Name:

**\*\* ONLY TEXT AND IMAGES APPEARING INSIDE THE RED BOXES WILL BE GRADED\*\***

1. Earlier in the semester you chose a pdb entry number for a protein that interests you. Write your pdb entry code in the red box:

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| INSERT HERE |

1. Make a phi/psi map for your protein using Jane Richardson’s Molprobity. The link to [Molprobity](http://molprobity.biochem.duke.edu/) and [Instructions for using Molprobity](https://ww2.chemistry.gatech.edu/~lw26/course_Information/4511/misc/molprobity_phi_psi_instructions.pdf) are on the course website. Insert the pdf image of your phi/psi map here Resize it so that it will fit on this page.

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1. Launch Pymol, set it up, and download the scorpion venom protein. To do this, copy and paste the text below into the command line of PyMol and hit return.

#-----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, 2

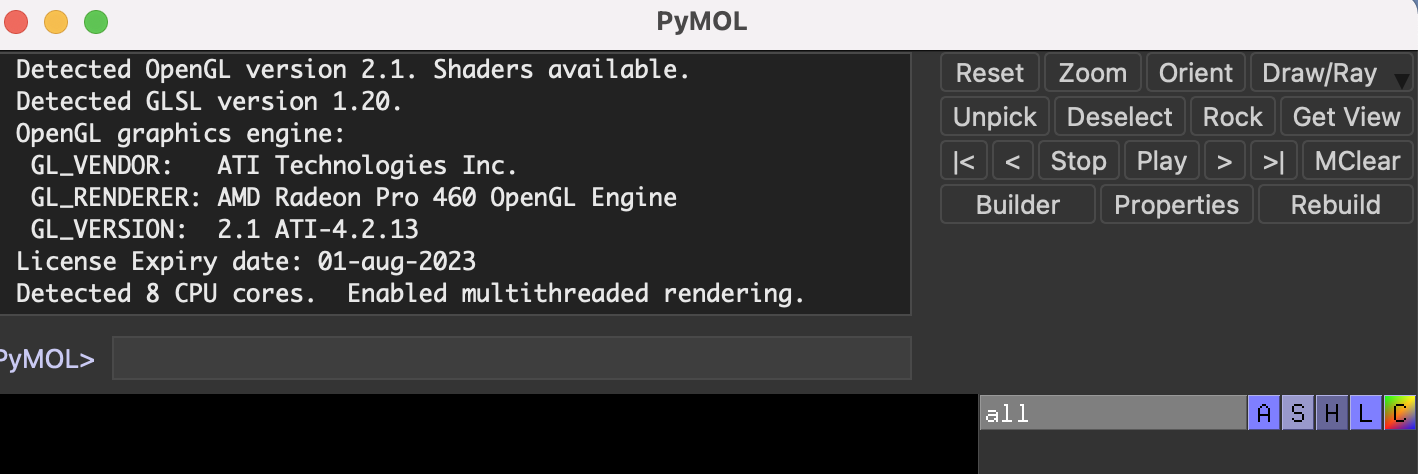
## End of Header: General Commands ##

fetch 1AHO

remove resn hoh

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

This is the command line, into which you should copy the commands above.



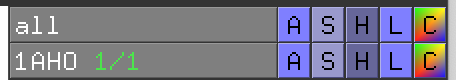


You will see the protein as a ribbon diagram on a white background.

Look on the right hand (RH) side of the PyMOL window and you will see

all  A S H L C

1AH0 A S H L C



“1AH0” is the PyMol object that contains the coordinates of the protein you have downloaded.

A S H L C are pulldown windows.

A = actions

S = show

H = hide

L = label

C = color

1. On the 1AHO pymol object panel

Click H (this is the hide panel)

Click Everything (hides everything; everything should disappear)

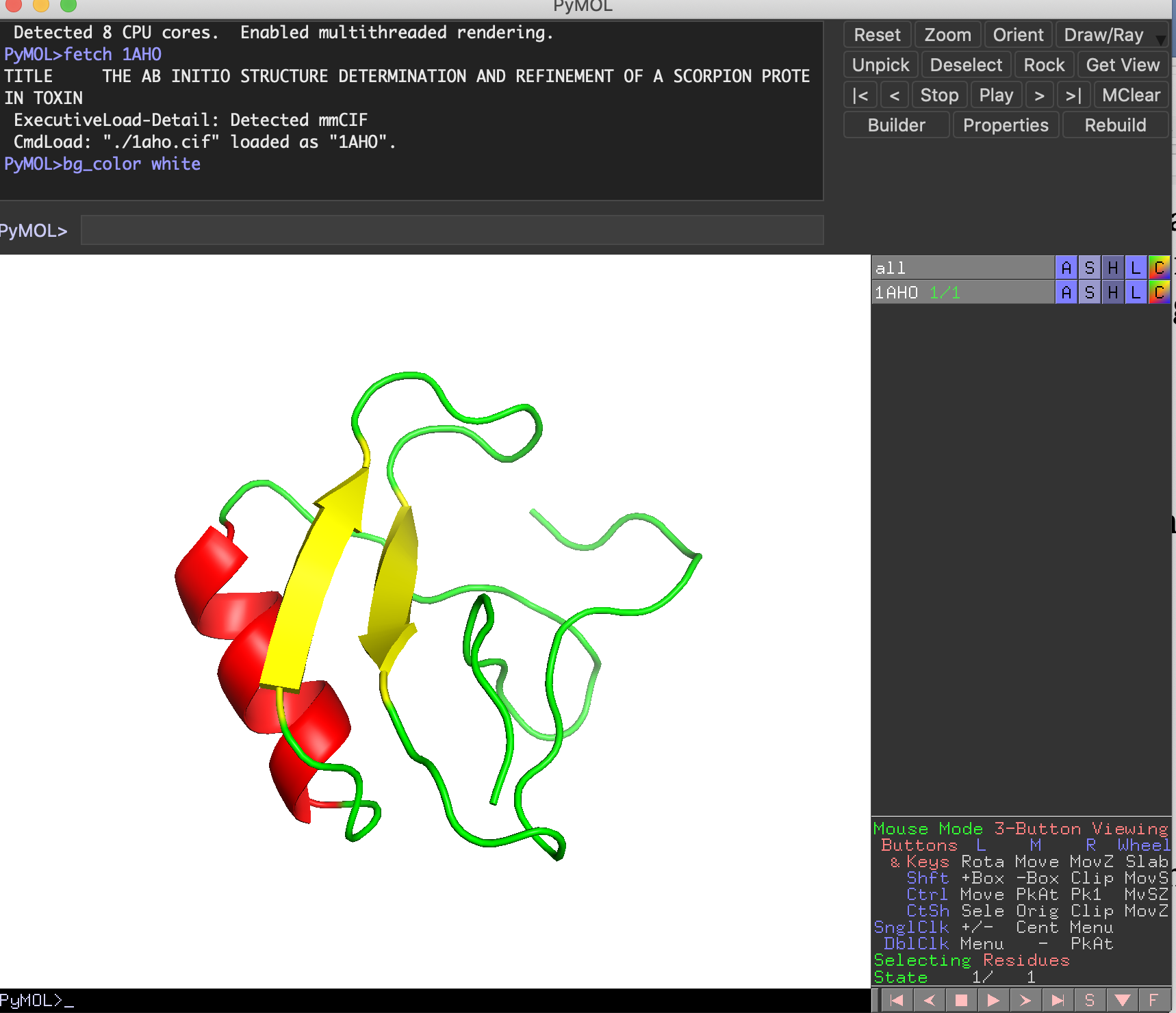
Click S (this is the show panel)

Click Cartoon (shows cartoon; the protein will show as a cartoon)

Click C (this is the color panel)

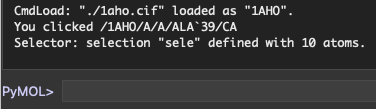
Click by ss and choose a Helix Sheet Loop color scheme; (colors by secondary structure; the loops, a-helices and b-strands show in different colors;)

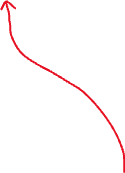
Your display should look like this:





1. Get Info. Click somewhere on the protein (anywhere). After you click, above the command line you will see information about the atom that you clicked on.





object

segment (segi)

chain

residue name (resn)

residue identifier

(i.e., the amino acid number (resi)

atom (C alpha)

1. PyMOL allows you to display the sequence of the protein.

Command line option

set seq\_view, 1

turns it on

or

set seq\_view, 0

turns it off

Menu Option

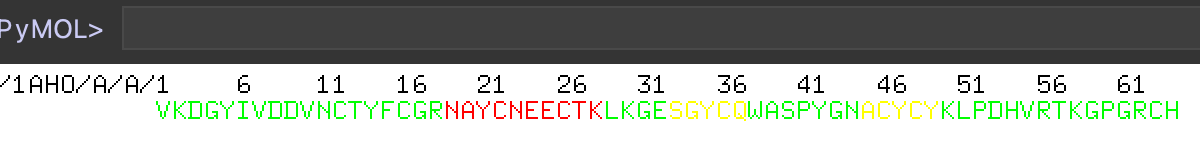
To display the sequence look on the bottom right of the window, and click S.

Graphical user interface, text

Description automatically generated



After you click S, you will see the amino acid sequence below the command window. The residues are color coded to correspond to color scheme used, which in this case matches with secondary structure. The first loop region is green, from resi 1 through resi 18.



This is the color scheme

loop; resi 1-18

a-helix; resi 19-28

loop; resi 29-32

b-sheet; resi 33-37

loop; resi 38-44

b-sheet, resi 44-49

loop, resi 50-64

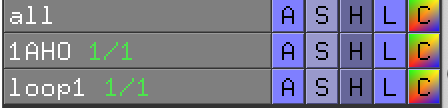
(Note: The 1 letter code is immediately under the corresponding residue number. Amino acid 16 is C (C is under the LH digit of 16). Amino acid 21 is Y.

1. PyMOL allows you to make new “objects”; as many as you like, each with its own set of attributes. To illustrate this feature, and to learn how to work with objects, make some objects from subsections of this protein that are associated with different elements of secondary structure.

To create an object called loop1, containing amino acids 1 through 18, type

**PyMOL>** create loop1, resi 1-18

You will see object loop1 in the RH panel.



Now you have three objects (and one selection (sele), which can be ignored for now).

all is a default object and you will not use it.

1AHO contains the protein plus all the waters, ions and ligands in the 1AHO coordinate file.

loop1 contains amino acids 1-18 of the protein.

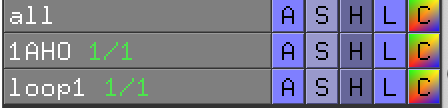
1. Now go to “H” button of loop1 and hide everything, then show it as stick

Click H (for loop 1)

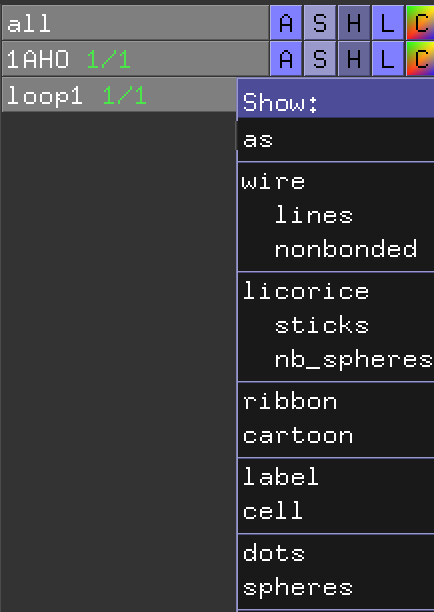
Click everything

Click S (for loop 1)

Click licorice sticks





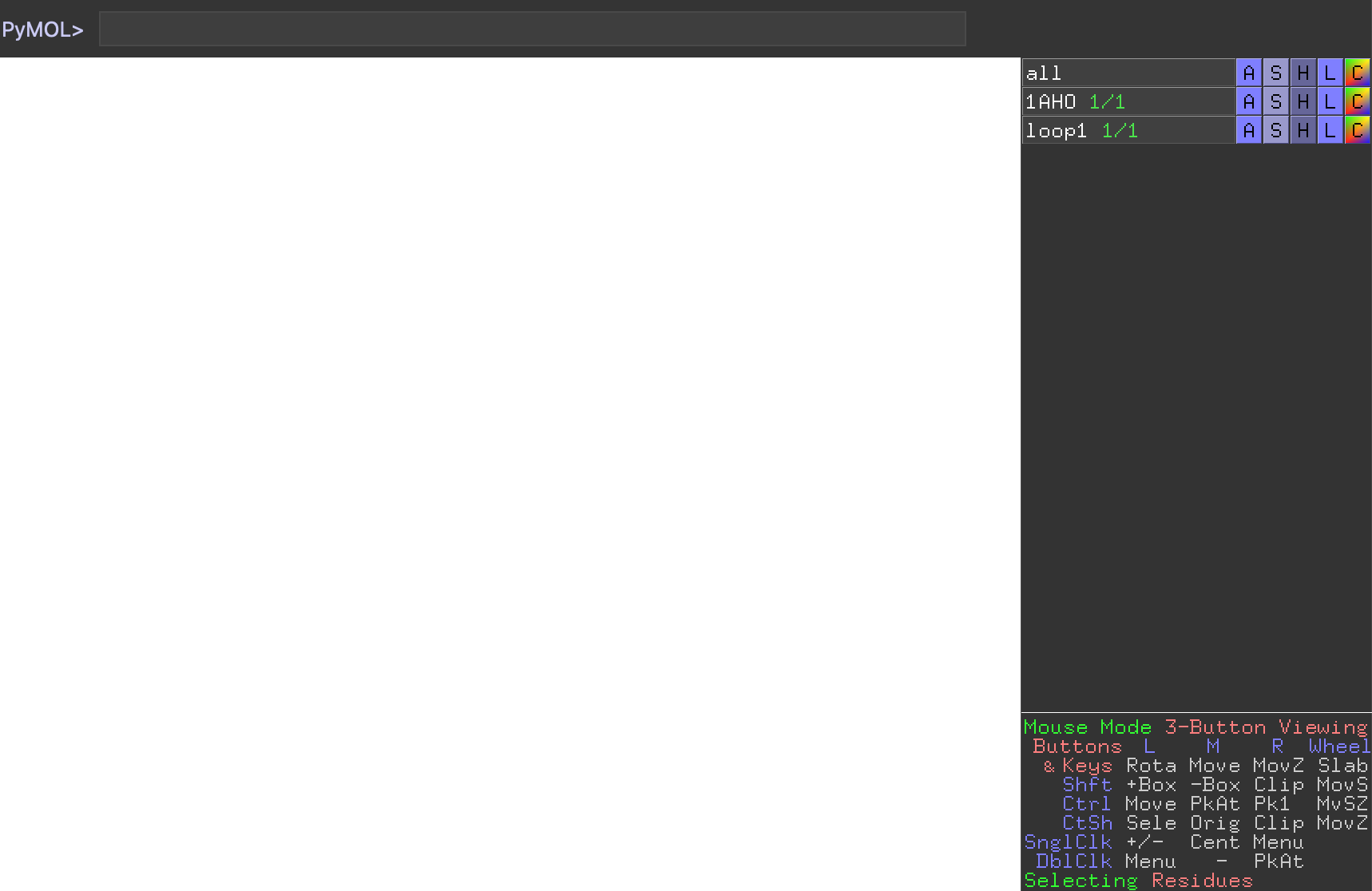




Click C (color)

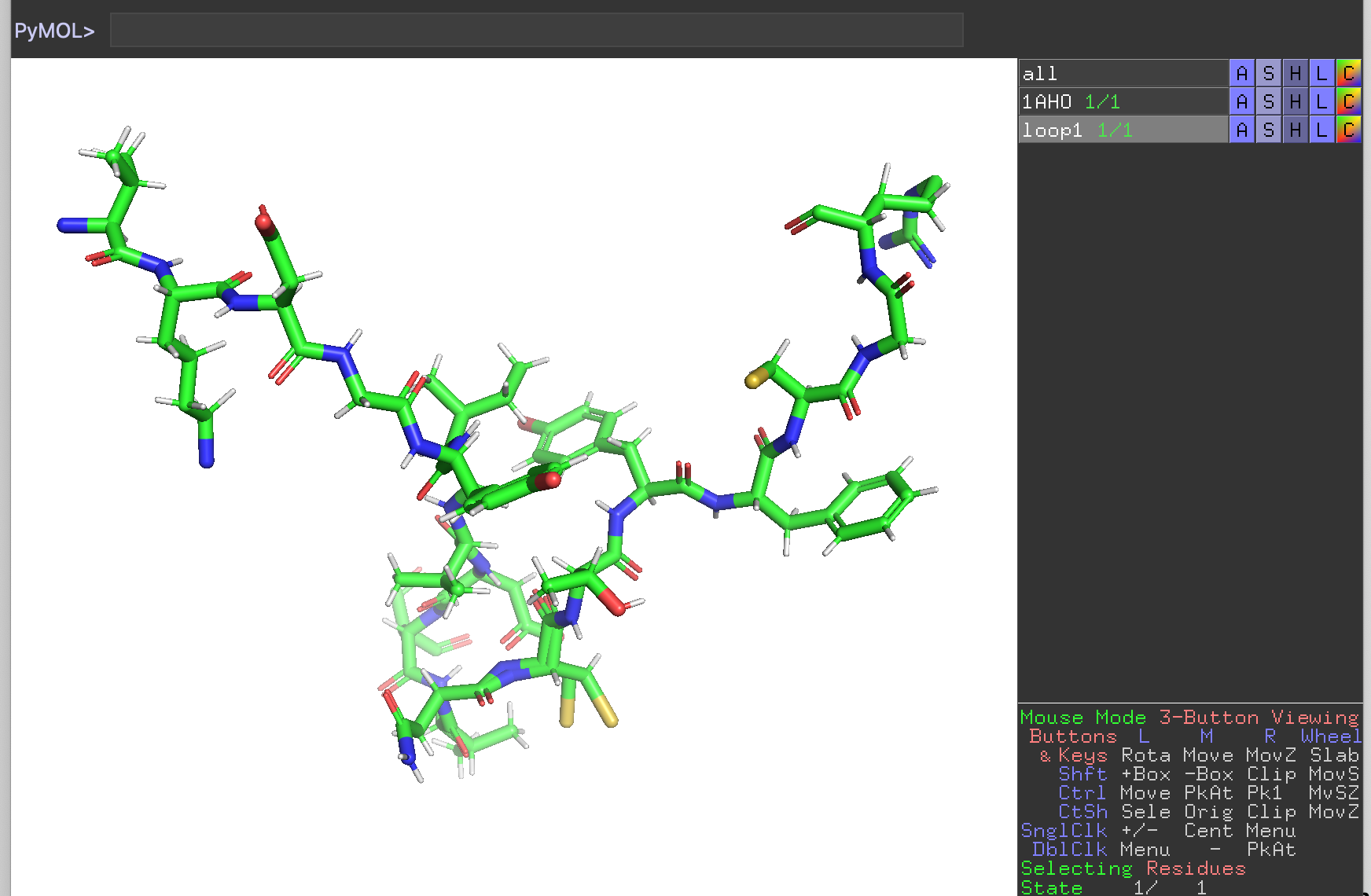
Click by element (color atoms by element type)

Turn all objects off by clicking on all





Turn on loop1 by clicking on loop1





You should see loop1, the object that you just created, in the stick representation.

1. Now make more objects. Make multiple objects of structural elements of this protein by copying and pasting the following (all together) into the PyMOL command line. Hit return after you copy and paste.

**PyMOL>**

#----------------------------------copy from this line--

create helix1, resi 19-28

create loop2, resi 29-32

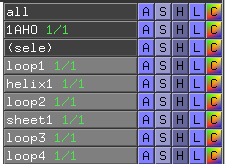
create sheet1, (resi 33-37 or resi 44-49)

create loop3, resi 38-44

create loop4, resi 50-64

#-----------------------------------to this line------------

The sidebar should look like this



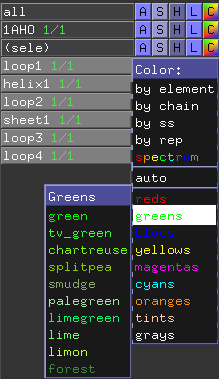
When you get to this point be sure to use the File -> Save Session As… feature to save your work, so that you can come back to it later, if you need to, or so that you can go back to a particular point if you make an error.

Now make each of your new objects into a surface representation. For each new object (H everything, S, surface). Note: surface might be slow to load.

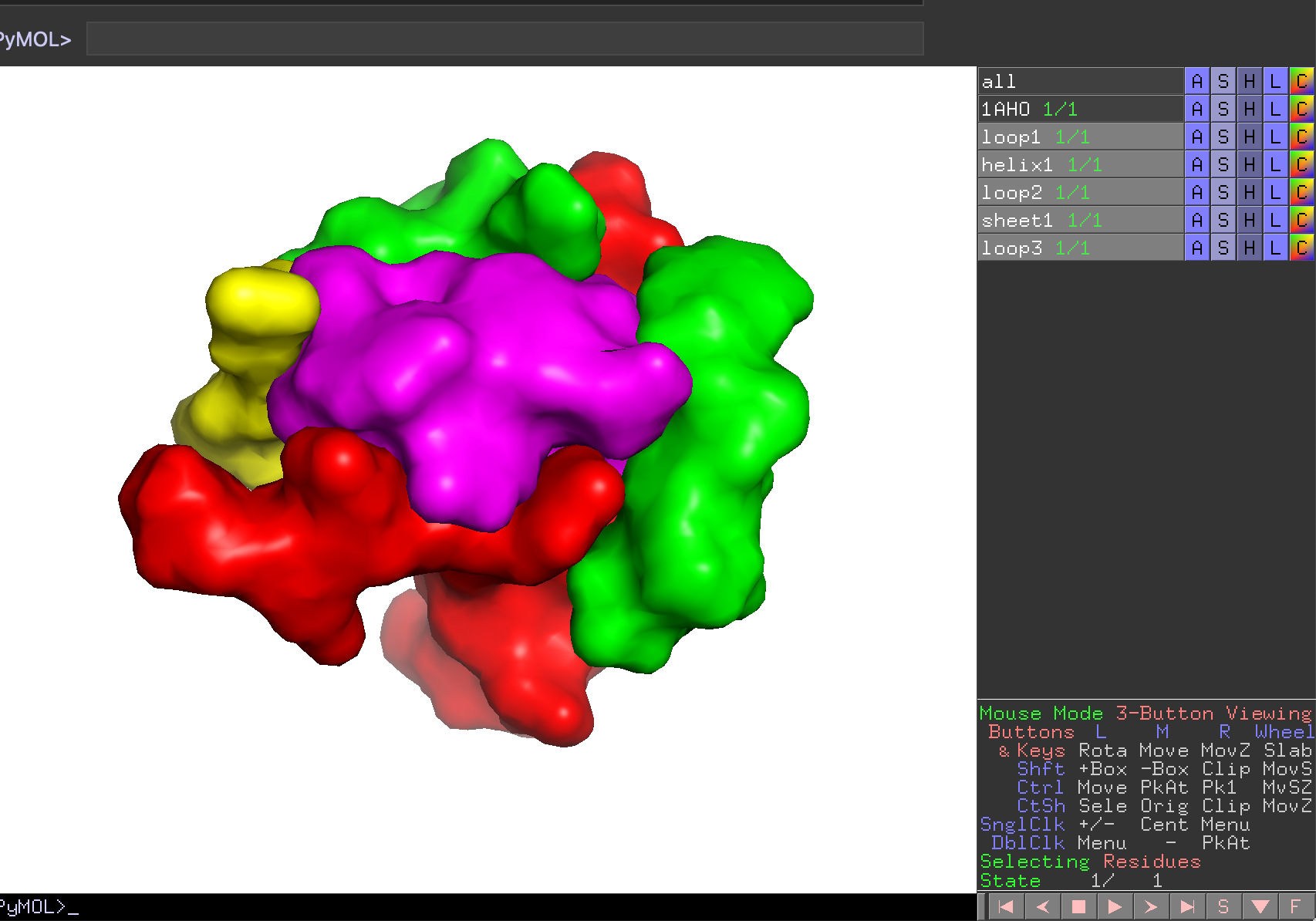




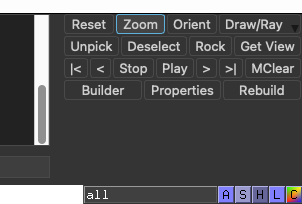
Then, give each object a different color (C).



It should look something like this.



Note: if your molecule is not centered on the screen click Zoom at the top RH side.

 or just type **PyMOL>**zoom into the command line

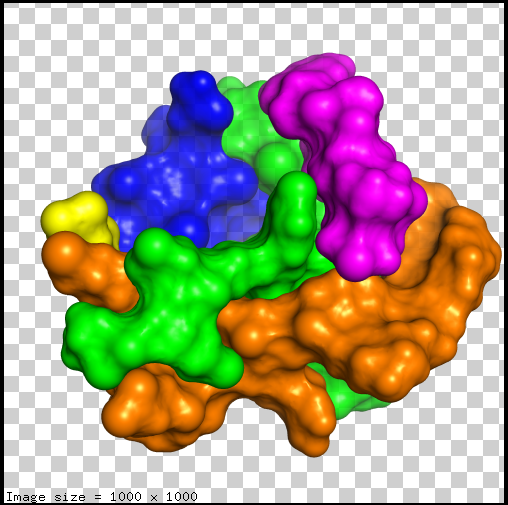
Use File -> Save Session

(To save your place in PyMol)

1. Export an image. Type

**PyMOL>**ray 1000, 1000 (to ray trace at 1000x1000 pixals)

It should look like this



Without clicking in the molecule viewing window,

**PyMOL>**save my\_pymol\_image.png (make up a good name and save your image as a png file).

**PyMOL>**pwd (to check which directory your image was saved in)

**PyMOL>**ls\*.png (shows all .png files in the current directory)

1. Insert the png image here. Resize the image to fit on this page.

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| INSERT HERE |

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

**PyMOL>**

#-----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, 2

## End of Header: General Commands ##

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

1. Type: **PyMOL>**fetch ZZZZ   
   (where ZZZ is the pdb entry code of your protein)
2. Use the commands you learned in section (f) to:   
   (i) display your protein as a cartoon, and

(ii) color it by secondary structure.

1. Export a beautiful .png image of your protein.
2. Insert the .png image of your protein.

|  |
| --- |
| INSERT HERE |

1. Write a paragraph describing your protein. What is the overall shape? Is it single or multiple domains? What is the dominant type of secondary structure in the 3D structure of your protein? What is the dominant type of secondary structure in your phi/psi map (see the ‘General Case’ map of your protein from Molprobity and compare it to Lehninger Table 4.1 and Figure 4-9 (8th Ed.: Figure 4-8)). Do the phi/psi map and 3D structure agree?

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| INSERT HERE |

1. Save the document Assignment\_12\_lastname.docx.