

# Biophysical Chemistry I, Fall 2010

## Homework Assignment #3, due Sept. 30

1. Download the 1IL8 entry from the PDB. If you examine the structure in VMD, you will see that it consists of two polypeptide chains. In two to four sentences, qualitatively describe the nature of the interface between the two chains.
2. In two to four sentences, describe the biological context for interleukin-8.
3. Your analysis task is to compute the amount of buried surface area as chains "A" and "B" come together. The buried surface area is given by the sum of the surface areas of chain "A" (by itself) and chain "B" (by itself) minus the surface area of the structure consisting of both chains together. To do this in VMD, you will need to use the TCL scripting component. Here are a couple of places to start:
  - (a) Learn about the "atomselect" command to create atom selections:  
<http://www.ks.uiuc.edu/Research/vmd/current/ug/node118.html>.
  - (b) Use the "measure sasa" command to get surface areas: see  
<http://www.ks.uiuc.edu/Research/vmd/current/ug/node133.html>.
4. A rough(!) estimate of the hydrophobic driving force for bringing the two chains together is that the "surface burial energy" (in kcal/mol) is 0.005 times the amount of buried surface area (in  $\text{\AA}^2$ ) [Sitkoff, Sharp & Honig, *J. Phys. Chem.* 98:1978, 1994.] What does this give you for a burial free energy?