

# Making measurements in molecular visualization software

Purpose: Some of the most common tasks in molecular visualization and analysis include measuring distances between atoms, and measuring dihedral angles. You should be comfortable doing this in several packages.

## Using Rasmol

1. What is the length of the longest dimension of calmodulin?
2. Open the file `~/rosetta_workshop/tutorials/day02/sample_files/1CLL.pdb` in stick mode
3. Use **Settings** → **pick Distance**, and choose two atoms from the most distant residues at opposite ends of the protein.

## Using Pymol

1. Open a pregenerated session showing one helix from the potassium channel:  
`pymol ~/rosetta_workshop/tutorials/day02/sample_files/alpha_helix.pse`
2. Use **Wizard** → **Measurement** to measure several several (i, i+4) H-bonds (you can hide side chains to simplify the display)
3. You can change the **drop-down** box called Distances to Angles or Dihedrals
4. An alternate method is to **ctrl-middle-click** on two atoms (producing pk1 and pk2), then type distance. **Ctrl-right-click** on the background to clear the picked atoms.
5. The command-line syntax to do distance and angle measurements looks like this example. This is particularly useful for putting into custom scripts.  
`get_dist ///A/102/O, ///A/106/N`  
`get_angle ///A/103/N, ///A/103/CA, ///A/103/CB`  
`get_dihedral ///A/103/N, ///A/103/CA, ///A/103/C, ///A/104/N`

## Using Chimera

1. Measure the dihedral angles of one residue in a helix and one residue from a beta sheet.
2. Restore the session: `chimera ~/rosetta_workshop/tutorials/day02/sample_files/dihedrals.py` One segment of helix and one of sheet have been shown in stick mode in this small cytochrome.
3. Use **Tools** → **Structure Analysis** → **Angles/Torsions** (you can do Distances analogously)
4. Select 4 sequential backbone atoms in the beta strand, then “**Create**” angle measurement.
  1. Select atoms in order: C, N, CA, C to measure phi
  2. Select atoms in order: N, CA, C, N to measure psi
  3. Select atoms in order: CA, C, N, CA to measure omega
5. If you have time, you may repeat with a turn of the helix.