MMOD101: Workshop “Visualizing 3D structures with Pymol”

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Requirements:
Pymol http://www.pymol.org
3-button mouse

PyMOL is a molecular modeling software used for making publication-quality renders of biochemical structures. Using PyMOL, it is possible to make high quality images, analyze and manipulate structures.

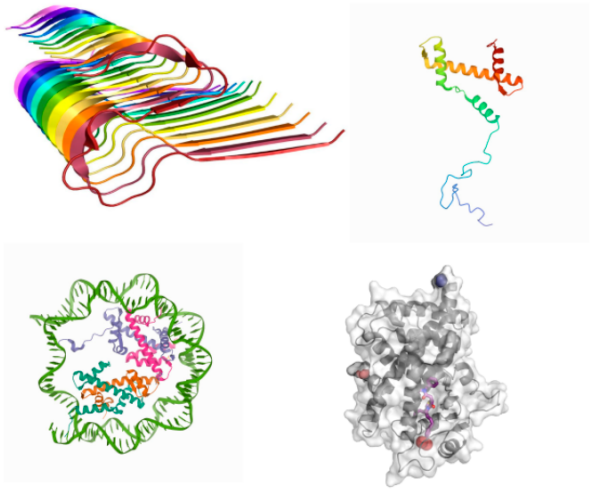

Figure 1: Example of structure visualization

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1 User interface orientation

Below is the PyMOL window:

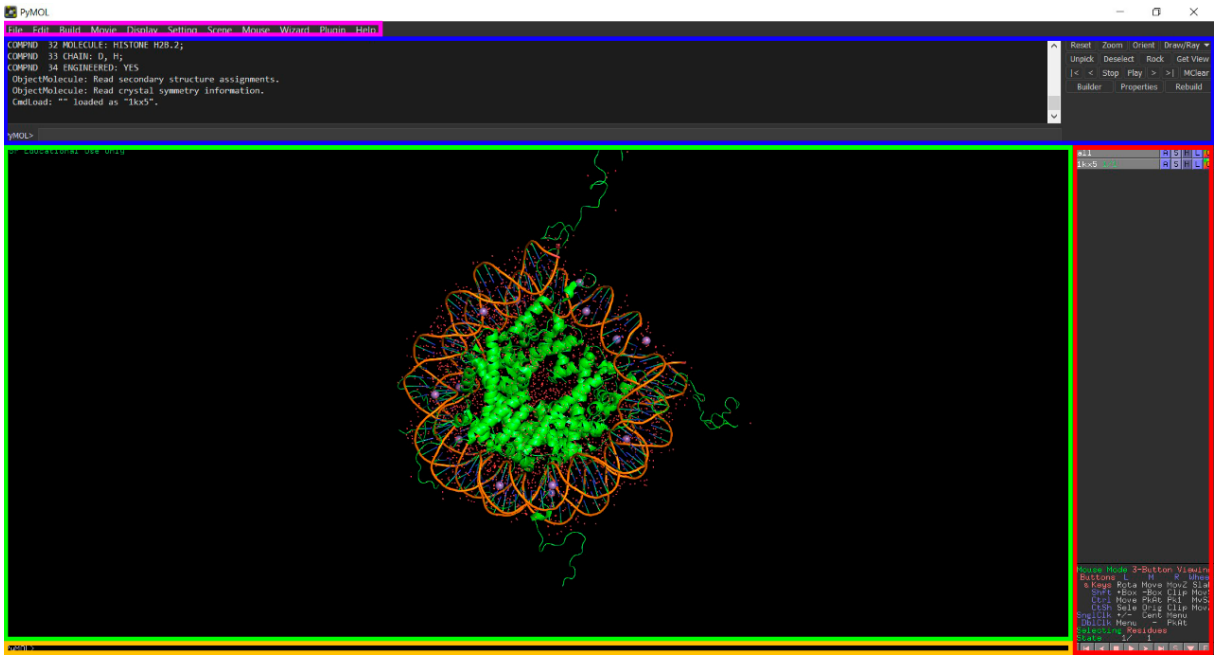

Figure 2: User interface

- **"Upper Control Panel"** - you can work with commands (open file, color "selection", etc.)
- **"Command line"** - this line mostfully use pro users, in this course we won't work with that line
- **"Object Control Panel, Mouse Control Legend"** - here you can work with objects, change mouse control and work with scene control buttons.
- **"Toolbar"** - on this bar we have usefull tools for work.
- **"Display area"** - try to play with the mouse controls.

2 Download and open PDB structure

In Toolbar click **File** and select **Get PDB**, then a dilog window will open:

Write **1kx5**

Click **Download** and the selected structure will load.

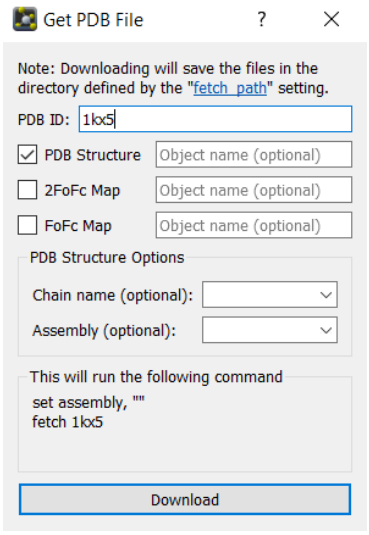

Figure 3: Dialog window

Also if we downloaded file structure from internet, we can open it from our desktop, as we see i have this file type **.pdb** on my desktop that called 1kx5:

Figure 4: Desktop file

We can open it by double clicking on it or we'll go to **Upper Control Panel** and write this command: (**fetch 1kx5**)

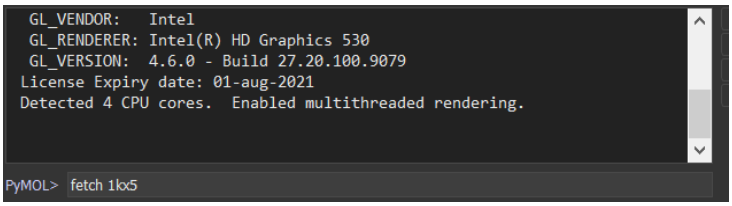

Figure 5:

Then press **Enter** and strusture will open

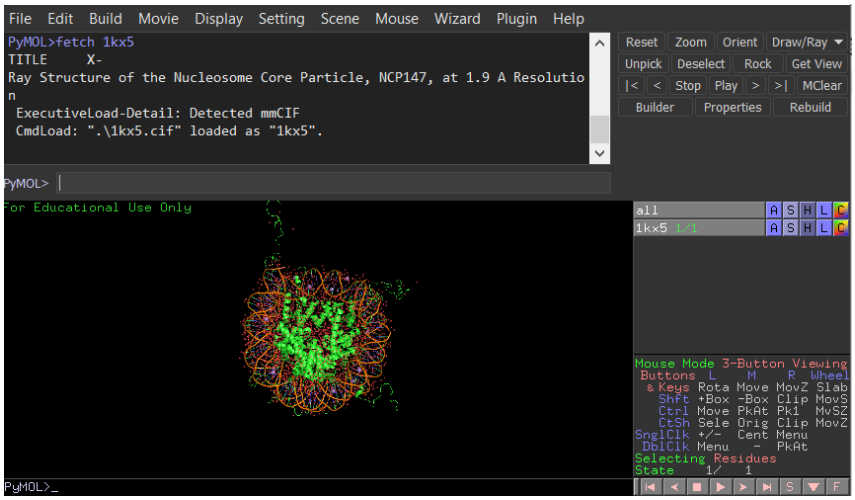

Figure 6:

Basic mouse control:

- **Left click:** rotates the model, click in the center allows free control. As you drag around the edges, it will rotate around the Z axis.
- **Right Click:** zoom and out structure.
- **Middle Mouse Button:** when you click on a squirrel, it moves around the preview window without rotating.

3 Rotating, translating, setting clipping planes, projection type, centering (actions) etc.

- **Rotating:** press **Right mouse button** and move mouse.
- **Translating:** ...
- **Setting clipping planes:** you can scrool mouse wheel to move clipping planes
- **Projection type:** in **Toolbar** click on **Display** and select **Orthoscopic View**
- **Centering:** Press **Action** button and select **center**. The structure will rotate around “center point”. Also you can select **orient**, it will rotate structure in comfortable, front view.

  CTRL+ Left Click: will center veiw on object you click
- **Double Left Click on structure lement:** will open quick tool menu of structure

4 Structure visualization modes (presets, lines, sticks, spheres)

- **Presets:** press **Action** button near structure name block, in **Preset** section and click on **Publication** you have chosen one of several types of projection.
- **Lines/sticks/spheres:** press **Show** button, aim on **as** and select **lines/sticks/spheres**

5 Making selections (by chains, sequence, etc.).

To make chain selection you need to Double click left mouse button on element you want to select, then aim on “chain” and select “sele”

Sequence selection: in right bottom angle you can see **Scene Control Panel**, press S panel button opens the protein sequence, than you can select section you need.

Figure 7: Scene Control Panel

6 Pymol selection language

Try to use this command:
>show spheres, solvent and chain A
To make structure look default write:
> as cartoon
List of commands you can see on this site

7 Molecular surfaces

Press **S**(Show) button, then aim on **as** and select surface
Also you can write command:
>as surface

8 Structure alignment

For alignment to write command, or in Toolbar select **Plugin>Align** in opened window choose structures and press OK
Here is a command > align structure1, structure2
If i have these strustures 1) 1kx5 2) 1kt4
I'll write > align 1kx5, 1kt4

9 Manipulating, moving structure (actions)

If you have a certain amount of structures, and you want to move them relative to each other, follow this steps:

1) Look at **Mouse Control Legend** and press on **Mose Mode**, it must change to 3- Butoon Editing
2) To rotate structure relative to each other press **Shift + Left Mouse Button**, to move it press **Shift + Middle Mouse Button**
3) Also you can bend elements of your structure, press on element you want to bend **CTRL + Left Mouse Button**

10 Adding H-atoms.

To add Hydrogen atoms, you must use command >h_add (name of sele, structure)

11 Calculating charge

Press **A**(Action) button, **Compute>Charges>formal charge sum**

12 Morphing, visualizing conformational transitions.

To morph structures, press **A**(Action) button, **Generate>Morph>to molecule(choose the molecule)**

13 Coloring structure by parameters (B-factors)

spectrum b, blue_red, minimum=10, maximum=50
spectrum count, rainbow_rev, chain A, byres=1

14 Comparing PDB with electron density.

Go to **Plugin > APBS Electrostatics** in opened window press **Run**

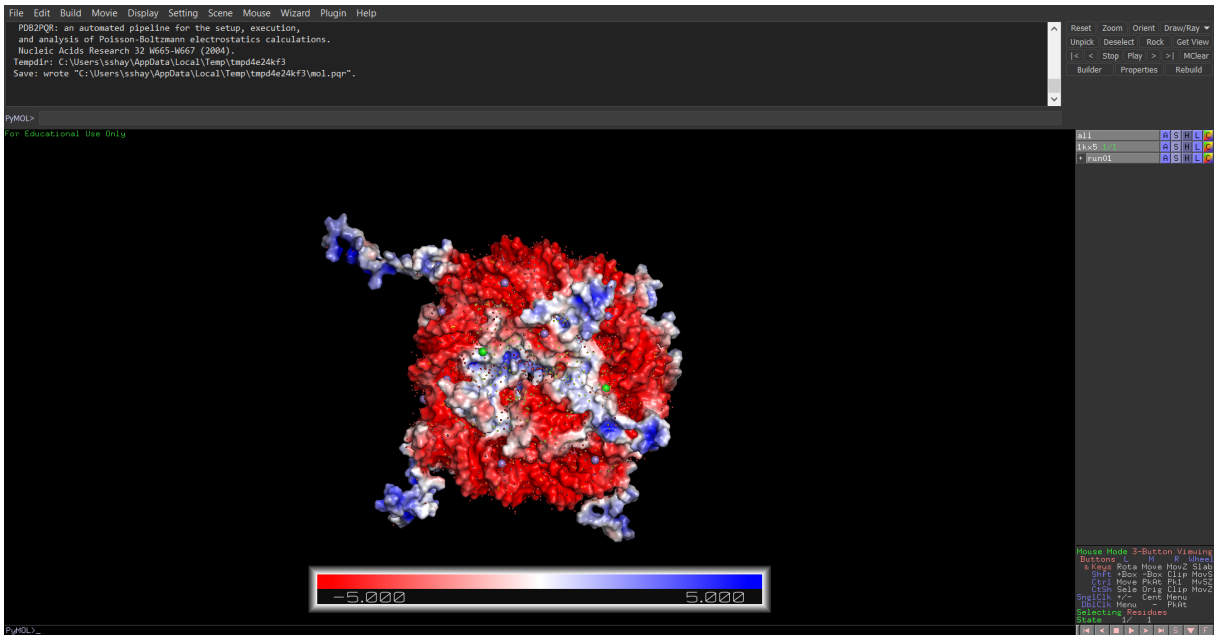

Figure 8: APBS Electrostatics

15 Scripting

In PyMOL scripts are wery useful tool. Script in PyMOL - is a file with list of commands, that helps you to save time.

Some of them you can look on this site

16 Object control panel

If you look to the right of the **Display area**, you will notice an area with different **blocks** including the PDB name "1kx5". This is called the back-end GUI:

Blocks -

You can hide elements from your **Display area** by clicking on the **block** with their name.

Let's pay attention to these buttons:

Each of these letters corresponds to an option for visualization:
A: Action, allows the user to orient the camera and move the protein around, edit the structure.
S: Show, will show a representation type of the visual, such as cartoon, spheres, sticks.
H: Hide, will hide a representation type of the visual.
L: Label, allows the labelling of different aspects of the visual.

Figure 9:

Figure 10: Blocks

Figure 11: Buttons

C: Color, will color the visual based on the user selection.

Let's also pay attention to this panel located in the lower right corner.

Figure 12: Scene Control Panel

The S panel button opens the protein sequence, it will be displayed at the top of **Display panel**.

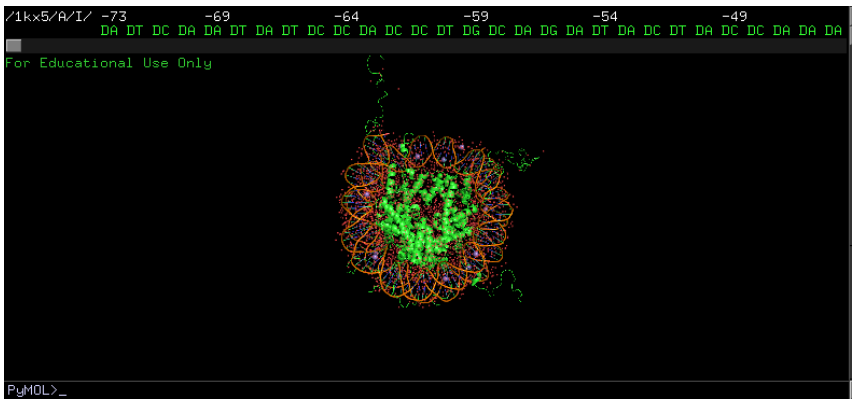

Figure 13:

The sequence can also be selected and colored.
In this image, we have selected 21 atoms, this can be seen in the **Upper Control Panel**, we can observe

that on our structure the selected segment of the sequence is displayed as pink squares.

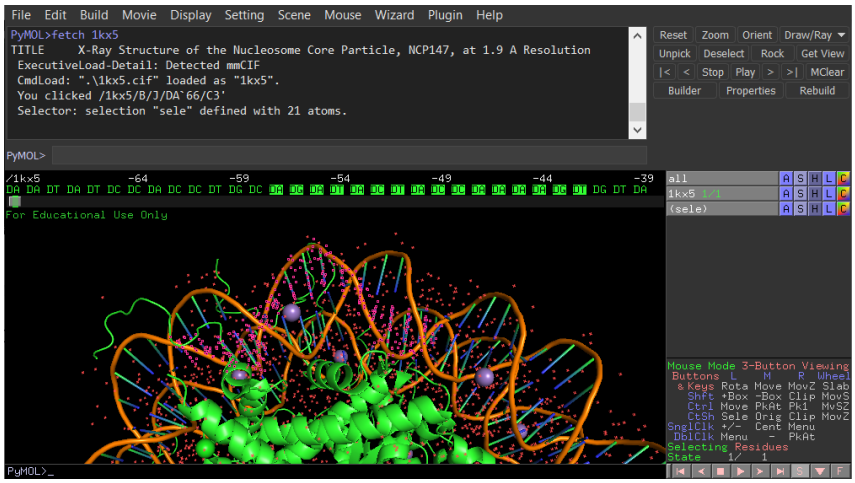

Figure 14:

Also, a new **block** called **(sele)** has appeared, with which you can further work, let's say you need to color this segment of the sequence, press **C** and choose the color.

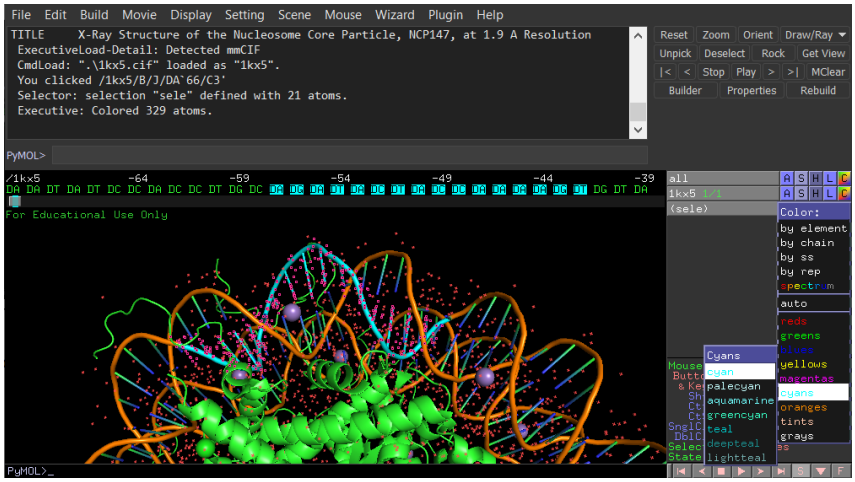

Figure 15:

We see how this segment is colored in the color we need.
With the help of the **H** button we can hide the selected segment.

And the selected segment disappears.
To return it, click on the button **S** and select the **cartoon** line, below you can see that our segment is displayed back.

17 Toolbar

The interface also contains most of the tools needed to use PyMOL. We will break down each tool individually in a square corresponding to the color in the picture below.

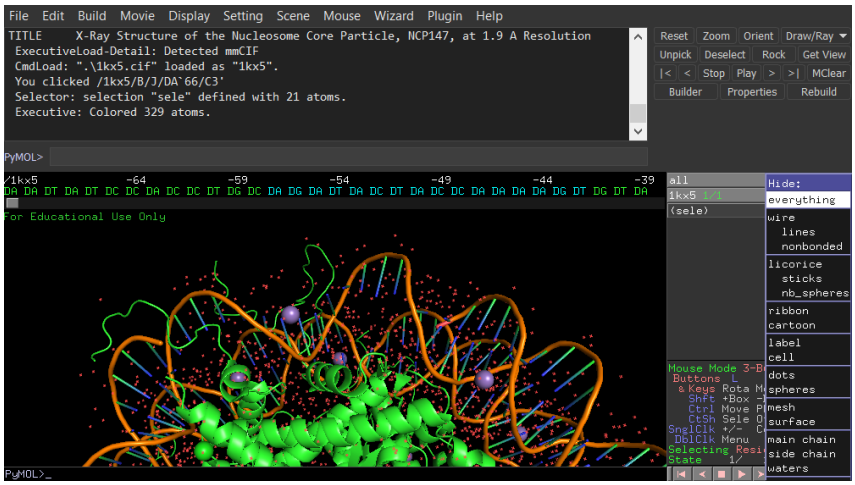

Figure 16:

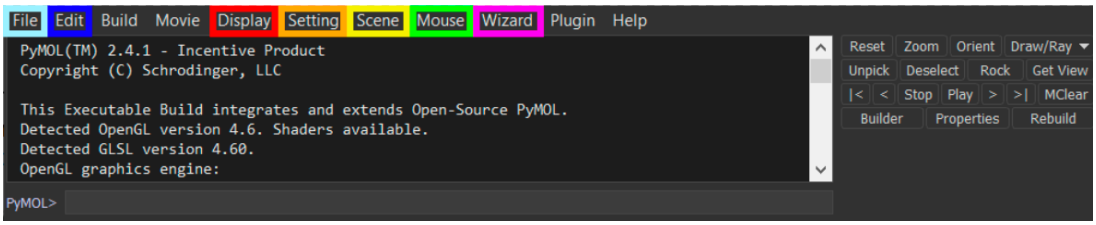

Figure 17:

File

As with most programs, this tab is used to open, save and export files. When you click on it, the following options appear:

- **"New PyMOL Window":** Allows you to open a new window, you can have multiple open at once.
- **"Open" and "Open Recent…":** Opens either structures to view in PyMOL or entire PyMOL .pse sessions.
- **"Get PDB…":** Allows you to fetch a model of a PDB and directly import into the session.
- **"Save Session" and "Save Session As…":** Saves the current session as a .pse file. A .pse file is a PyMOL session file.
- **"Export Molecule…":** Allows you to export a model on screen to a file format (e.g. .pdb)
- **"Export Image As":** Exports the current view on screen to an image.
- **"Export Movie As":** Export the current movie timeline to a video file.
- **"Reinitialize":** Reruns all the settings and display options currently enabled.

Edit

This tab allows you to redo or undo things in PyMOL

- **CTRL + Z** and **CTRL + Y** are shortcuts that you can use
- The maximum number of atoms can be adjusted for large images, but in most cases it is best to leave the default settings.

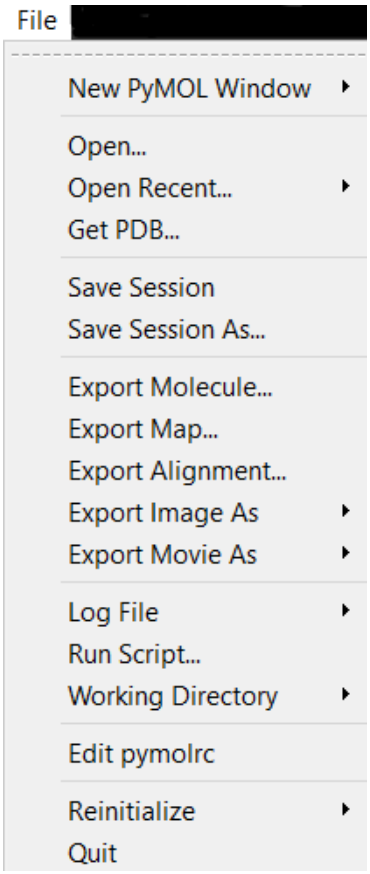

Figure 18:

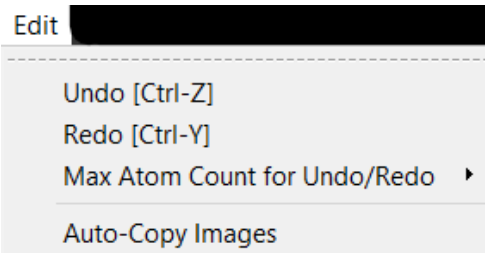

Figure 19:

Display

This tab houses the options that alter the display in the viewport of PyMOL

- **“Sequence”:** Displays the sequence of amino acids or nucleic acids in a protein or piece of DNA above the preview
- **“Sequence Mode”:** Changes what the sequence displays
- **“Background”:** Option to change the color and type of background visible
- **“Color Space”:** Houses settings for different color spaces, can allow for different aesthetic appearances
- **“Quality”:** Provides options for the level of quality of the visualization shown. This option is useful for less powerful computers

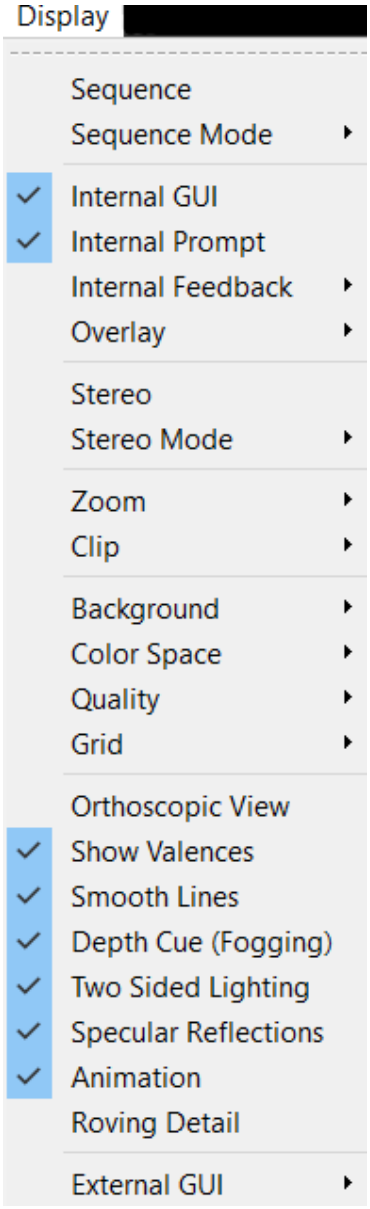

Figure 20:

- **“Grid”:** Allows the option to display objects in a grid
- **“Orthoscopic View”:** Toggles the orthoscopic view setting, which slightly distorts the preview window to enhance depth perception
- **“Show Valances”:** Toggles the visibility of valences in models
- **“Depth Cue (Fogging)”:** Toggles fog that helps with depth perception

Settings

This tab holds the settings for the representations of structures on screen

- **“Edit All...”:** This will bring up a menu of all the advanced settings available in PyMOL, this will be explored further in the advanced tutorial

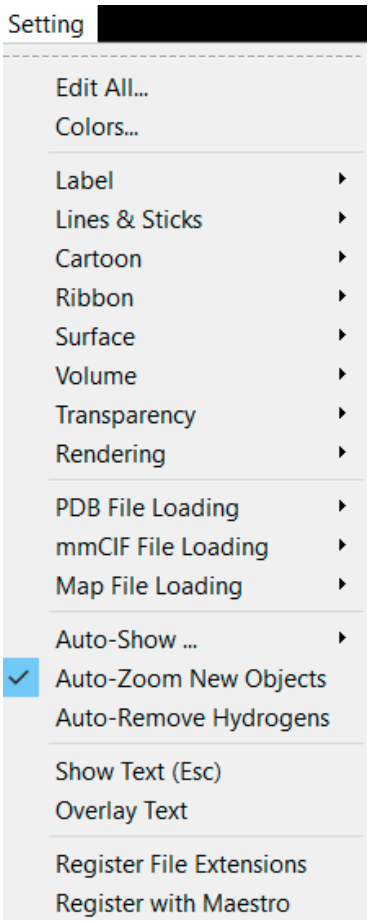

Figure 21:

- **"Colors..."**: Allows you to change the color of atom types, and of preset colors available in the menu (ie make all phosphorous green)
- **"Label" "Transparency"**: Allows you to tweak settings of visualization.
- **"Auto-Zoom New Objects"**: Will force zoom to objects as they are loaded in
- **"Auto-Remove Hydrogens"**: Removes hydrogens from objects as they are loaded in

Scene

This allows for the storage of perspectives and visualizations as scenes that can be retrieved at a later point. This is very useful for moments when multiple representation types are necessary for a single protein.

- **"Next"**: Switches to the next scene, can be called by using the [PgDn] key
- **"Previous"**: Switches to the previous scene, can be called by using the [PgUp] key
- **"Append"**: Makes a new scene from the settings currently present, automatically assigning the name as a number
- **"Insert Before" and "Insert After"**: Does the same as Append, but will create the scene before or after the current scene toggled on
- **"Update"**: Overwrites the current scene

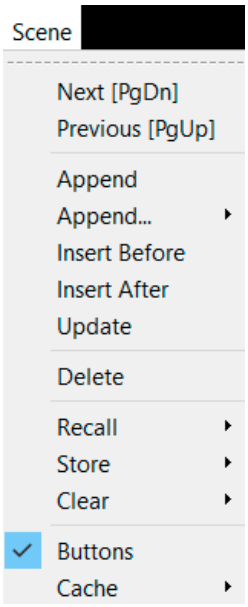

Figure 22:

- **“Delete”:** Deletes current scene
- **“Recall”:** Will toggle a scene from a list of F1 to F12. Scenes can also be recalled by using the buttons at the bottom left of the screen
- **“Store”:** Allows you to store a scene from F1 to F12
- **“Clear”:** Clears a scene F1 to F12

Mouse

This tab provides the options

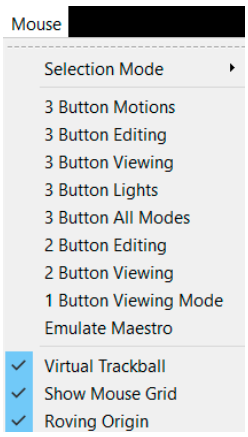

Figure 23:

- **“Selection Mode”:** Houses the different selection modes for picking parts of the model on screen
- **“Emulate Maestro”:** Sets the mouse control settings to that of Maestro, and allows the user to select by dragging a box across the screen

Wizard

This tab provides special modes that provides useful tools to measure, change appearance, etc.

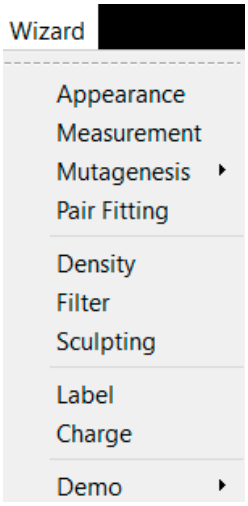

Figure 24:

- **“Appearance”:** Allows the user to quickly toggle through showing certain aspects of the visualization (ie quickly hide and show sticks)
- **“Measurement”:** One of the most useful, measures the distance between two objects
- **“Mutagenesis”:** Allows the user to mutate residues or nucleic acids by rotation, substitution, etc.
- **“Label”:** Can toggle the labels for certain residues of the visualization
- **“Demo”:** Allows the user to play around with some demonstrations of what PyMOL can do, let’s choose **Representation** and we’ll see:

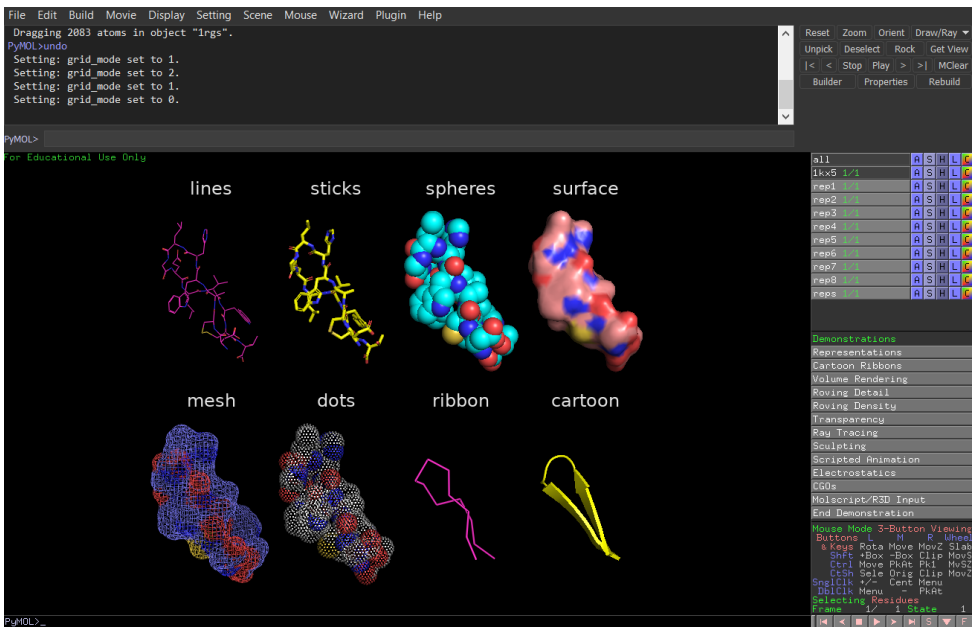

Figure 25: