

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

$$V_{tot} = \sum_{i=1}^N \sum_{j=1}^{i-2} V_{lr}(r_{i,j}) + \sum_{i=1}^{N-1} V_{bl}(r_{i,i+1}) + \sum_{i=1}^{N-2} V_{ba}(\theta_{i,i+1,i+2}) + \sum_{i=1}^{N-3} V_{da}(\phi_{i,i+1,i+2,i+3}),$$

where $r_{i,j} = |\vec{r}_i - \vec{r}_j|$, \vec{r}_i locates the

center of monomer i , σ is the diameter of the monomer, $V_{lr}(r_{i,j}) = 4\epsilon_h \left[\left(\frac{\sigma}{r_{i,j}} \right)^{12} + C \left(\frac{\sigma}{r_{i,j}} \right)^6 \right]$ with $C=-1$ and $\epsilon=\epsilon_h$

when $i,j=B,B$, $C=1$ and $\epsilon=\epsilon_L=2/3\epsilon_h$ when $i,j=LL, LB$, and $C=0$ and $\epsilon=\epsilon_h$ when $i,j=NN, NL, NB$, and ϵ_h is the Lennard-Jones energy scale, $V_{bl}(r_{i,j}) = \frac{k_b}{2}(r_{i,j} - \sigma)^2$, k_b is the spring constant, $V_{ba}(\theta_{i,j,k}) = \frac{k_\theta}{2}(\theta_{i,j,k} - \theta_0)^2$, k_θ is

the bend spring constant, $\theta_{i,j,k} = \cos^{-1} \left(\frac{\vec{r}_{i,j} \cdot \vec{r}_{k,j}}{r_{i,j} r_{k,j}} \right)$, 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 $\cos(\phi_{i,j,k,l}) = (\vec{r}_{i,j} \times \vec{r}_{k,j}) \cdot (\vec{r}_{j,k} \times \vec{r}_{l,k}) / \left(\left\| (\vec{r}_{i,j} \times \vec{r}_{k,j}) \right\| \left\| (\vec{r}_{j,k} \times \vec{r}_{l,k}) \right\| \right)$ and

$\sin(\phi_{i,j,k,l}) = \vec{r}_{j,k} \cdot \left[(\vec{r}_{i,j} \times \vec{r}_{k,j}) \times (\vec{r}_{j,k} \times \vec{r}_{l,k}) \right] / \left(\left\| (\vec{r}_{i,j} \times \vec{r}_{k,j}) \right\| \left\| (\vec{r}_{j,k} \times \vec{r}_{l,k}) \right\| \right)$.

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 $V_{lr}(r_{i,j}) = 4\epsilon_h \left[\left(\frac{\sigma}{r_{i,j}} \right)^{12} + C \left(\frac{\sigma}{r_{i,j}} \right)^6 \right]$ applies only to non-adjacent

amino acids.