CB&B752/MCDB452/MB&B752/MCDB752/CPSC752
Homework 1

Problem 1:

For the BLN model protein discussed in class (see J. D. Honeycutt and D. Thirumalai, "The nature of folded states of globular proteins," Biopolymers 32 (1992) 695 & T. Veitshans, D. Klimov and D.Thirumalai, "Protein folding kinetics: timescales, pathways and energy landscapes in terms of sequence-dependent properties", Folding and Design 2 (1997) 1-22) which includes Lennard-Jones-like long-range (V_{lr}), bond length (V_{bl}), bond angle (V_{ba}), and dihedral angle (V_{da}) interactions, calculate the total potential energy, given by $V_{tot} = \sum_{i=1}^{N}\sum_{j=1}^{i-2} V_{lr}\left(r_{i,j}\right) + \sum_{i=1}^{N-1} V_{bl}\left(r_{i,i+1}\right) + \sum_{i=1}^{N-2} V_{ba}\left(\theta_{i,i+1,i+2}\right) + \sum_{i=1}^{N-3} V_{da}\left(\phi_{i,i+1,i+2,i+3}\right)$, where $r_{i,j} = \left|\vec{r}_i - \vec{r}_j\right|$, $\vec{r}_i$ locates the center of monomer i, σ is the diameter of the monomer, $V_{lr}\left(r_{i,j}\right) = 4\varepsilon_h\left[\left(\frac{\sigma}{r_{i,j}}\right)^{12} + C\left(\frac{\sigma}{r_{i,j}}\right)^{6}\right]$ with C=-1 and $\varepsilon=\varepsilon_h$ when i,j=B,B, C=1 and $\varepsilon=\varepsilon_L=2/3\varepsilon_h$ when i,j=LL, LB, and C=0 and $\varepsilon=\varepsilon_h$ when i,j=NN, NL, NB, and ε_h is the Lennard-Jones energy scale, $V_{bl}\left(r_{i,j}\right) = \frac{k_b}{2}\left(r_{i,j} - \sigma\right)^2$, k_b is the spring constant, $V_{ba}\left(\theta_{i,j,k}\right) = \frac{k_\theta}{2}\left(\theta_{i,j,k} - \theta_0\right)^2$, k_θ is the bend spring constant, $\theta_{i,j,k} = \cos^{-1}\left(\frac{\vec{r}_{i,j}\bullet\vec{r}_{k,j}}{r_{i,j}r_{k,j}}\right)$, and θ_0 is the equilibrium bend angle, $V_{da}(\phi_{i,j,k,l}) = A(1+\cos(\phi_{i,j,k,l})) + B(1+\cos(3\phi_{i,j,k,l}))$, where A and B constants and where $\phi_{I,j,k,l}$ is defined by $\cos\left(\phi_{i,j,k,l}\right) = (\vec{r}_{i,j}\times\vec{r}_{k,j})\cdot(\vec{r}_{j,k}\times\vec{r}_{l,k})/\left(\left|(\vec{r}_{i,j}\times\vec{r}_{k,j})\right|\left|(\vec{r}_{j,k}\times\vec{r}_{l,k})\right|\right)$ and $\sin\left(\phi_{i,j,k,l}\right) = \vec{r}_{j,k}\cdot\left[(\vec{r}_{i,j}\times\vec{r}_{k,j})\times(\vec{r}_{j,k}\times\vec{r}_{l,k})\right]/\left(\left|(\vec{r}_{i,j}\times\vec{r}_{k,j})\right|\left|(\vec{r}_{j,k}\times\vec{r}_{l,k})\right|\right)\cdot$

Calculate the total potential energy V_{tot} for the configuration of the (N=46) polymer $B_9N_3(LB)_4N_3B_9N_3(LB)_5L$ in the file config.dat.

Download the file config.dat from the course website, which lists the positions of the 46 monomers corresponding to the ground state of the BLN model $B_9N_3(LB)_4N_3B_9N_3(LB)_5L$ in the following format:
r_{x1} r_{y1} r_{z1}
r_{x2} r_{y2} r_{z2}
…
r_{xN} r_{yN} r_{zN}

All above constants can be found in Protein folding kinetics: timescales, pathways and energy landscapes in terms of sequence-dependent properties", Folding and Design 2 (1997) 1-22). The final energy value should be in terms of ε_h.

Note: The long range energetic interaction $V_{lr}\left(r_{i,j}\right) = 4\varepsilon_h\left[\left(\frac{\sigma}{r_{i,j}}\right)^{12} + C\left(\frac{\sigma}{r_{i,j}}\right)^{6}\right]$ applies only to non-adjacent amino acids.