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Mechanical Strength of Beta-Solenoid Proteins Under Bending and Twisting Simulations[1] AMANDA PARKER, KRISHNAKUMAR RAVIKUMAR, DANIEL COX, UC Davis — We present a study of the mechanical properties of seven beta-solenoid antifreeze proteins, using molecular dynamics simulations. The goal is three-fold: (i) to collect and organize data on a range of beta-solenoid proteins, (ii) to investigate the validity and reproducibility of common techniques of measuring the mechanical strength of proteins computationally, and (iii) to find evidence for relationships between attributes of these proteins and their mechanical strength. The proteins studied vary in length, number of turns, amino acids per turn, handedness, cross-sectional area, and number of sides. The mechanical properties of the proteins are measured by conducting and analyzing bending and twisting simulations, in multiple directions, for each protein. The results are validated in part by repeating the procedure, for each direction, for each protein. Values for the bending and twisting moduli are calculated and tabulated.

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