Assignment 9

version 1.0

1. Launch Pymol
2. Set up Pymol by copying and pasting the following (all at once) into the command line

#-----first line in copy------------------------------------------------------------------------

## Header: General Commands ##

# delete all objects and reset pymol

reinitialize

# set the background color to white

bg\_color white

# make the background transparent for ray trace

set ray\_opaque\_background, 0

# set the ray trace mode

# normal color

set ray\_trace\_mode, 0

# normal color + black outline

#set ray\_trace\_mode, 1

# black outline only

#set ray\_trace\_mode, 2

# turn off shadows during ray trace

set ray\_shadows, 0

# set the mouse mode for laptop.

config\_mouse one\_button

# get rid of double bonds and skinny bonds to H

set stick\_h\_scale, 1

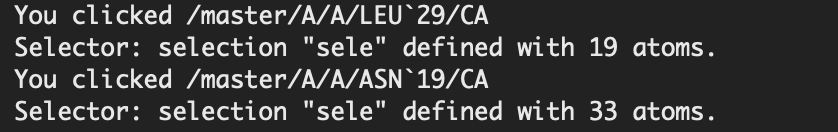
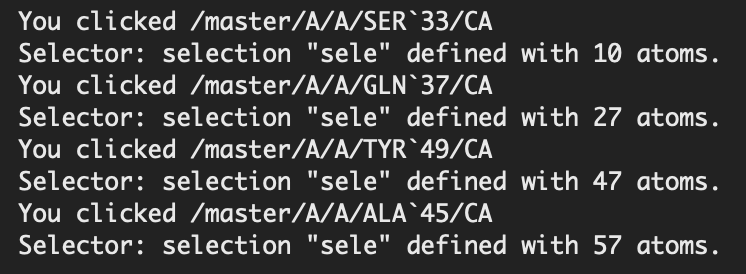
set valence, 0

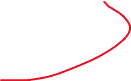
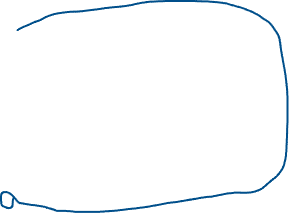
# high quality surfaces

set surface\_quality, 3

## End of Header: General Commands ##

#-------last line in copy---------------------------------

1. Get your protein  
   Type:   
   fetch ZZZZ, master  
   where ZZZ is the pdb code of your protein.  
   This is a slight variation of what we did previously with the fetch command. The command as used here downloads your coordinates into PyMol and puts them into an object called “master”)
2. Use the commands you previously learned to  
   (i) display your protein (the master object) as a cartoon (this is the default),  
   (ii) color it by secondary structure,  
     
   (iii) create an object (called helix1) that contains an a-helix  
     
   If your protein does not have an a-helix (rare but not impossible) see \* at the end of section e.  
     
   To create the object, first identify an a-helix by looking at the ribbon structure in PyMol,  
   then click on the ribbon on either end of the helix,  
   look just above the command line and you will see something like this  
     
   type  
   create helix1, resi 19-29  
   (your residue identifiers (amino acid numbers) and residue names (amino acid types) will not be the same as what I have typed here)  
   (PyMol is case sensitive, and the syntax (commas, etc) must be exact).  
     
   If the command above selects multiple helices, change it to  
   create helix1, resi 19-29 and chain A  
     
   (iv) create an object (called sheet1) that contains a 2 stranded b-sheet  
   for this you will have to identify both strands and click on a total of four places to identify the start and stop of each of the two strands  
     
     
   type  
   create sheet1, resi 33-37 or resi 45-49  
   (note the boolean operator “**or**”. Do not use “and” here, it won’t select anything for your object)  
     
   (v) create an object (loop1) that contains a loop region of at least 7 amino acids



1. In this section we will study your a-helix.   
   The commands below convert all of your sidechains to alanine (easier to see), add hydrogens and draw hydrogen bonds. Please look through the commands and get a general sense of what each is doing. You will need to use them later on.  
   Copy and paste the following  
     
   #---------start copy --------------  
   # center the display on helix1  
   zoom helix1  
   # strip away the sidechains  
   ﻿remove helix1 and not (backbone or name CB)  
   # add hydrogen atoms to object helix1  
   h\_add helix1  
   # find helix1 backbone atoms (either O or H) that are within hydrogen bonding distance of each other (2.3 Å). Put these distances in an object called hbond1)  
   distance hbond1, (name O\* and helix1), (name H\* and helix1), 2.3  
   # color the hydrogen bonds and set the dash width etc  
   color black, hbond1  
   set dash\_width, 5, hbond1  
   set dash\_gap, 0.4, hbond1   
   # Set the atom colors  
   color wheat, name C\* and (helix1)  
   color red, name O\* and (helix1)  
   color blue, name N\* and (helix1)  
   # set the display as stick  
   hide everything, helix1  
   show sticks, helix1  
   #---------end copy --------------  
     
   Save images of each object in two views, rotated by approximately 90°.  
   use   
     
   ray 1000,1000  
   save image\_name\_view1.png  
     
   save 2 images (different views) of your   
   master object, (name the images image\_name=master\_pdbid),   
   helix (use image\_name=helix\_pdbid),   
   sheet (image\_name=sheet\_pdbid), and   
   loop (image\_name=sheet\_pdbid)   
     
   \* If your protein does not have one of the secondary elements required for this assignment (i.e., it does not contain any a-helix or b-sheet) then use PDB entry 3IBF just for the missing secondary element. Use your protein for as much of this assignment as possible.
2. Hydrogen Bonds   
     
   Measure and record all the hydrogen bonding distances, O to H within the a-helix.  
   Make a table of these distances and determine the average and standard deviation.   
     
   Measure and record the hydrogen bonding angles, N to H to O (you need the wizard for this). (For this you will need to use Wizard -> Measurement (on the top menu), then go to the pull down measurement menu (on the bottom right) and set measurement to angle.)   
   Make a table of these angles and determine the average and standard deviation.  
     
   Measure and record the hydrogen bonding angles, C’ to O to H (note that C’ is usually called C in coordinate files)  
   Make a table of these values and record the average and standard deviation.
3. Phi and Psi (For this you will need to use Wizard -> Measurement (on the top menu), then go to the pull down measurement menu (on the bottom right) and set measurement to dihedral. A torsion angle is the same thing as a dihedral angle). A torsion angle is defined by 4 atoms, so you will have to click on 4 atoms for each torsion angle.   
     
   Measure and record all of the phi torsion angles in your a-helix. Phi is defined by C’-N-Ca-C’. Coordinate files will usually call these atoms C-N-CA-C. The numbering is C(j)-N(j+1)-CA(j+1)-C(j+1)   
     
   Measure and record all of the psi torsion angles in your a-helix. Psi is defined by N-Ca-C’-N. The numbering is N(j)-CA(j)-C(j+1)-N(j+1).  
     
   Measure and record all of the phi and psi torsion angles in your b-sheet and in your loop.  
     
   Graph the phi/psi pairs of your a-helix, b-sheet and loop using the layout of a standard Ramachandran plot.
4. Insert all the images, tables and graphs into a file called Assignment\_9\_lastname.docx. Clearly label each image, table and graph.