1. Load *ala-ala-ala.gro* and *ala-ala-ala.xtc* from last lab into VMD.
   (a) Go to *Extensions→Analysis→Ramachandran Map*
   (b) Select "0" from the *Molecule* drop down
   (c) Type "resid 3" into the *Selection* box and hit ENTER. (You should now only see one yellow dot on the Ramachandran plot).
   (d) Click "Create 3-d histogram"
2. Where are the peaks in this plot? What does this tell you about the conformational preferences of Ala?
3. Repeat the same steps for the *ala-gly-ala* and *ala-pro-ala* simulations. (These can be found in the *md-files* directory).
4. Where are the peaks in this plot? What does this tell you about the conformational preferences of glycine and proline? Can you justify these observations in terms of the amino acid side chain?
5. Download *phi-psi.zip*. This has a list of $\phi/\psi$ angles acids calculated for simulations of *ala-X-ala* peptides like the simulations you looked at above. (If you want to see how this was calculated, check out *md-files/phi-psi.tcl*).
6. By a very loose definition, $\alpha$-helices have $\phi \in [-180°, -30°]$ and $\psi \in [-90°, +10°]$. For an amino acid of your choice, what fraction of the time does it spend in the $\alpha$-helical conformation over the simulation?
7. Estimate the change in conformational entropy if this amino acid was placed at a position in a protein that constrained it to be helical, with the bounds: $\phi \in [-70°, -30°]$ and $\psi \in [-70°, +10°]$.
8. Estimate the conformational entropy change for ALA-ALA-ALA-ALA-ALA-ALA to fold into a helix (e.g. $\phi \in [-70°, -30°]$ and $\psi \in [-70°, +10°]$).
9. Estimate the conformational entropy change for GLN-ALA-ARG-HIS-PRO-ALA to fold into a helix (e.g. $\phi \in [-70°, -30°]$ and $\psi \in [-70°, +10°]$). What is the free energy difference, at 298 $K$, for folding this peptide into a helix, as opposed to a chain of six ALA?
10. What assumption(s) do you have to calculate these differences in energy? How might those assumptions affect your estimate?