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Search for Length Dependent Stable Structures of Polyglutamaine Proteins with Replica Exchange Molecular Dynamic[1] ALEXANDER KLUBER, ROBERT HAYRE, DANIEL COX, University of California Davis — Motivated by the need to find beta-structure aggregation nuclei for the polyQ diseases such as Huntington's, we have undertaken a search for length dependent structure in model polyglutamine proteins. We use the Onufriev-Bashford-Case (OBC) generalized Born implicit solvent GPU based AMBER11 molecular dynamics with the parm96 force field coupled with a replica exchange method to characterize monomeric strands of polyglutamine as a function of chain length and temperature. This force field and solvation method has been shown among other methods to accurately reproduce folded metastability in certain small peptides, and to yield accurately de novo folded structures in a millisecond time-scale protein. Using GPU molecular dynamics we can sample out into the microsecond range. Additionally, explicit solvent runs will be used to verify results from the implicit solvent runs. We will assess order using measures of secondary structure and hydrogen bond content.

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