

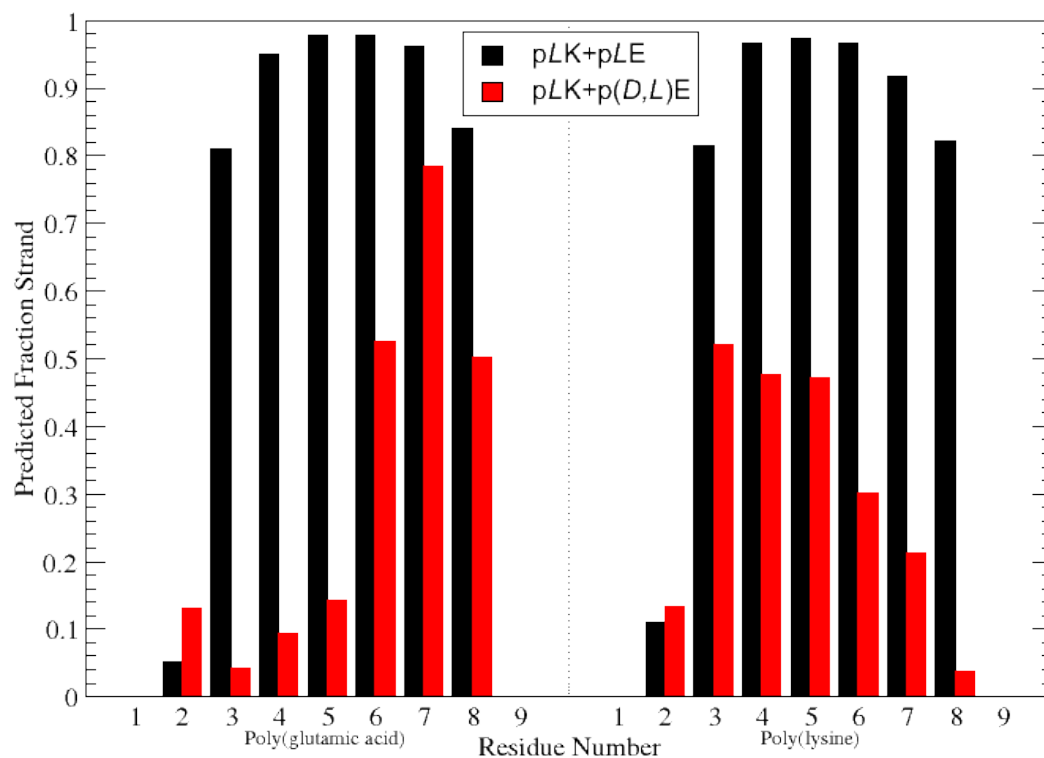
Supplementary Information: A Molecular View of the Role of Chirality in Charge-driven Polypeptide Complexation

K.Q. Hoffmann,^a S.L. Perry,^{ab} L. Leon,^{ac} D. Priftis,^a M. Tirrell^{ac} and J.J. de Pablo^{*ac}

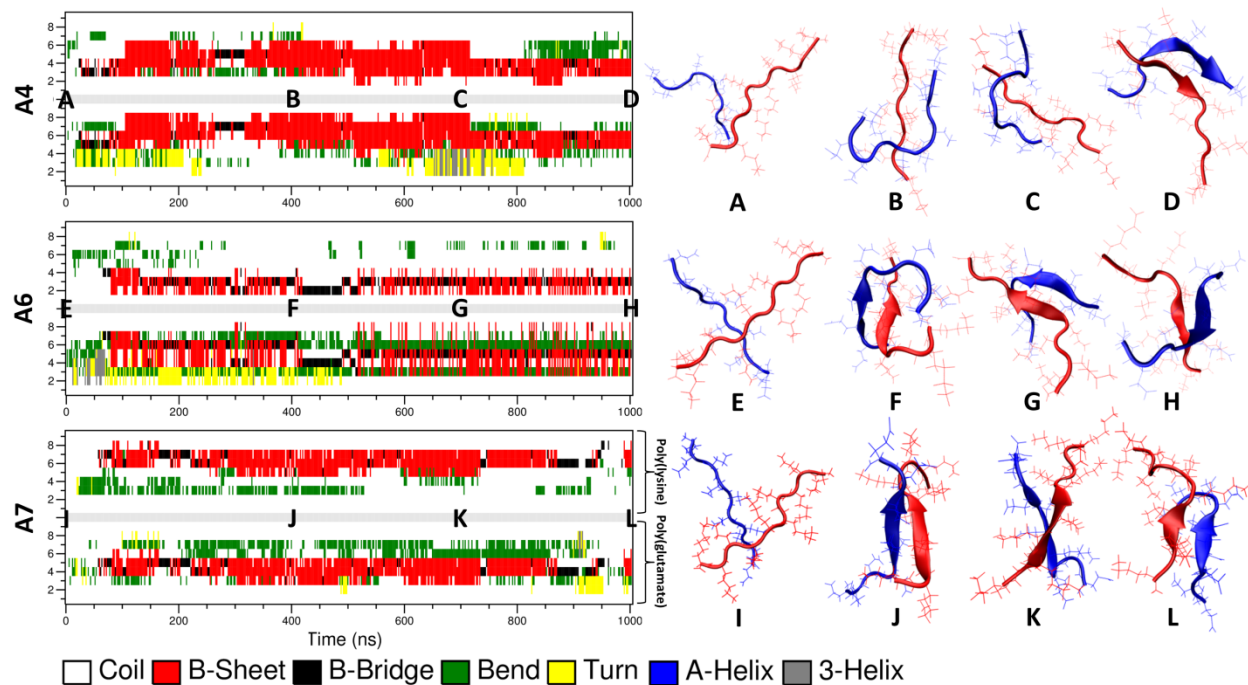
^a Institute for Molecular Engineering, University of Chicago, Chicago IL 60637, USA. E-mail: depablo@uchicago.edu.

^b Department of Chemical Engineering, University of Massachusetts Amherst, Amherst MA 01003, USA

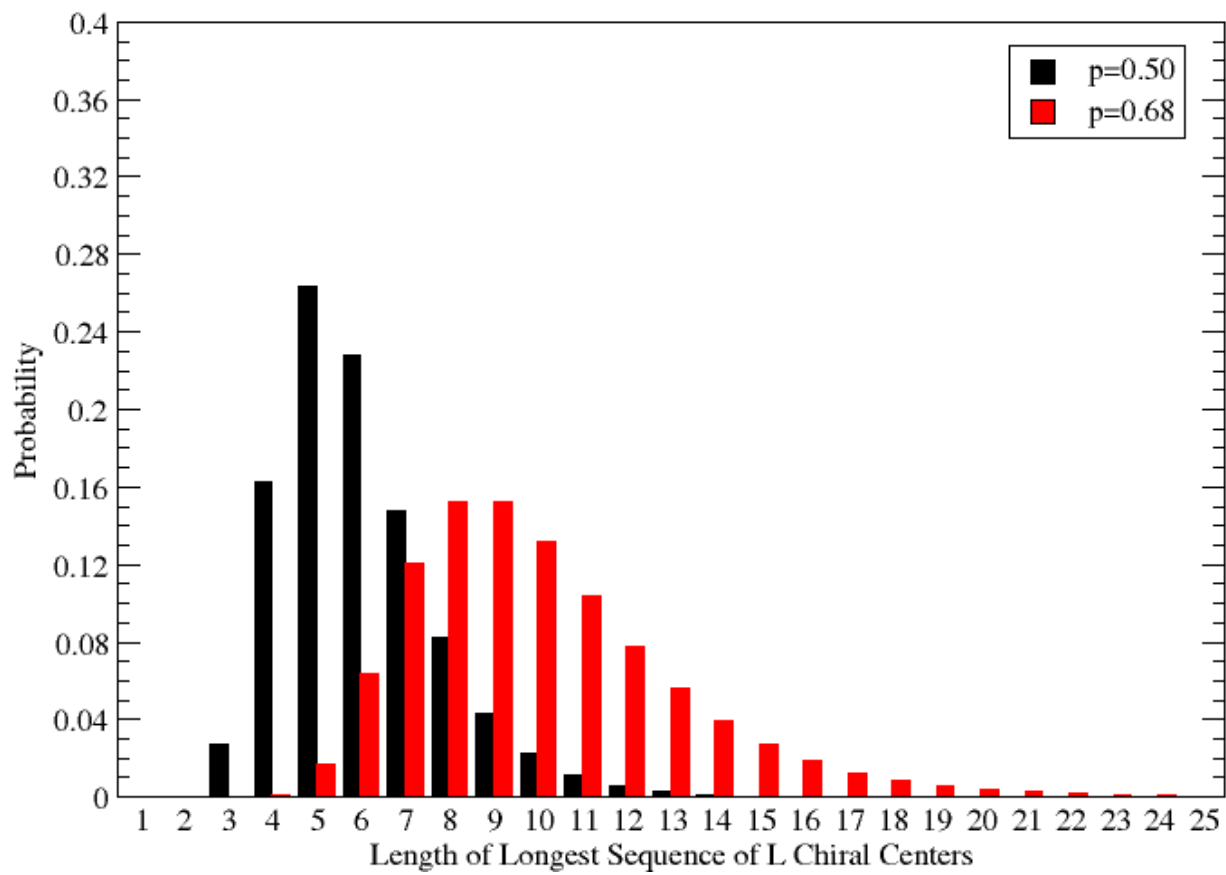
^c Institute for Molecular Engineering, Argonne National Laboratory, Argonne, IL70439, USA



Supplementary Figure S1. Average fraction of time each residue is in a strand (β -Sheet or β -Bridge) for pLK+pLE (black) and pLK+p(D,L)E (red).



Supplementary Figure S2. Secondary structure of each residue vs. time for various MD simulations of polypeptide pairs. “A” denotes a non-homochiral sequence. These sequences are given in Table 1. The PGLu chains are the bottom half of each figure, while the PLYs chains are in the top half. At each time, the secondary structure of each residue along the y-axis is denoted by the color. For example, red indicates a β -sheet structure. The structures of PLYs and PGLu are shown at 0, 400, 700, and 1000 ns for each pair. PLYs is shown in red, and PGLu is shown in blue.



Supplementary Figure S3. Distribution of maximum consecutive sequence of L-amino acids for a chain 100 residues long when the probability that each residue is L is 0.5 (black) and 0.68 (red).