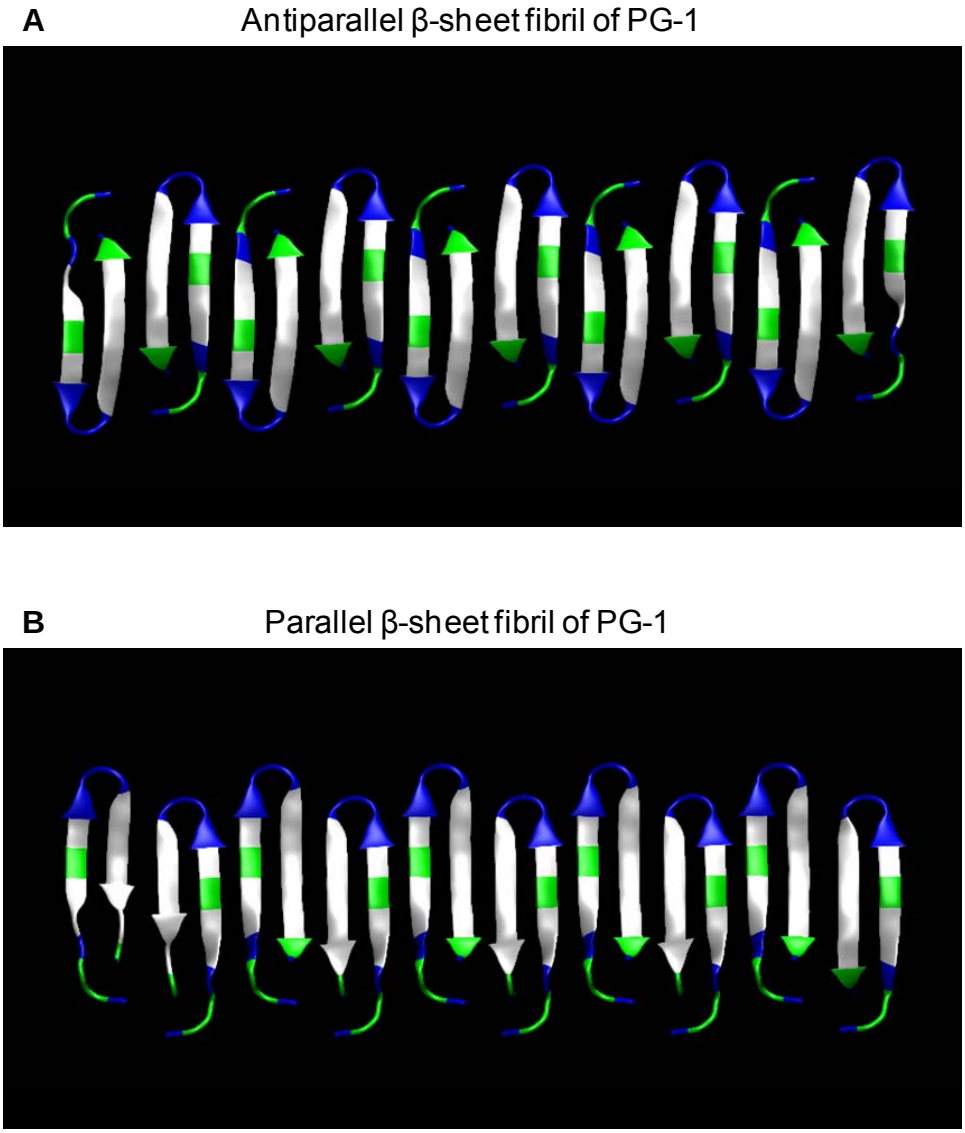

FIGURE S1 Pre-assembled planar β-sheet fibrils of PG-1. Initially, the PG-1 peptides are assembled to form the (*A*) antiparallel (turn-next-to-tail) and (*B*) parallel (turn-next-to-turn) β-sheets in a multimeric NCCN packing.

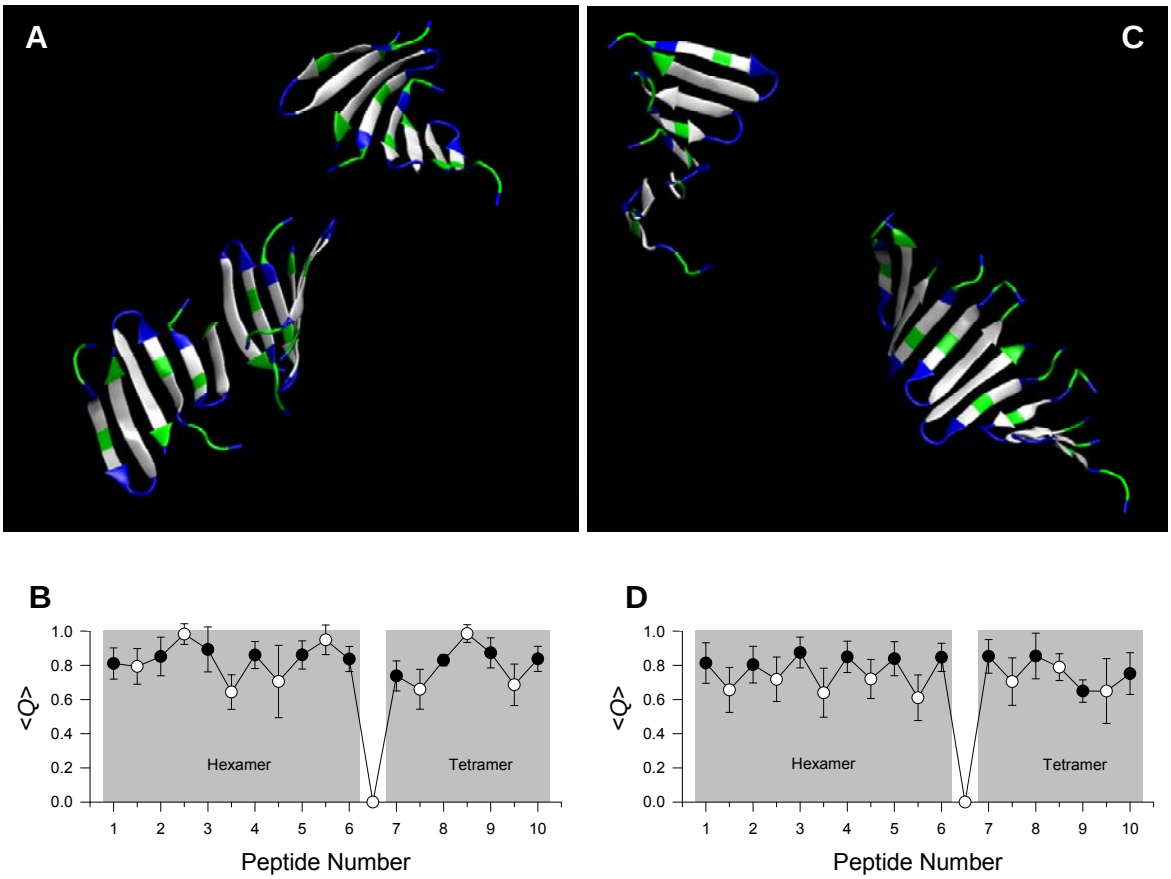

FIGURE S2 Snapshots of fibril structures in water at the end simulations in a ribbon representation for the (*A*) antiparallel and (*C*) parallel β-sheet fibrils of PG-1. In the peptides, hydrophobic residues are shown in white, polar and Gly residues are shown in green, and positively charged residues are shown in blue. Average fractions of intramolecular (solid circles) and intermolecular (open circles) backbone H-bonds, *Q*, as a function of peptide number for the (*B*) antiparallel and (*D*) parallel β-sheet fibrils of PG-1. Both antiparallel and parallel β-sheet fibrils break into 2 parts; hexamer and tetramer. Crossed β-sheet structures are distinct in the small PG-1 β-sheets.