

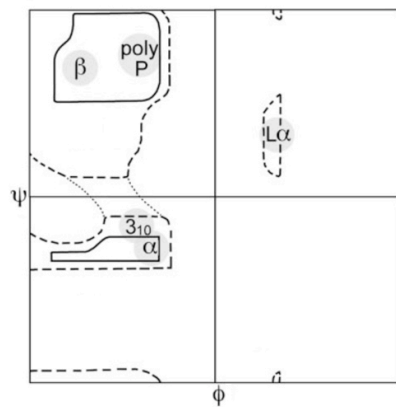


Tasks on the Computer:

In any protein chain, the secondary structures are manifest in two dihedral angles called ϕ and ψ .

1. Using a quick search on the internet, report what atoms make up the two angles. Enter the three atoms required for each angle.

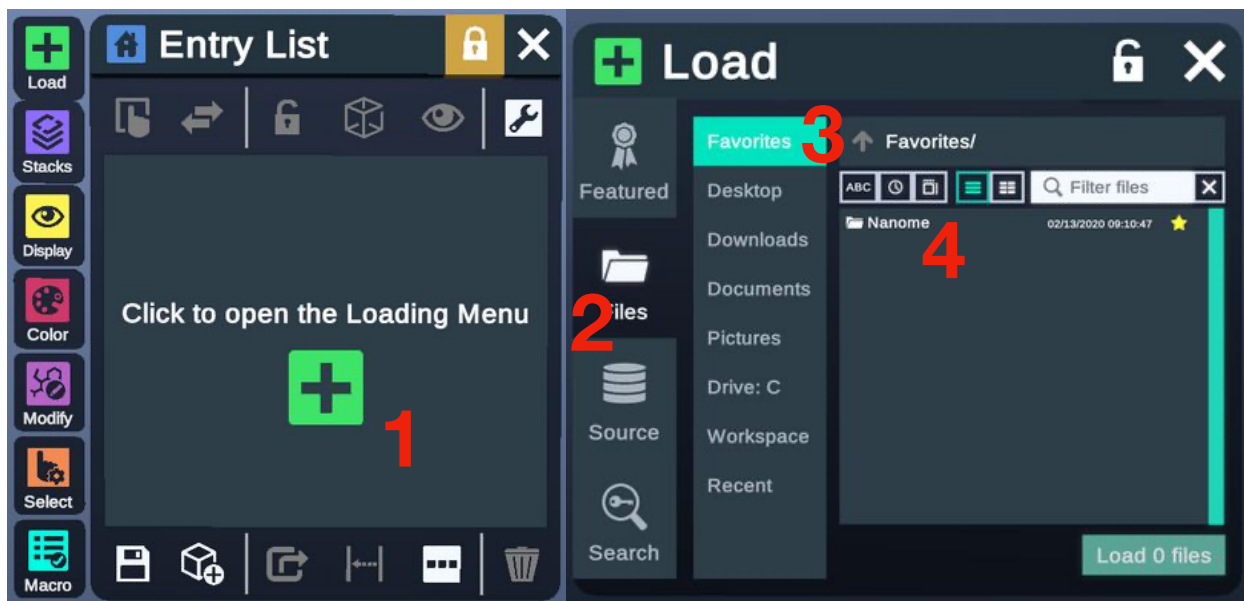
Different ranges in values of ϕ and ψ leads to different secondary structures. A plot of ϕ vs. ψ distribution is known as the Ramachandran plot. Here's a general version of such a plot:





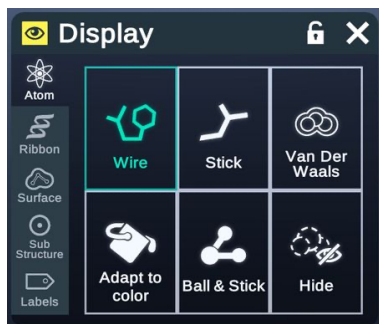
Tasks in VR:

1. Open Nanome and load the Alanine-helix.pdb file by using the load module from favorites/Nanome/Task-X/

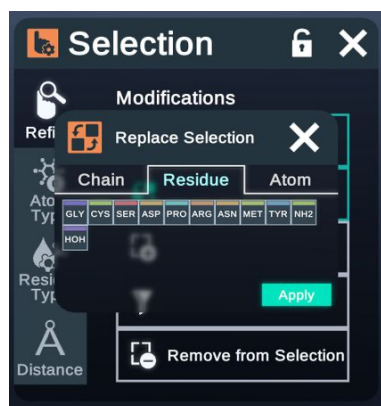


Inspect the structure.

2. Use the Display panel to set the representation of the whole molecule to ball and stick.



3. Use the select panel to select residues 9 and 10, and label them by residue number.



4. From the measurement tool (hold X), use the **dihedral** option to measure the ϕ and Ψ of residues 9 and 10 of the helical structure. What are the values? How do they compare to the Rama plot you see above?
5. Use the torsion tool to select one of the angles you just measured and change it to a different value which falls outside the normal region of alpha helices on the Rama plot.
6. Measure your angle again and report its value.
7. Show the clashes on your molecule. Does the new angle lead to any steric clashes?

Proline is a well-known helix-breaker. In this part we are going to mutate a residue and examine its effect on the helical structure.

8. Use the mutation tool to mutate residue 15 to to proline. Examine steric clashes and watch for ϕ and Ψ . Why do you think proline is a helix-breaker?
9. Use the camera module to take a picture of your peptide with the angle labels, mutation and the whole molecule clearly visible.