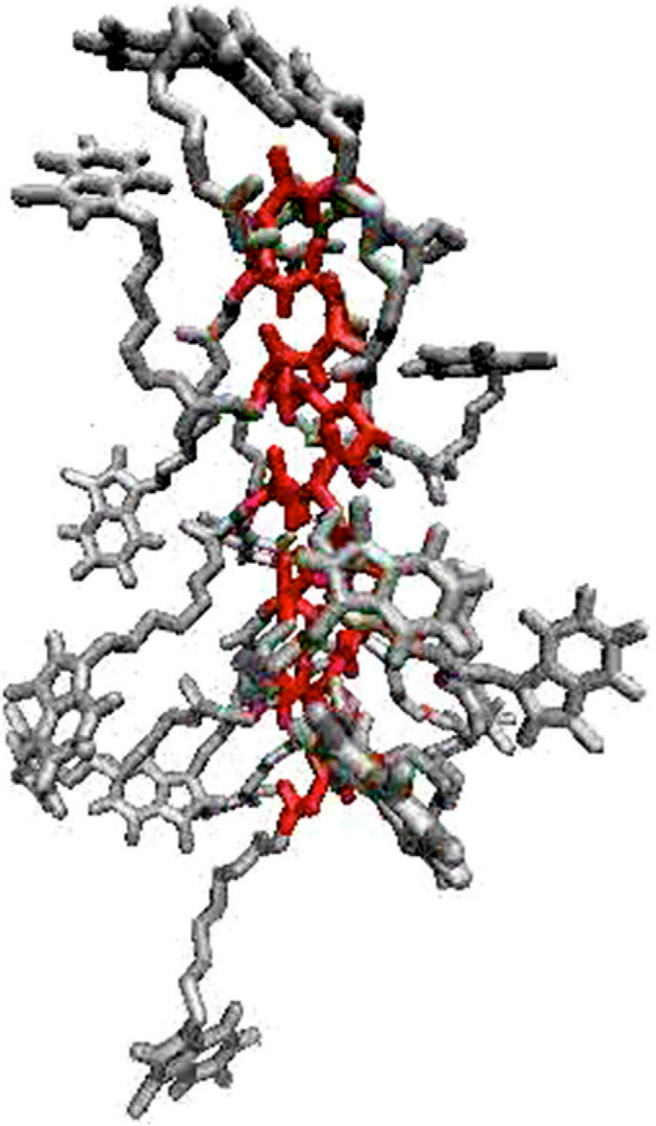
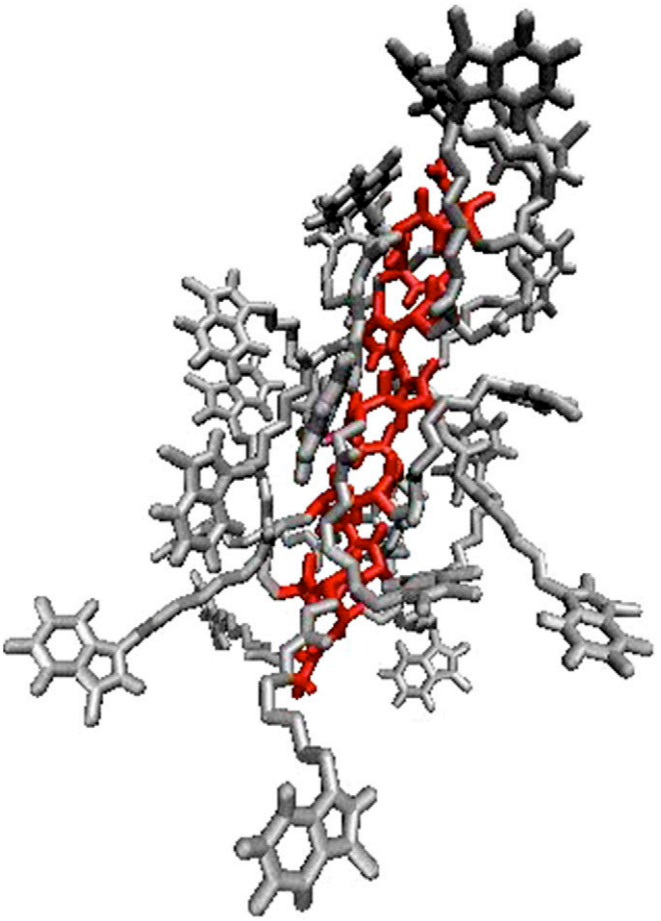
Supporting Information

Xiong et al. 10.1073/pnas.1507893112



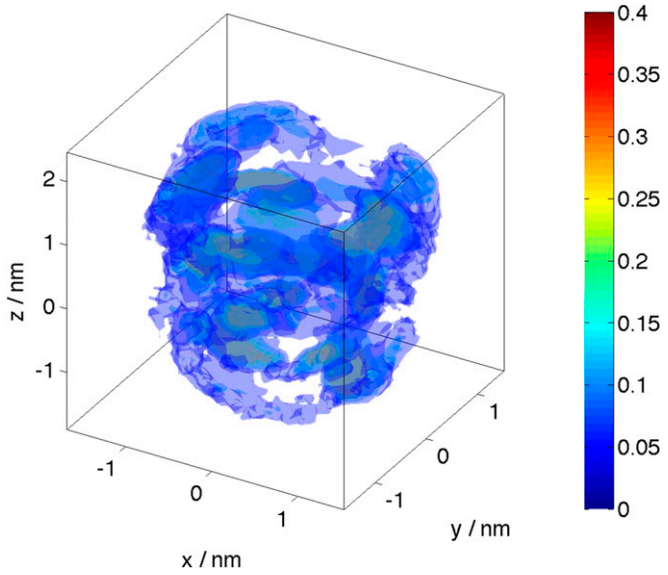
Movie S1. Movie of the 68-ns production simulation with frames rendered every 150 ps. For clarity of viewing, the peptide backbones in each configuration have been mutually aligned to a single reference configuration and water molecules removed. The peptide backbone is colored in red and the side chains in gray. This movie was produced using VMD (14).

Movie S1



Movie S2. A 360° rotation around a representative peptide configuration. For clarity of viewing, the water molecules have been removed and the backbone and side chains colored in red and gray, respectively. This movie was produced using VMD (14).

Movie S2



Movie S3. Fly-around of the 3D probability distribution of the side chain N_{12} atoms around the α-helical backbone. Histograms were compiled over the simulation trajectory using a grid comprising cubic cells of size 0.1 × 0.1 × 0.1 nm, and the probability density function computed by normalizing by the total count and the cell volume. The value of the probability density in any one cell ranged from 0 to 3.7 nm^{-3}. Four contours in the probability density are plotted at 0.05, 0.1, 0.2, and 0.3 nm^{-3}. Because the positive charge in the cationic side chains resides primarily in the termini, this distribution may be considered a proxy for that of the positive charge. This movie was produced using MATLAB (15).

Movie S3

Other Supporting Information Files

SI Appendix (PDF)