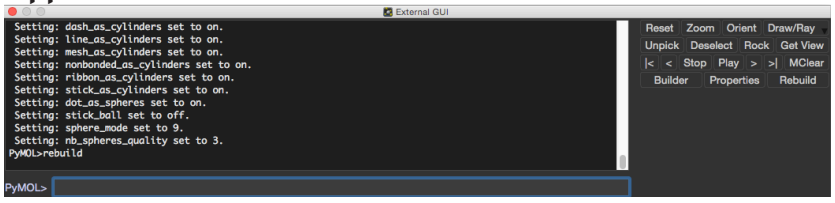
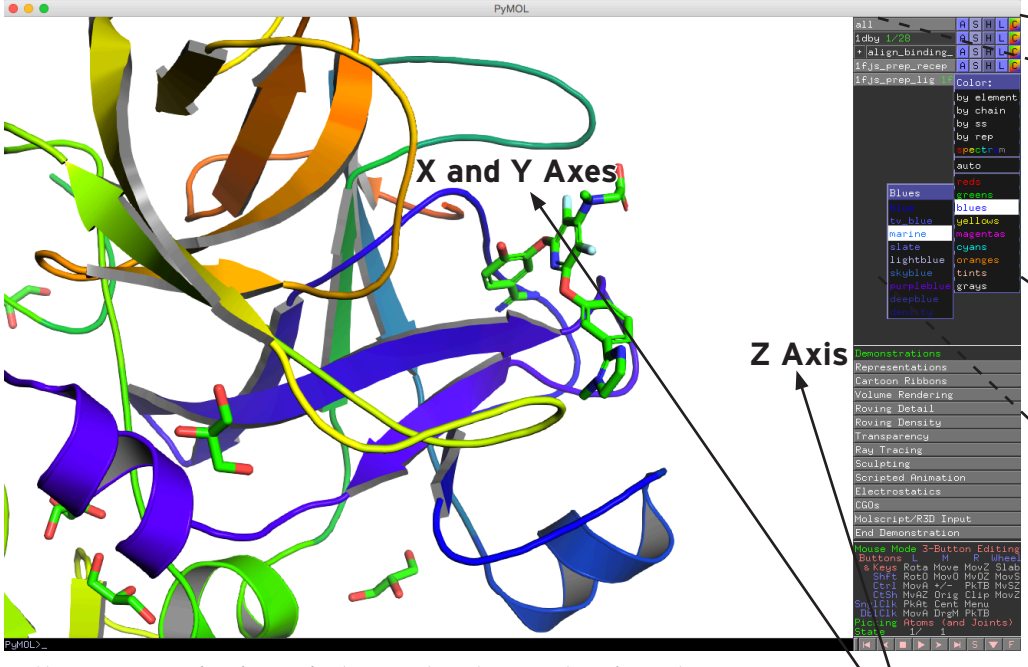
PyMOL User Interface

Upper Control Window



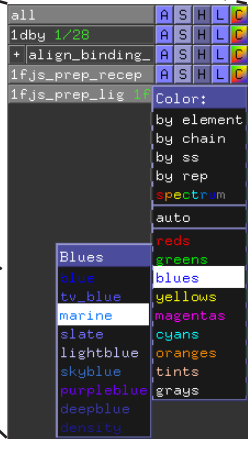
The **Upper Control Window** is where the main drop down menus are located. These menus control files, settings, and tools. Other points of interest in this window are the Ray button in the top right and the command line entry point along the bottom.

PyMOL Viewing Window



In the **PyMOL Viewing Window** molecules can be viewed and directly interacted with. In this window, the camera and molecules can be moved and rotated, sets of atoms can be selected directly by clicking on the molecule or by clicking in the Sequence Viewer located at the top, scenes can be changed and updated via the scene buttons in the lower left hand corner, movies can be controlled with the movie bar controller in the bottom right, and model representation of individual atoms can be changed by right-clicking on the molecule to call up pop-up menus.

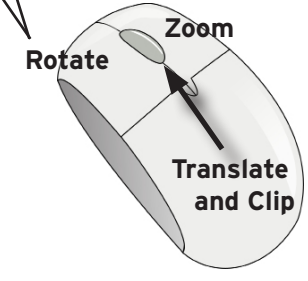
Object Control Menu



The **Object Control Menu** is used to control atoms/ molecules (called objects), and sets of atoms/molecules (called selections). This menu and its many pop-up menus allow a lot of control over how objects are represented in the **PyMOL Viewing Window**.

A=Action S=Show H=Hide L=Label C=Color

Mouse Controls



PyMOL's mouse controls for moving the camera in the **PyMOL Viewing Window** utilizes a virtual track ball. Holding the left mouse button while the pointer is inside the molecule will cause the camera to rotate along the X and Y axes. If however the pointer is outside the molecule, the camera will rotate along the Z axis.

Common Operations in PyMOL

Loading Molecules

Upper Control Window:

File > Get PDB

Command Line:

load "file name"

fetch "pdb_code"

Mouse Controls

Left button:

Hold: rotate

Click: select (residues by default)

Right button:

Hold: zoom

Click: pop-up menu

Center button:

Hold: translate

Click: center on atom

Scroll: adjust clipping plane

Representations

PyMOL has many options when it comes to representing molecules many of which can be controlled from the **Object Control Menu** via the single letter pop-up menus A S H L C and can be applied to both objects and selections.

Example commands:

S **> as > cartoon**

shows a cartoon representation only

S **> sticks**

adds sticks to the current representation

H **> waters**

hides waters from the current representation

A **> preset > ball and stick**

classic ball and stick representation

L **> residue**

labels residues with three letter code and number

C **> blues > marine**

colors the representation marine

Selections

Selections in PyMOL are sets of atoms and are differentiated from objects by the use of ( ) in the Object Control Menu. The default selection is (sele) which is automatically created upon selecting any atom or residue. To start a second selection, rename (sele) and deselect it, then start a new selection.

Creating selections:

Left mouse button

Clicking on the molecule will select/deselect resides by default

Sequence Viewer

Display-> Sequence

Left click and drag on sequence to select/deselect large portions of the molecule

Renaming a selection:

A > rename selection > delete and retype new name

Display and Settings

Many display options and other effect settings can be controlled from the Display and Setting drop down menus located in the **Upper Control Window.**

Example Commands:

Display > Sequence

starts up the Sequence Viewer

Display > Background > White

sets the background color white

Setting > Transparency > Surface > 50%

sets transparency of all surfaces to 50%

Setting > Rendering > Shadows > None

turns off shadows during ray tracing

Setting > Edit All...

brings up a new window with all settings

Scene Control

Scenes are snapshots of the PyMOL viewing area that include all of the representation information as well as the camera position. Changing and updating scenes is very easy from the **PyMOL Viewing Window** if you turn on the Scene Buttons.

Example Commands:

Scene > Append

stores a new scene

Scene > Buttons

toggles the interactive scene buttons in the **PyMOL Viewing Window**

Measurement Wizard

PyMOL has a built-in measurement tool, for distances, angles, dihedrals, and neighbors.

Wizard > Measurement

starts the measurement wizard (distance by default)

Click Distances to toggle measurements > pick atoms as directed

Programmed Movies

PyMOL is a very powerful moviemaker with many sophisticated options, however there are also several pre-programmed movie options available for the beginner to use.

Example Commands:

Movie > Program > Camera Loop > Y-roll-> 4 sec

creates a movie that rotates 360˚around the Y-axis in 4 seconds

Movie > Program > Scene Loop > Nutate > 4 sec

creates a movie that loops through stored scenes and oscillates them for 4 seconds

Saving and Exporting Files

It is important to save your work and very easy to export your figures and movies.

Example Commands:

File > Save Session As...

saves the entire contents of your PyMOL session

Click Ray, then

File > Export Image As > PNG...

exports a ray traced image

Movie > Ray Trace Frames, then

File > Export Movie As > MPEG/QuickTime

exports the current movie and ray traces every frame

Further Help

PyMOL has a diverse and active community, and much of PyMOL's functionality can be learned from community-sponsored resources and professional support.

visit www.pymol.org/support

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