



Homework 05

- is to be submitted for grading after 1 week in class; no late submissions are accepted
- show your work neatly – if I do not understand logic in your steps, you will lose points
- make a sincere effort to understand the problems; otherwise you may not do well on the presentation and on the exams

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1. Using the “Complete Rotamer Library” given in the lecture notes, for ubiquitin compute the size of the conformational search space if

- A) all amino acid side chains are repacked
- B) just the core amino acid side chains are repacked
- C) all amino acid side chains are redesigned
- D) just the core amino acid side chains are redesigned

Explain your logic in distinguishing core from non-core amino acids. Rationalize the number of “rotamers” you use per amino acid.