Problem set 5

Due November 24, 2026

1. Derive the formula for the end-to-end distance of a wormlike chain with total length L and persistence length a that has ta sharp bend with angle β at length l.

2. Using the UNRES server (`https://unres-server.chem.ug.edu.pl`), run Langevin dynamics simulations for polyglycine chains with 10, 20, 30, and 40 residues (run 200,000 MD steps as per standard settings; the results of calculations of Problem set 4 can be used), starting from random-generated structures at $T = 300$ K and 350 K. Compute the average end-to-end distance from each run. Make log-log plots of the distance vs. chain length. By using linear regression determine the scaling coefficient ν at both temperatures.