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Estimates of Twisting and Bending Rigidities of Beta-Solenoid Proteins Using Molecular Dynamics[1] AMANDA PARKER, KRISHNAKUMAR RAVIKUMAR, DANIEL COX, UC Davis — The use of beta-solenoid proteins as functionalizable, nano-scale, self-assembling molecular building blocks has many applications, including in templating the growth of wires or higher-dimensional structures. By understanding their mechanical strengths, we can more efficiently design the proteins for specific functions. We present a study of the mechanical properties of seven beta-solenoid proteins, where we use GROMACS molecular dynamics software to produce force/torque-displacement data, implement umbrella sampling of bending/twisting trajectories, produce PMFs, extract effective spring constants, and calculate rigidities, for two bending and two twisting directions for each protein. In particular, we examine the differences between computing the strength values from force/torque-displacement data alone and PMF data. In addition to the analysis of the methods, we report estimates for the flexural and torsional persistence lengths for each protein, which range from approximately 0.5-3.4 μm.

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