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Molecular Dynamics Simulations of Alpha-synuclein MARIA SAMMALKORPI, CARL SCHRECK, ABHINAV NATH, DAVID DEWITT, ELIZABETH RHOADES, COREY O'HERN, Departments of Chemical Engineering, Physics, Mechanical Engineering and Materials Science, and Molecular Biophysics and Biochemistry, Yale University — We investigate the conformational dynamics of single alpha-synuclein proteins, which have been implicated in amyloid diseases such as Parkinson's and Alzheimer's disease, in solution using unconstrained and constrained all-atom, explicit solvent molecular dynamics simulations. The constraints on inter-residue separations are obtained from our single-molecule FRET measurements of eleven FRET pairs that span the protein. By comparing the simulation data satisfying different combinations of FRET constraints, we are able to identify those constraints that are most important in determining the radius of gyration and key features of the contact map of the protein.

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