Challenge 1

LCVC Module 2 – 2021/2022

Access the Google Colab Notebook at:

https://colab.research.google.com/drive/1BfIIZHmD0DVZ9Iy4fwCn30uLbVmaK5OF?usp=sharing

1. Mutate residue 48 to be of type ALA, ARG and SER.
2. Homework: Make a GIF/movie with all possible mutations for residue 48 (other than PRO).

3. Load the default Dunbrack Rotamer Library.
4. Apply a different (random) rotamer to residue 48 (in the original structure, may have to reload the pose).
5. Loop over 5 random rotamers for residue 48 and show all the rotamers in a GIF/movie.
6. Homework: Make a GIF/movie showing multiple residues changing rotamers simultaneously.