Assignment 3

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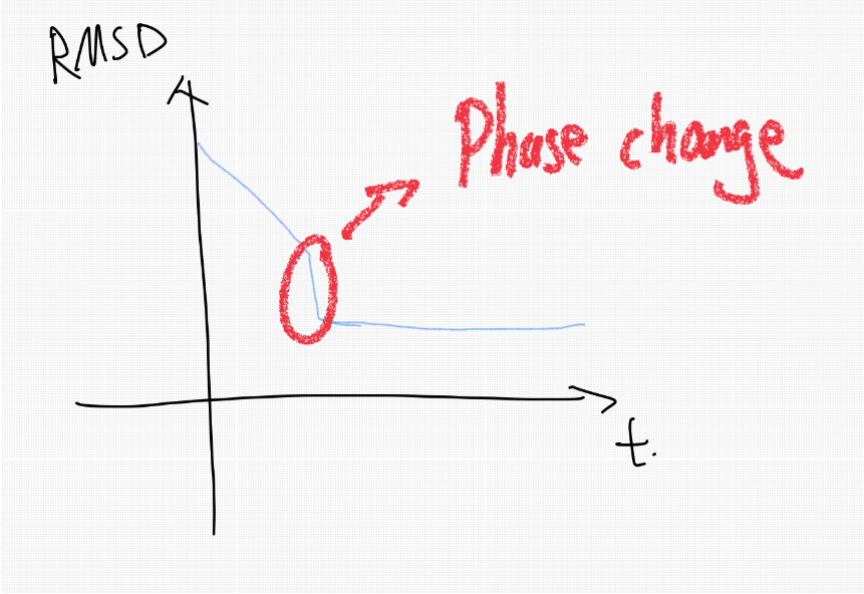
1 Problem 1

From statistical mechanics, we know the following rule. When there is a phase change, some function related to the structure of the system will change abruptly. More specifically, you could calculate **RMSD** for the system under investigation. Over time, you should see a discontinuity in the plot of time versus **RMSD**. That's when a phase change occurred.

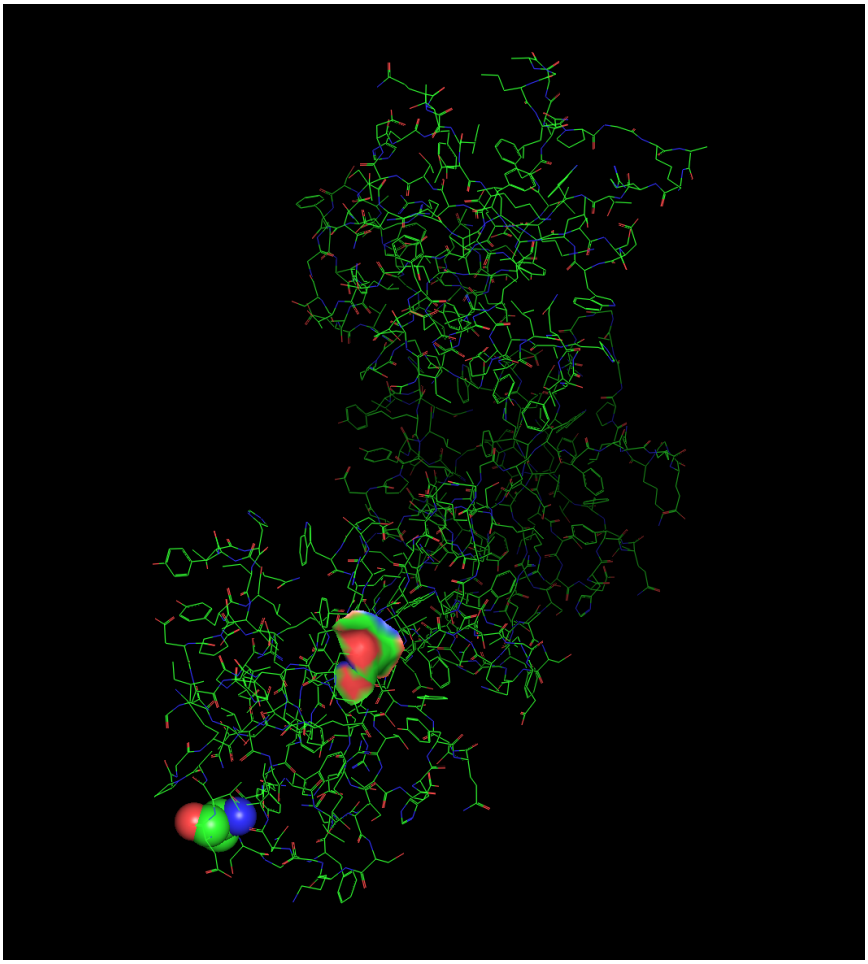
A plot may look something like this.



2 Problem 2

In a folded protein, I expect to find hydrophobic amino acids in the **innerds** of the structure. Conversely, I expect to find hydrophilic amino acids on the **outside** of the folded protein. This is basically due to the need to minimize energy in the folded state of a protein.

- Hydrophobic Amino Acid: Alanine
- Hydrophilic Amino Acid: Aspartic Acid
- I have illustrated the protein: BARNASE MUTANT WITH ILE 88 REPLACED BY ALA (1BRJ). In addition, I illustrated the hydrophobic amino acid, Alanine, as balls. I also illustrated the hydrophilic amino acid, Aspartic Acid, as surface.



3 Problem 3

4 Problem 4