DRAFT CHAPTER OF THE OFFICIAL PyMOL MANUAL (For PyMOL Sponsors)

A first installment

Although this is not Chapter One, this is the first chapter we are posting for your use and feedback, a part of our expanded documentation system for PyMOL sponsors.

This chapter is intended to get new users up and running on PyMOL, without plodding through a formal review of every detail. It is planned as an early chapter of a comprehensive manual, so you will find many references to chapters that are not included here. Nonetheless, we think you may find it helpful, especially if you are a new user. Please email help@schrodinger.com if you find it in any way confusing or incomplete for a user's first encounter with PyMOL.

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X. HITTING THE GROUND RUNNING

This chapter introduces the **PyMOL** *interface,* **PyMOL's** *capabilities, and the commands and representations you need for creating and saving images. The aim is not complete coverage, but simply to help you get off and running. The information here corresponds to* **PyMOL version 1.2.r1.**

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PyMOL Layout and Features

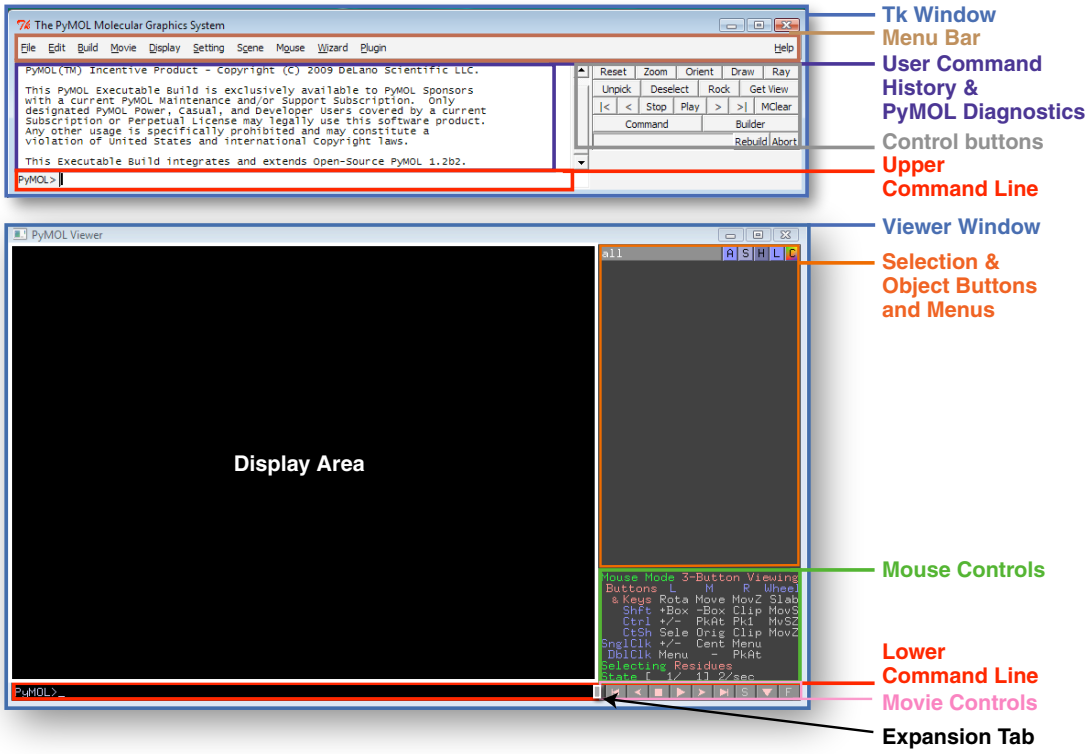


Figure X.1 The PyMOL user interface on a Windows PC

PyMOL user interfaces on various computers

There are some differences in appearance (and a few differences under the hood) between the versions of PyMOL that run on Windows™ Personal Computers (PCs), Unix/Linux systems, and Macs™. For the user, most of the differences are cosmetic. In this chapter, we usually show the Windows interface (because most PyMOL users have Windows), and illustrate the differences on the Mac where they count. The Unix/Linux version of PyMOL looks a lot like the Windows version.

When you launch PyMOL on a PC (see Figure X.1), two windows appear, one right above the other (they are really two separate windows). The top PC window has a Tk logo at the top left. We'll call this the Tk window (some menus call it the Tcl Tk GUI window). Below it is the PyMOL Viewer window.

The Tk window contains, at top left, a bar of PyMOL pull-down menus, a white box for displaying the command history and diagnostic messages, and a live area for typing in commands at the bottom left. To the right is a bank of button controls. Below the Tk window, the Windows PyMOL Viewer window contains the Display Area, the lower command line, and several other types of controls in a panel to the right of the Display Area.

When you launch MacPyMOL (see Figure X.2), the PyMOL menu appears in the Apple™ menu bar at the top of the screen. On the desktop, you'll find one window containing the Display Area and all the other controls and command lines.

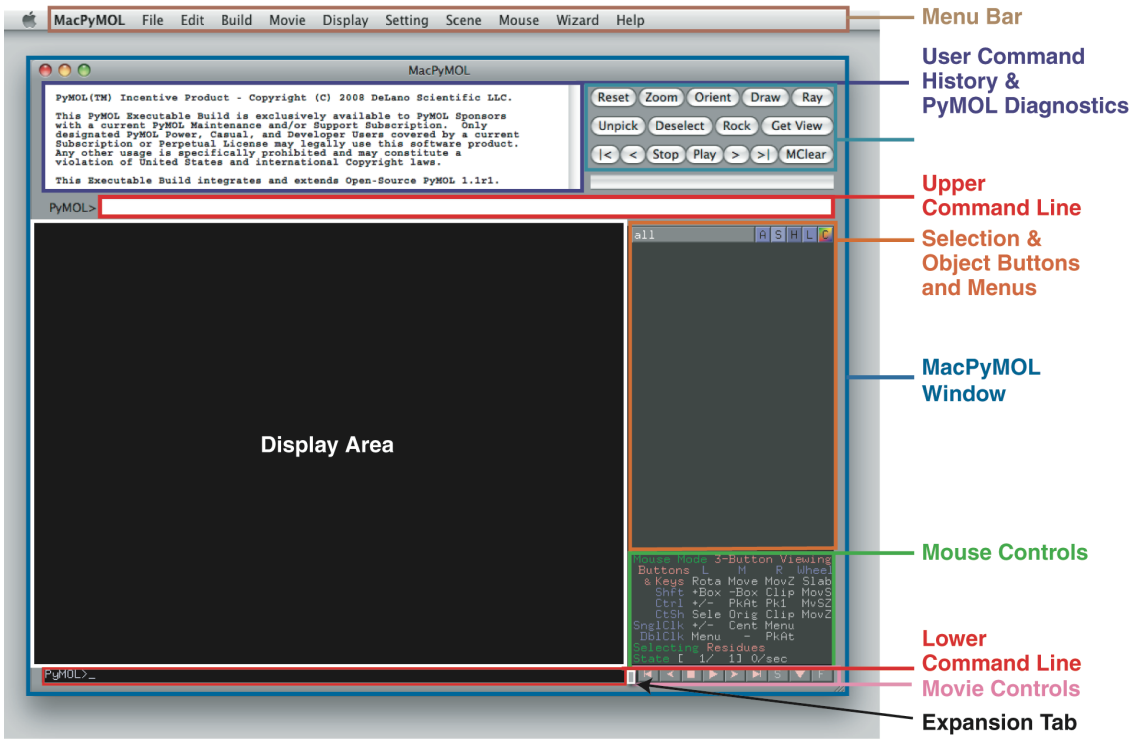


Figure X.2 The MacPyMOL user interface

The main difference between the Mac and the Windows PyMOL interface is the number of windows. On the Mac, the topmost menus are incorporated in the Apple menu bar, and all the other controls are in one window below. On Windows, the topmost bar of menus shares the Tk window with the command history, upper command line, and a bar of control buttons.

Controls and information are presented on the right-hand side of the MacPyMOL User interface (Figure X.2) and the Windows PyMOL Viewer (Figure X.1). These include a list

of names for each object and selection you create, as well as a bank of pop-up menus for each object and selection. A block of mouse configuration information, a tab for expanding the Display Area, and a line of VCR-style movie control buttons are also on the right side of the Display Area. A secondary command line runs under the Display Area on the left.

Demonstration Wizard

PyMOL contains a set of demonstrations to give you a taste of its capabilities. We suggest you check them out now by opening PyMOL.

You may want to get into the habit, starting now, of checking that the Caps Lock key on your keyboard is not enabled when you launch PyMOL. When the Caps Lock is enabled, PyMOL's mouse controls do not work properly.

Launch the demonstration wizard by choosing the **Wizard** pull-down menu from the Tk menu bar on Windows, or from the Apple menu bank on the Mac. Then select **Demo** and **Representations** from the submenus to see the animation of the representation types (see Figure X.3).

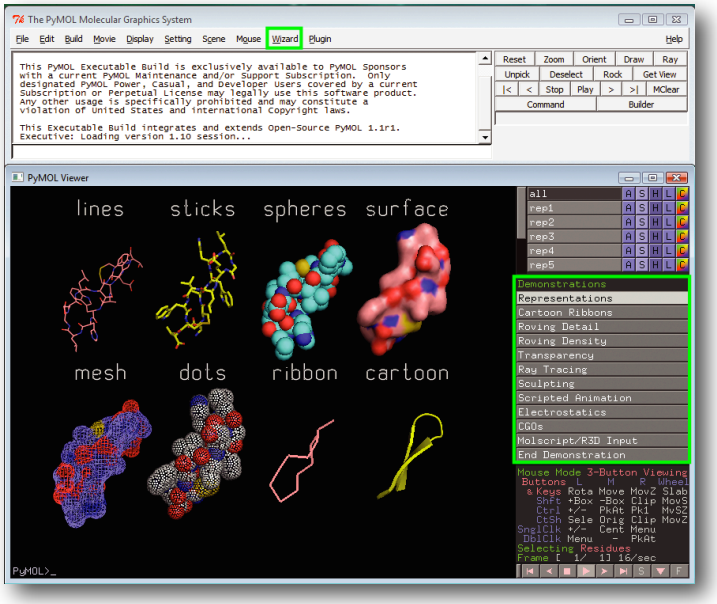


Figure X.3 The demonstration wizard shows ten PyMOL capabilities. Choose any one of them from the **Wizard / Demo** menu (the Wizard menu is outlined here in the top green box), and a list of all the demos will appear in the objects & selections list to the right of the Display Area (also shown here boxed in green, on the right).

To view the other demonstrations, left-click on the buttons listing **Representations**, **Cartoon Ribbons**, etc., to the right of the Display Area. Some of the demonstrations are

interactive and require a three-button mouse to work. This is an important point. *To get the most out of PyMOL, you need a three button mouse.*

Before you left-click on **End Demonstration** at the bottom of the list, left-click on **Representations** once more so you can examine the bank of control buttons (shown in Figure X.4). On the left is a list of the object names, **all**, **rep1**, **rep2**, **rep3**, **rep4**, and **rep5**. However, there are eight different objects in the demo. To view the complete list, drag down on the scroll slider to the left of the names until you can see the last four, **rep6**, **rep7**, **rep8** and **reps**.

Figure X.4 There is a scroll slider (here boxed in green) to the left of the object names list.

The demonstration wizard is scripted to show some of PyMOL's capabilities, but many functions are not accessible from these scripts. To dig in, the next step is to load a coordinate set. Left-click on **End Demonstration** to clear the Display Area and the list of objects & selections.

Loading a Molecule

PyMOL accepts commands in a variety of ways. For example, to load the molecular coordinates from a PDB file, you can use the **Open...** dialog box under the **File** menu; or, with PyMOL closed, you can drag a PDB file icon from anywhere on your computer onto the PyMOL program icon; or, if you are connected to the internet, you can load molecules directly from the PDB website, using the PDB identifier for the coordinate set. (An updated list of all the file format types PyMOL accepts, and the methods for loading are found online.) For example, make sure your computer is online, launch PyMOL, then left-click in the upper command line and type

```
PyMOL> fetch 1acj
```

(and enter, or return). 1acj is a PDB identifier. PyMOL will download the PDB file to your User folder. If you are not online, but you have access to a PDB file, go ahead and open it in PyMOL from the **File / Open...** menu, which allows you to navigate to the file as you would in any other program, depending on your operating system.

The first thing you'll notice is that your command is echoed in the command history area above the upper command line. Then, once PyMOL has located the PDB file (and downloaded it to your User folder when you use the `fetch` command), it will display a representation of the molecule in the Display Area, and echo the header information from the PDB file in the command history area (see Figure X.5). The default representation is lines, colored by element (oxygens red, nitrogens blue, carbons green, etc.).

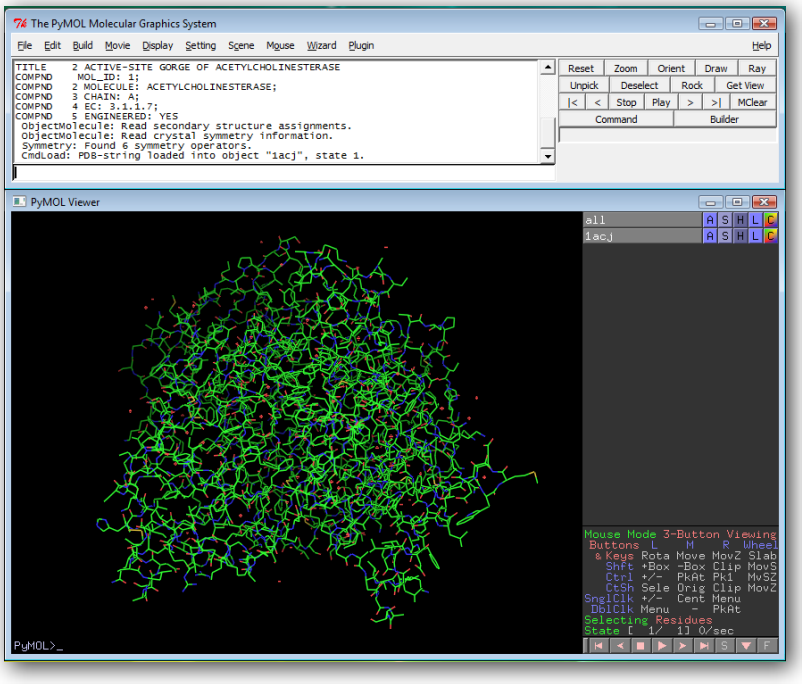


Figure X.5 Here, PyMOL has loaded and displayed **1acj** in a **lines** representation.

Visualization Presets

When PyMOL has loaded 1acj, the lines representation appears in the Display Area, and the object name **1acj** appears in the objects & selections list. To the right of the object name, a row of A S H L C buttons appears. The buttons in this row apply only to the object **1acj**. You can load or create any number of coordinate sets in a PyMOL session. A new object and row of buttons will appear for every coordinate set you load, or selection you create (Making selections is treated in this chapter, under Making and Representing Selections). The object name **all** appears at the top of the list. The row of buttons next to the object name **all** applies to every object you have loaded.

Left-clicking on **A** displays a pop-up cascading menu of Actions that PyMOL can perform on the object named in that row. Left-clicking on **S** displays a list of representations and atom types that PyMOL can Show; **H** displays a similar list of representations and

atom types to Hide; **L** displays Labels that you can add or clear; and left-clicking on **C** gives you a cascading pop-up menu of Colors (**A S H L C** buttons are treated in this chapter, mostly under Representations). We are aiming for a submenu under **A** Action / **Preset** (see Figure X.6).

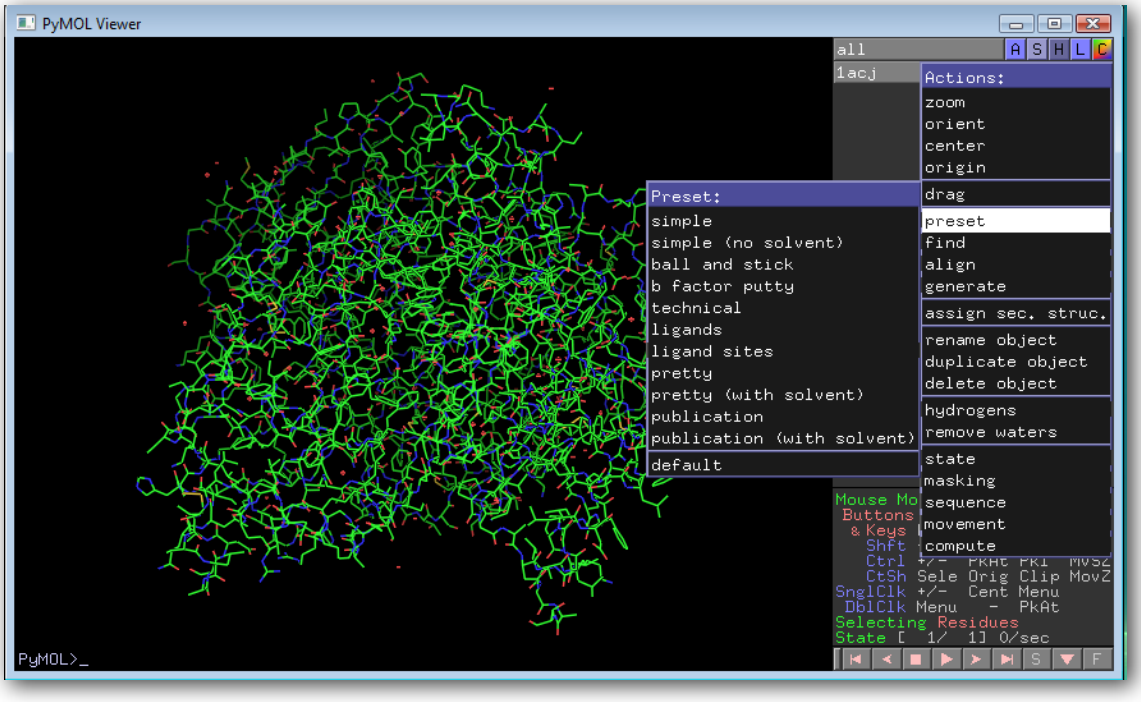
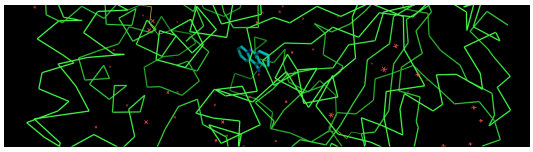


Figure X.6 Left-clicking on the **A** Action button, and then left-clicking on **preset** brings up a cascading menu of preset representations from which to choose. In this case, there is only one set of coordinates loaded into PyMOL, so left-click on the **A** Action button in either the **1acj** row or the **all** row. Here, none of the presets has been chosen yet.

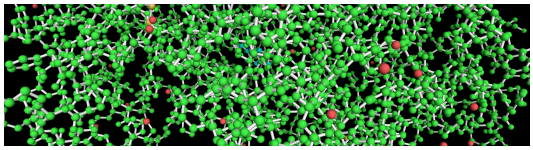
PyMOL provides you with a set of built-in preset representations for visualizing proteins, nucleic acids, and ligand complexes. For example, the **ligands** preset enables you to visualize the polar contacts made between proteins and ligands. When you apply the **ligands** preset, the **1acj_pol_conts** object name appears in the list of objects & selections to the right of the Display Area. You can toggle the display of polar contacts by left-clicking on the name **1acj_pol_conts.** With polar contacts enabled (gray background behind the object name), you can also display the number of Ångstroms between the contacting atoms by left-clicking on the **S** Show pop-up menu next to **1acj_pol_conts** and choosing **labels**. Left-click on the **H** Hide pop-up menu and choose **labels** to hide the distance measurements.

Other presets worth trying at this point include **technical**, **ligand sites / transparent surface**, and **publication**. Table X.1 shows examples of the visualization presets that include solvent (some presets hide solvent molecules).

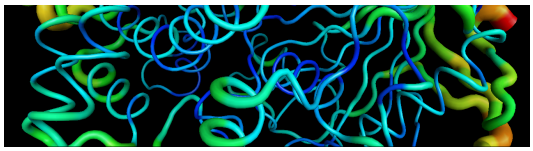
Table X.1 Visualization Presets



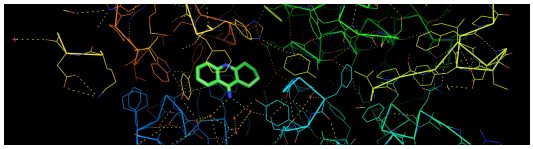
simple (with or without **solvent**) A C-alpha trace of the main chain is shown with a **ribbon** representation.



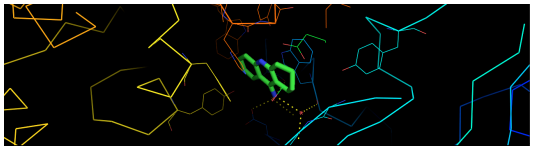
ball and stick Bonds are shown with **stick** representation (stick_radius set* to 0.1). Atoms (and solvent) are shown as **spheres** (sphere_radius set to 0.25).



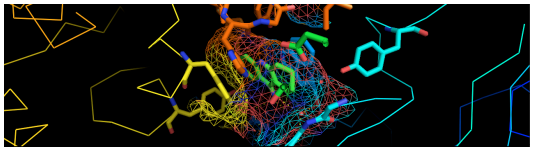
b factor putty This preset runs a script to calculate the diameter of the **cartoon putty** in proportion to the crystallographic *B*-factor. Solvent is not shown.



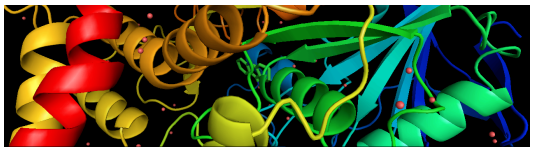
technical The backbone is shown in a **ribbon** representation. Side chains are **lines**, ligands are **sticks**, and polar contacts are dashed lines. Solvent is shown with crosses.



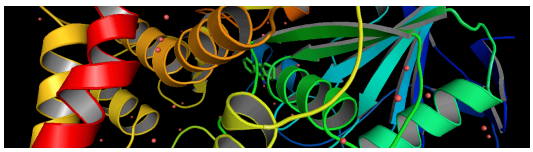
ligands PyMOL zooms in on a ligand, shown as **sticks**, with polar contacts as dashed lines. The protein backbone is shown as a **ribbon**, side chains as **lines**, and solvent as crosses.



ligand sites (mesh surface) PyMOL's camera zooms in on a ligand site, representing it as a **mesh surface**, with **stick** representation for the site side chains and ligand.



pretty (with or without **solvent**) The protein is in **cartoon** representation and the ligand is in **sticks**. Cartoon settings include **round helices** and **fancy flat sheets**.



publication (with or without **solvent**) The protein is in **cartoon** and ligand in **sticks**. The cartoon settings include **fancy helices**, and **sheets**, and **highlight color**.

*PyMOL's settings are an advanced topic, treated in Chapter XX, and on the web.

Navigation

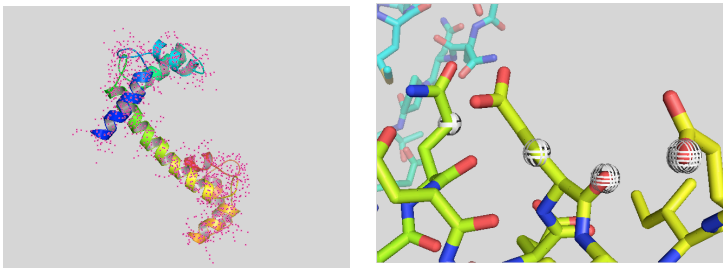


Fig. X.7 If you click in the PyMOL Display Area without dragging, you may cause pink boxes or white globes to appear. For now, just left-click in a blank area to be rid of them. (See Selecting with the Mouse and Chapter XYZ for the functions of the globes and boxes.)

Dragging the mouse — middle button pressed — for translations

Figures X.7 through X.11 guide you through the basic mouse-dragging operations. The black arrows represent your cursor in the Display Area, and the green arrows represent paths for moving the cursor. Figures on the left are "before" you drag. Figures on the right are "after." To match the figures, connect to the internet, launch PyMOL, and type in the upper command line

```
PyMOL> fetch 3cln
```

(and enter, or return). PyMOL will download coordinates for calmodulin from the PDB. Choose **Display / Background / Light Grey** from the top bank of menus. Find the object name **3cln,** pull down the **A** Action menu, **preset**, then **publication**.

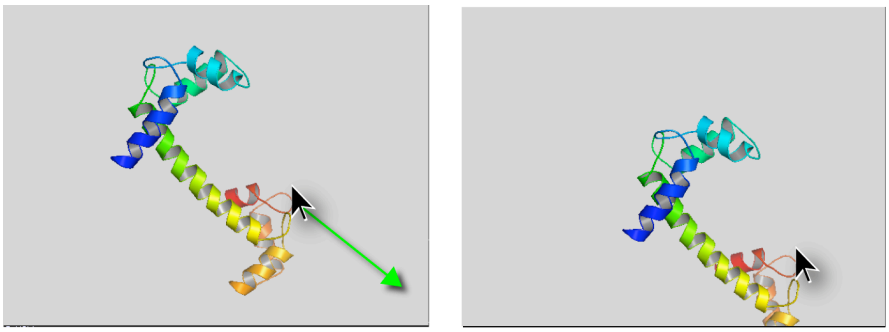


Fig. X.8 First place the mouse so the cursor shows on or near the molecule in the Display Area. Push down on the middle mouse button and drag. The molecular representation will translate in the plane of the screen (picture plane).

Dragging the mouse — left button pressed — for rotations

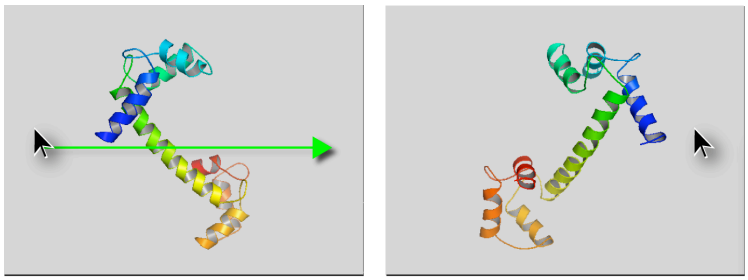
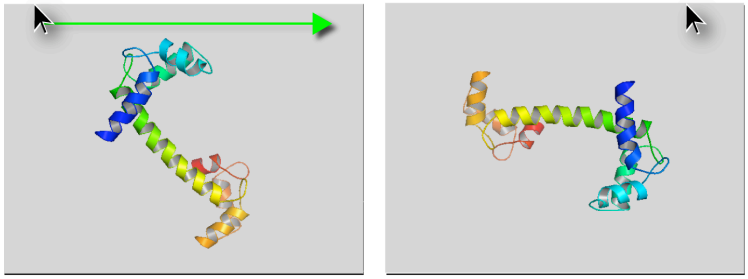
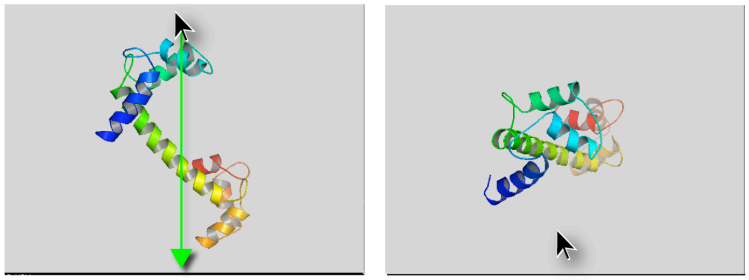


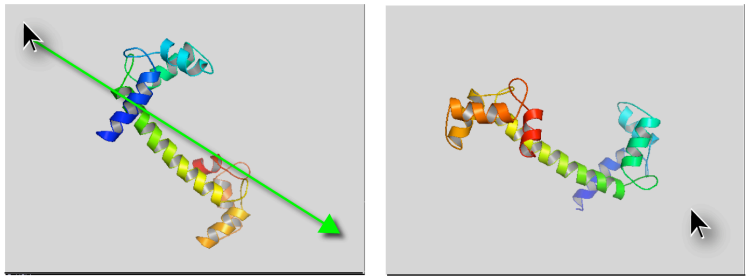
Figure X.9 Dragging the mouse straight across, starting with the cursor at mid-screen height, produces rotation out of the picture plane. The rotation axis is oriented vertically in the picture plane.



Dragging the mouse along an edge of the screen produces rotation in the picture plane. This works at top, bottom, left and right edges. The rotation axis is perpendicular to the picture plane.



Dragging the mouse straight vertically with the cursor at center screen-width produces rotation out of the picture plane. The rotation axis is oriented horizontally in the picture plane.



Dragging the mouse diagonally, starting with the cursor at any position, produces a rotation about an axis that pierces the picture plane at an angle.

The PyMOL Trackball (See Figure X.10.) When you press and drag using the left mouse button, the rotation behavior depends on where the cursor is when you start, and the direction in which you drag. For simple rotation about an axis located in the picture plane, always move the cursor along a horizontal or vertical line that passes through the center of the Display Area. In contrast, for rotation about an axis perpendicular to the

screen, drag along one of the edges of the Display Area. Moving the mouse in an intermediate path between these two extremes will generate mixed behavior, and enable you to rotate the molecule about any axis you wish.

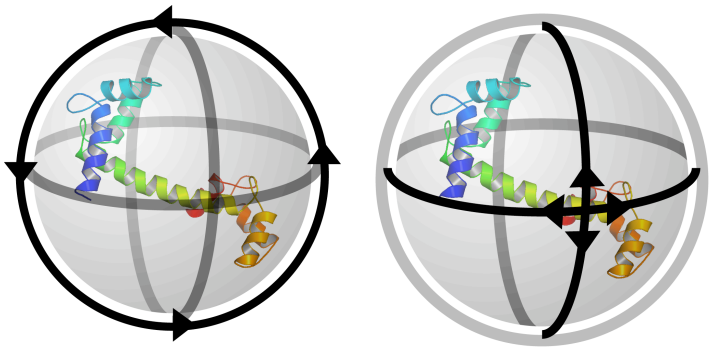


Figure X.10 Dragging the mouse with the cursor in the Display Area with the left mouse button depressed rotates the display like a virtual trackball.

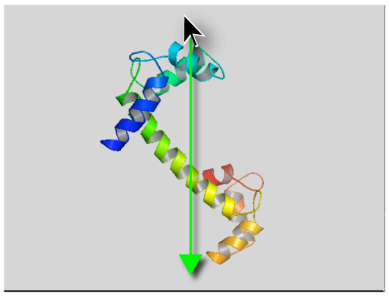
To understand what is going on when you drag the mouse with the left button depressed, imagine what would happen if you pressed your index finger against a heavy bowling ball, and then moved your finger in some arbitrary direction while continuing to press. If you moved your finger near the top of the ball in the center, then the ball would simply roll in the same direction as your finger. However, if you pressed the side of the ball, then the ball would tend to rotate about the axis pointing at you from the center of the ball. If your pushed from someplace between the center and the edge of the ball, the response would be a combination of rolling and rotation. That is essentially how PyMOL's virtual trackball works. The positions of PyMOL rotation axes are treated more specifically in Chapter XX.

If you prefer, you can disable the virtual trackball by deselecting **Virtual Trackball** in the **Mouse** menu (at the top of your screen on a Mac, and at the top of the Tk window on a Windows PC or Unix system). Rotation will then be restricted to axes in the picture plane.

Reset and zoom

Investigations with PyMOL can take you far afield from the default view of your molecule that PyMOL presents when you first load the coordinates. You can always get back to the original view. Left-click the **Reset** button (just to the right of the white command history and diagnostics area) to restore the original view of your molecule. If you have simply moved the virtual camera too deeply inside a structure, and need a longer view, the **Zoom** button will pull the camera out toward you so you can see the entire molecule in the Display Area. Then the right mouse button can be used to gradually zoom back into the structure with a renewed perspective on your position. In the Saving and restoring sessions section, we'll show how to save and restore program states. In Chapter XYZ, we'll show how to save views of a molecule in a log file, or script.

Dragging the mouse — right button pressed — for zooms



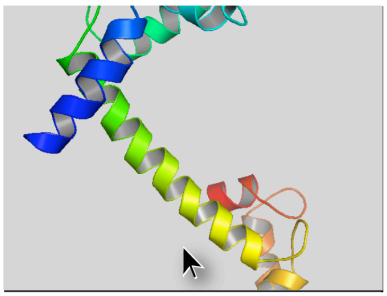
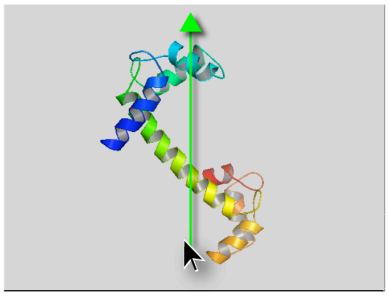
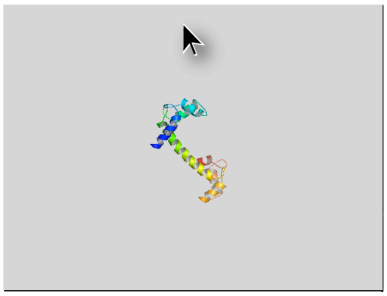


Figure X.11 With the right mouse button pressed, dragging the mouse toward you, moving the cursor down the Display Area, will enlarge the image.





With the right mouse button pressed, dragging (pushing) the mouse away you, moving the cursor up the Display Area, reduces the image.

Clipping with the scroll wheel

Clipping gives you the ability to focus on interesting parts of your molecule while eliminating interference from other parts. A black background with a **lines** representation is a good combination for manipulating clipping planes (see Figure X.12). Reset the viewer window to the original view by left-clicking the **reset** button; choose **A** Action **/ preset / default**, and choose **Display / Background / Black** from the top bank of menus. Place the cursor in the Display Area, and try rolling the mouse scroll wheel backward, toward you. Various portions of the molecule should disappear from both the front and the back of the molecule. Now roll the scroll wheel in the reverse direction, forward, away from you. Portions of the molecule that previously disappeared should now reappear. This is the simplest way to control clipping in PyMOL.

Now press the keyboard Shift key and continue to hold it down while scrolling. PyMOL will translate the clipping slab relative to the molecule. The molecule will not appear to move; just what is visible will change. Next, press the keyboard Control (CTRL) key and hold it down while you roll the mouse wheel. The molecule will appear to be moving toward you or away from you.

Whenever you use a key on the keyboard in combination with the mouse to control PyMOL, press the key first, and continue to hold it down while you use the mouse.

Clipping with the right mouse button

For finer control, hold down the Shift key and the right mouse button. Then drag the mouse vertically to move the front clipping plane, and drag horizontally to move the back clipping plane. Try adjusting the thickness of the clipping slab to display approximately one single layer of amino acids. Try rotating, panning (translating), and zooming using the left, middle, and right buttons. With some practice, you should be able to navigate to display interesting side chain interactions.

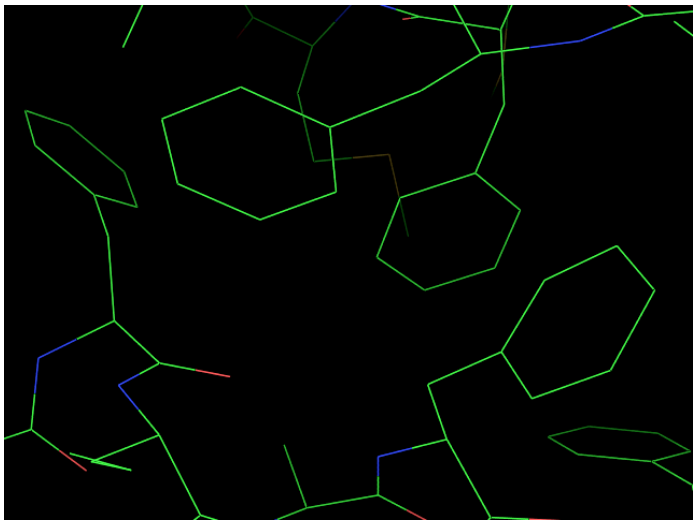


Figure X.12 In the **Default** preset (**Lines** representation), it is possible to spot interesting interactions and navigate to frame them. The sidechain arrangement shown here was found in the 3cln.pdb coordinate set.

We'll return to clipping in the Practice section.

Centering with the mouse — middle button click

An interesting way to navigate through a structure is to step from one center of interest to another. To see how this works, left-click on the **reset** button. Position the cursor over an atom of interest, and click and release the middle mouse button or wheel. PyMOL will then move the molecule so that the atom you middle-clicked over is at the center of the Display Area and the clipping slab. When you then rotate (drag the mouse with the left button depressed), the axis of rotation will go thru the central atom so you can see it from all sides. Middle-click on another atom and it will play the same central role.

Representations

Representation menus

Occasionally, a PyMOL preset will provide exactly the representation you need. However, you may want to control representations more closely. Representations are controlled using the **S** Show, **H** Hide, **L** Label, and **C** Color pop-up menus. Every object has its own set of pop-up menus, as does each selection (list of atoms) that the user defines.

When you use a **S** Show or **H** Hide menu for an object, the representation of all the atoms in the object are shown or hidden, and the changes are cumulative. For example, if you **S** Show **sticks**, **S** Show **spheres**, and then **S** Show **dots**, every atom in the object

will have all three representations active at once in the Display Area. If you then **H** Hide **spheres** and **H** Hide **dots**, only the **sticks** representation will remain visible.

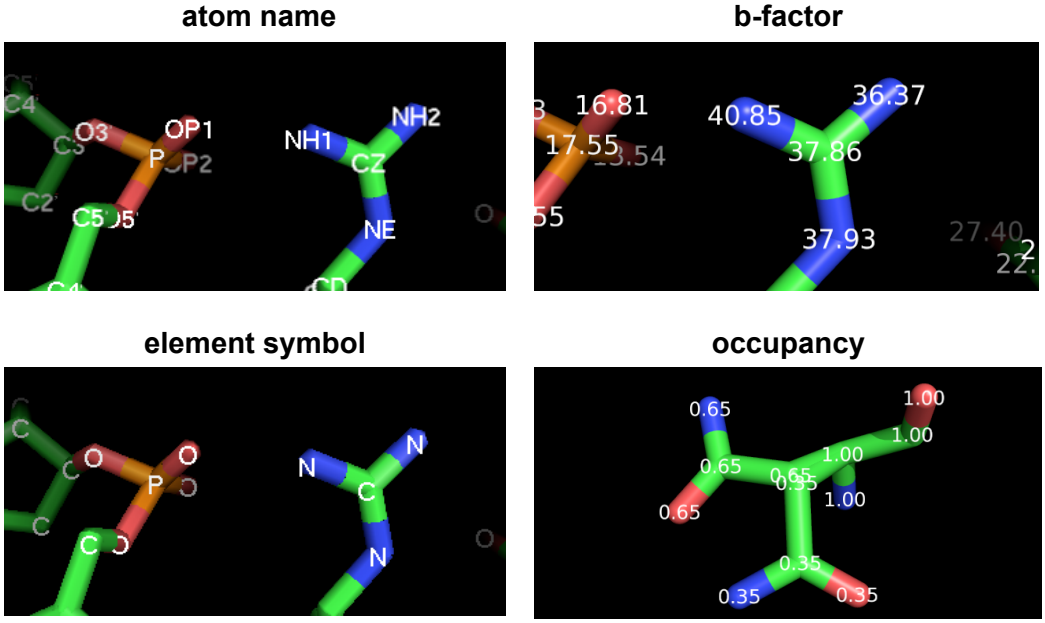
The **S** Show menu has a cascading **as** submenu (see Figure X.13, left), which enables you to hide all other representations while showing only the representation you choose. For example, if you **S** Show **/ as sticks**, and then **S** Show **/ as dots**, only the **dots** representation will remain visible. Take a moment to experiment with the **S** Show, **S** Show **/ as**, and **H** Hide pop-up menus and the various representations. Note that the **surface** and **mesh** representations take some time to compute for larger molecules.

nb_spheres in the **S** Show and **H** Hide menus refers to special small spherical representations of molecules that are not assigned bonds in the coordinate file, such as waters and simple ions. **nonbonded** refers the same molecular locations, represented as crosses. Figure X.13 describes the use of other entries in the **S** Show and **H** Hide menus.

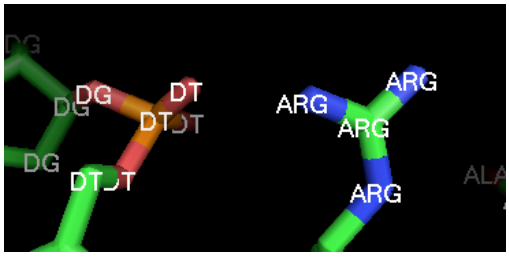
The **C** Color menu has several cascading submenus. There are alternatives for coloring atoms by element, and alternatives for distributing colors over chains or secondary structures (**ss**). Each color listed at the bottom of the menu has a submenu of variants.

As shown in Table X.2, the **L** Label menu is useful for identifying structures in close-up views of a molecule.

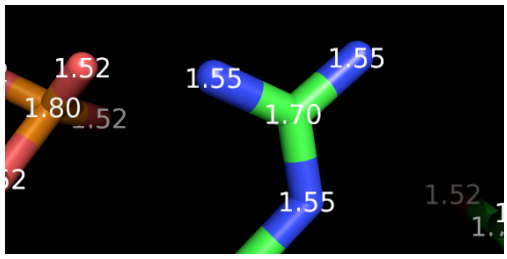
Table X.2 Examples of useful labels from the **L** Label pop-up menu



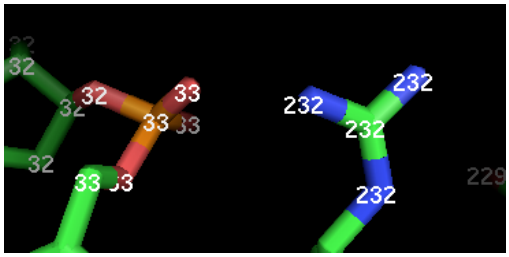
residue name



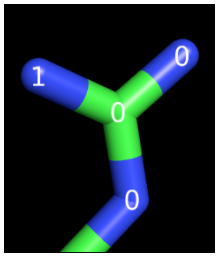
vdw radius



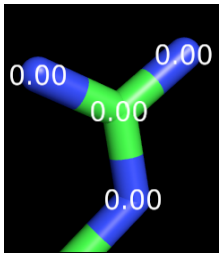
residue identifier



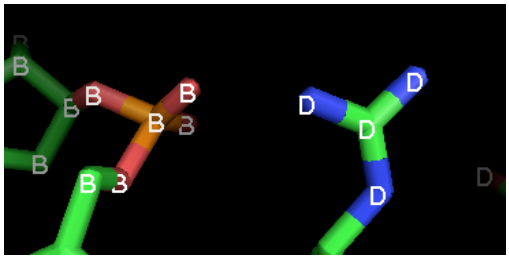
formal charge



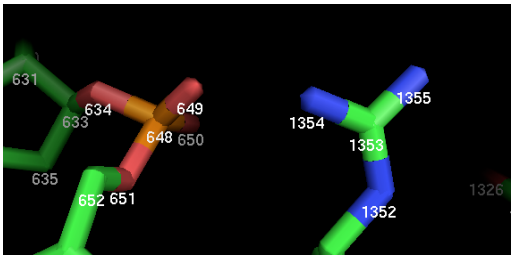
partial charge

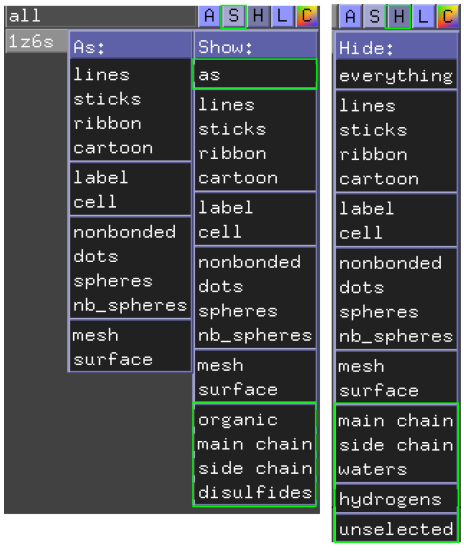


chain identifier



rank





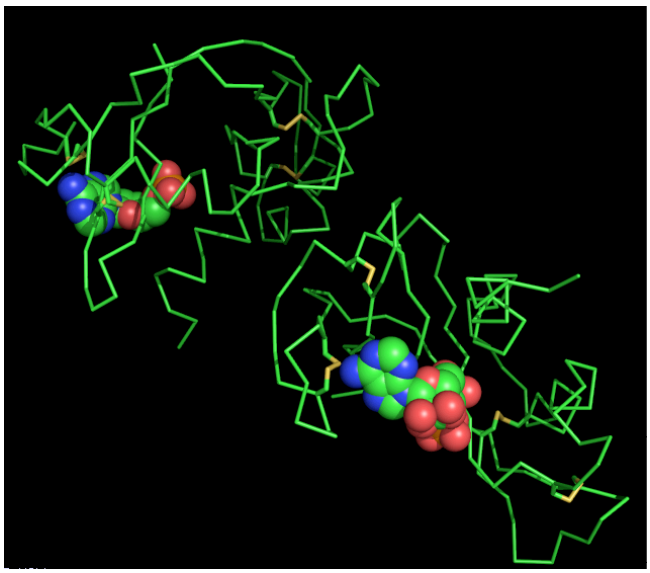


Figure X.13 In addition to the representations in the **S** Show menu, there are four atom-type key words (boxed in green on left); **organic**, **main chain**, **side chain** and **disulfides**. There are five atom-type key words (also boxed in green) in the **H** Hide menu. Here we use the PDB file 1z6s to demonstrate these options. The recipe for producing the figure on the right is:

```
PyMOL> fetch 1z6s
```

(and enter, or return).
Next to the **all** object name, choose **H** Hide **/ waters**.
Next to the **1z6s** object name, choose **S** Show **/ as ribbon**.
Next to the **1z6s** object name, choose **S** Show **/ disulfides / Show sticks**.
Next to the **1z6s** object name, choose **S** Show **/ organic / Show spheres**.

The **all** object name is at the top of the list of named objects & selections (user-defined lists of atoms). Choosing from the **all** menu enables you to apply actions and representations to all objects that are currently loaded into PyMOL. For example, if you wish to hide all representations of all objects, you can choose **everything** from the **H** Hide pop-up menu next to **all**. In Figure X.13, the **all** menu is used to hide waters.

Practice

Here we demonstrate the use of clipping with a protein-DNA structure, in which we isolate protein-DNA interactions. To follow along, type in the upper command line:

```
PyMOL> fetch 1zaa
```

(and enter, or return). Next to **1zaa**, choose **S** Show **/ as sticks**. Change the color scheme of the elements under the **C** Color menu by choosing the **by element** scheme with yellow carbons. This changes the color scheme for every chain (protein and DNA) in the 1zaa object.

Now, to distinguish the DNA chains from the protein, type in the upper command line to make the selection:

PyMOL> `select dna, chain a or chain b`

(and enter, or return). The PyMOL user interface changes in two ways. Pink boxes appear in the Display Area, associated with every atom that is in the DNA a chain OR DNA b chain. The selection name **(dna)** appears in the list of objects and selections. The parentheses signal that this is a selection. Make the pink boxes disappear by left-clicking on **Deselect** in the bank of control buttons to the right of the command history and diagnostics window. Left-click on the **C** Color button to the right of **(dna)** and choose **Cyans / cyan**, or any color you prefer.

Use the keyboard shift key and the right mouse button to adjust the thickness of the clipping slab to display approximately a single layer of amino acid and nucleotide residues. When you hold down the Shift key and the right mouse button, and drag the mouse vertically, the front clipping plane moves. Keeping the Shift key and right mouse button depressed while you drag horizontally will move the back clipping plane. Figure X.14 shows examples of protein-DNA interactions you can isolate in this way.

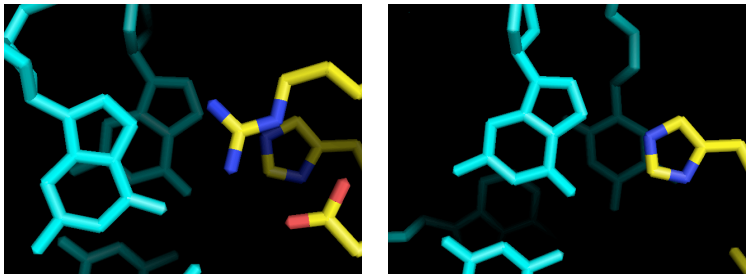


Figure X.14. On the left, the clipping plane focuses on DNA chain a, G7, and zinc finger protein residues Arg46 and Asp48 (PDB file 1zaa). On the right, His49 and DNA chain a, G6, come into view, and zinc finger residues Arg46 and Asp48 are clipped out.

Making and Representing Selections

When working with molecular structures, you may want to show different atoms using various representations and colors. In Figure X.13, we demonstrated this with a few key words that are available in the **S** Show and **H** Hide menus. However, you can only distinguish a few types of atoms from those menus, and doing so does not create a new selection.

PyMOL's selection methods enable you to select any atom or group of atoms within an object, or across multiple objects. These methods add the selection to the list of objects & selections to the right of the Display Area, enabling you to operate on them in a variety of ways, and to come back to them as convenient. The selection is highlighted in the Display Area by pink boxes centered over each atom in it. Typing is the most versatile way to make selections and give PyMOL commands (This is covered in Chapter XYZ). In this chapter, we focus on selections and commands created by clicks of the mouse.

Selections behave simply as lists of atoms, and do not have any properties of their own. They are used, instead, as arguments to PyMOL commands. Once you have named a selection of a group of atoms, you can apply any number of PyMOL commands to it, including those in the pop-up menus.

Selection names appear next to the Display Area, enclosed by a set of parentheses in order to distinguish them from object names. An object is the primary information set that PyMOL stores when it reads in a coordinate file. When an object is deleted from PyMOL, any selections from that object are useless, because they point to non-existent information. On the other hand, you can create and delete selections without changing PyMOL's memory of objects.

Selecting with the mouse

When you open PyMOL, the **Mouse Mode** is set to **3-Button Viewing**. This setting is shown to the right of the Display Area, below the space for the list of named objects & selections (see Figure X.15). The setting **3-Button Viewing** allows you to make selections by left-clicking the mouse over an atom in the Display Area. If the setting is 3-Button **Editing**, then you can toggle it to **Viewing** by left-clicking once on the word **Editing**. By default, in **3-Button Viewing** mode, PyMOL will select and deselect complete **Residues**. The **Selecting** setting (also shown in Figure X.15) can be toggled through groupings of **Residues**, **Atoms**, **C-alphas**, **Molecules**, **Objects**, **Segments**, **and Chains**, by left-clicking on the words that appear to the right of **Selecting**.

When you select an atom or group of atoms, pink boxes appear in front of the representation in the Display Area (Figure X.15). The selection name, which is **(sele)**, unless you rename it, appears at the bottom of the selection list with a gray background. As long as the selection remains active, that is, as long as the pink boxes remain in the Display Area and the background behind **(sele)** remains gray, you can make alterations to the selection using the pop-up menus in the **(sele)** row, or by more advanced methods (see Chapter XYZ). You can add to the group of selected atoms by left-clicking once above other atoms in the Display Area.

Deactivate the **(sele)** list by clicking once away from any atoms in the Display Area, by left-clicking once on **(sele)** in the list of objects & selections**,** or by left-clicking on **Deselect** (in the Tk window on a Windows PC, or in the top bank of buttons in the PyMOL window on a Mac). Any of these actions will deactivate the selection, toggle the area behind **(sele)** to black, and remove the boxes above the atoms in the Display area. Take some time to practice selecting and deselecting atoms, residues and other groups, and changing their representations.

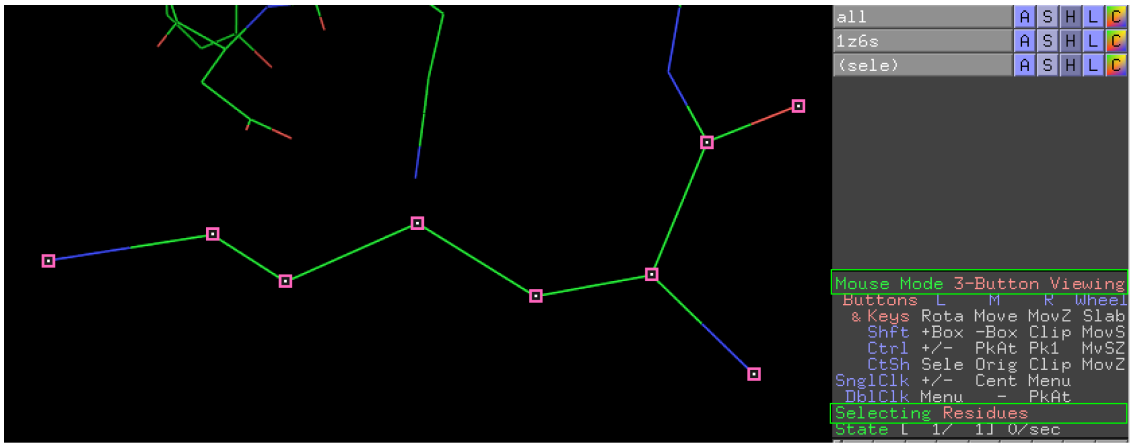


Figure X.15 PyMOL's Mouse Mode toggles between **3-Button Editing** and **3-Button Viewing**. You need the Viewing mode to make selections with the mouse. The default behavior when you left-click over any atom in the Display Area is that the entire residue is selected. Left-click to the right of the word "Selecting" to toggle through a list of types of groups you may select when you left-click over an atom in the Display Area.

Notice that, if you don't deselect between left-clicks over atoms in the Display Area, PyMOL adds the newly selected atoms to the group of atoms in the selection, **(sele)**.

Renaming selections

You can save PyMOL selections by renaming them. Giving meaningful names to selections helps you to navigate through a PyMOL session. To name a selection, left-click on the **A** Action menu next to **(sele)**, choose **rename selection**, and then enter the new name using the keyboard, and enter, or return. The new name will replace **sele**.

If you then left-click in the Display Area away from any atom, or left-click on the selection name in the objects & selections list (toggling the background from gray to black), or left-click on **Deselect**, the next atom or group of atoms you select will start a new selection with the default name **(sele)**. If you want to add to the list of atoms in a named selection, activate the selection (left-click on its name to make the background gray), and then left-click on the atom, residue, or other group that you want to add. Only one selection can be active at a time. An example of a representation created by left-clicking, selecting, and renaming is shown in Figure X.16.

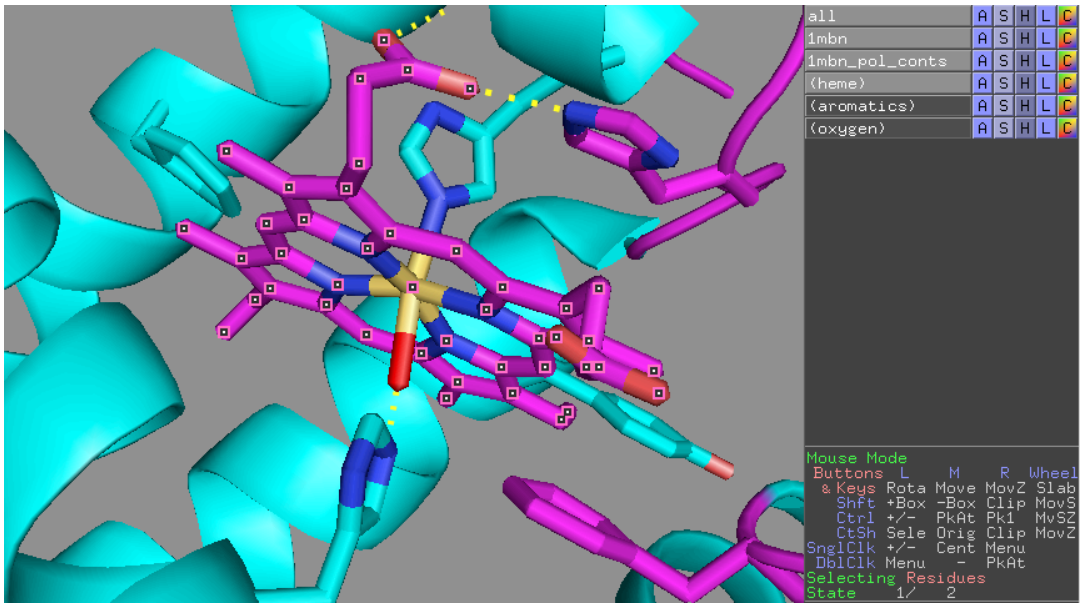


Figure X.16 This is the heme and surrounding aromatics from 1mbn, the first protein crystal structure ever solved, Kendrew's myoglobin. The recipe for producing the representation in this figure is: type `PyMOL> fetch 1mbn` (and enter, or return).
Choose **Display / Background / Gray**.
Choose **1mbn / A** Action **/ preset / ligands**.
Choose **1mbn / S** Show **/ cartoon**.
Choose **1mbn / H** Hide **/ ribbon**.
Choose **1mbn / C** Color **/ by ss /** helix sheet loop.
Left-click on an atom in the heme (in the Display Area) to select it. Rename **(sele)** as **(heme)**.
Choose **(heme) / C** color **/ by element /** NOS.
Left-click away from all atoms in the Display Area to deselect the heme. To make it easier to see the line representations, type
`PyMOL> set depth_cue=0`
Select aromatic residues around the heme by left-clicking on them in the Display Area.
Rename **(sele)** as **(aromatics)**.
Choose **(aromatics) / S** Show **/ sticks**.
Choose **(aromatics) / H** Hide **/ main chain**.
Choose **(aromatics) / C** color **/ by element /** NOS.
Left-click away from all atoms in the Display Area to deselect the aromatics. Set **Selecting** mode to **Atoms** by left-clicking. Left-click on the iron atom at the middle of the heme.
Choose **(sele) / C** color **/ yellows / yelloworange**.
Select by left-clicking on the oxygen ligand to heme. Rename **(sele)** as **(oxygen)**, show it **as sticks** and color it **reds / red**.
Left-click away from all atoms in the Display Area to deselect the oxygen.
Choose **1mbn / H** Hide **/ lines**.
Navigate with the mouse to match the view above.
Left-click on an atom in the heme to reactivate the selection and show the pink boxes. One selection, **(heme)**, is now active. The objects **all**, **1mbn**, and **1mbn_pol_conts** are also active.

Expanding and extending selections

Once you have created a selection, you can use the pop-up menus in the row of the selection name to change its representation. For example, the **S** Show **/ as sticks** action was used on the **(heme)**, **(aromatics)** and **(oxygen)** selections in Figure X.16.

Existing selections can be modified in a variety of ways to include additional atoms or to exclude atoms already in the selection. The aromatics selection in Figure X.16 was created in this way, by left-clicking on each representation of aromatic residues in the neighborhood of the heme in 1mbn. To perform a variety of other modifications, based on distances and other criteria, you can use the **modify** submenu under the **A** Action menu for a given selection. For example, in Figure X.17, the selection (heme) was renamed **(around heme)**. Then the selection was expanded by choosing **modify / expand / by 6 Å, residues** in the **A** Action menu for **(around heme)**.

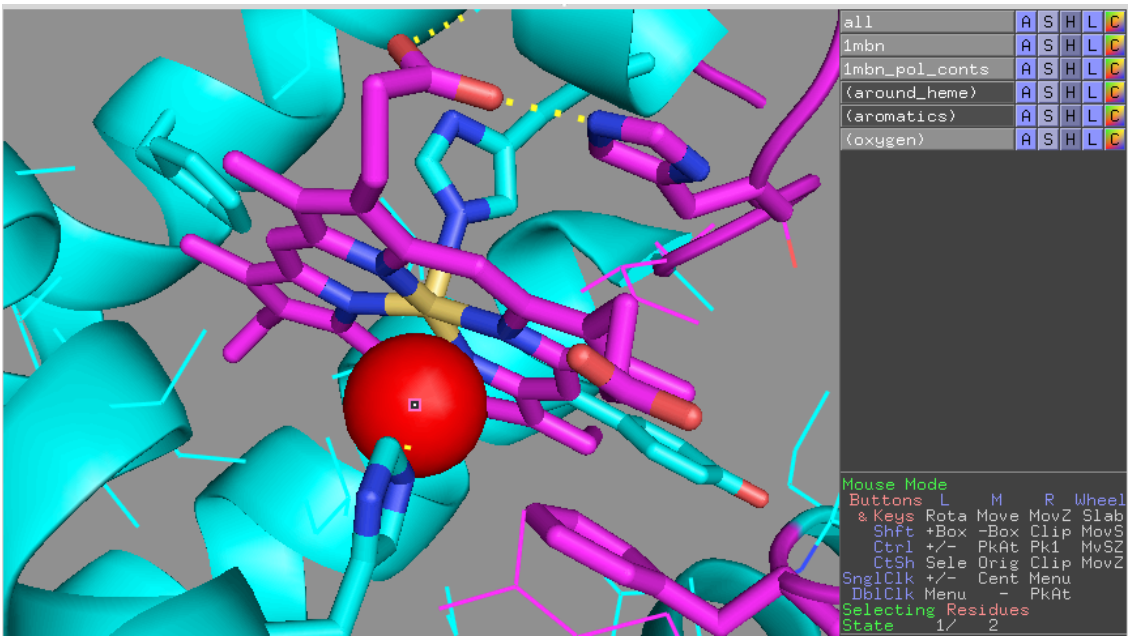


Figure X.17 Starting from Figure X.16,
Choose from the objects & selections list **(heme) / A** Action **/ rename selection** and type: `around heme`.
Choose from the objects & selections list **(around heme) / A** Action **/ modify / expand / by 6 Å, residues**.
Choose **(around heme) / S** Show **/ lines**.
The heme and all residues within 6 Å are shown as lines. However, the heme sticks representation hides the heme line representation.
Choose from the objects & selections list **(oxygen) / S** Show **/ as spheres**.

When you **expand** a selection, you choose the radius of the included area from the menu. When you **extend** a selection, you choose the maximum number of bonds within which to include atoms or residues in the selection.

Selecting and changing representations in sequence view

You can use sequence information to make selections by choosing the **Sequence On** option in the **Display** menu, or by left-clicking on the S (toggle switch) in the row of Movie

Controls. PyMOL will then display sequences for the active objects in a sequence viewer at the top of the Display Area. For proteins and polynucleotides, the default is the one-letter residue code. For ligands, PyMOL usually displays an abbreviated chemical name. Selected residues are highlighted in the sequence viewer (see Figure X.18).

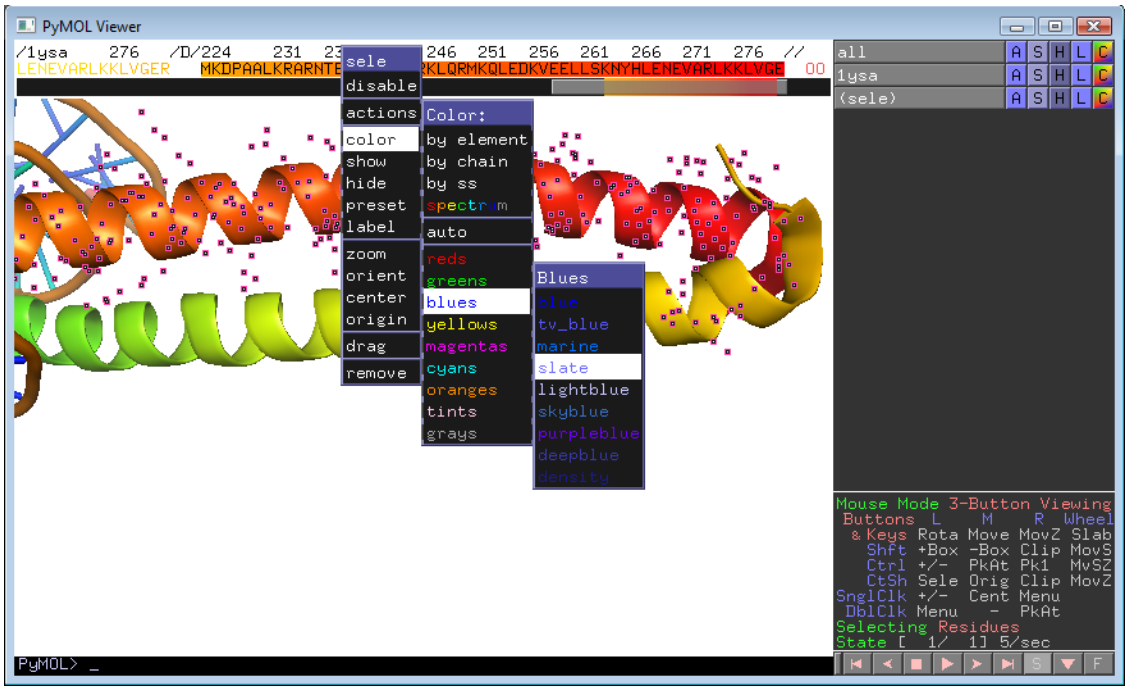


Figure X.18 A protein chain in **1ysa** was selected by dragging the cursor, left mouse button depressed, over its sequence in the sequence viewer. The rainbow color of the chain shows up behind the sequence to highlight it. The usual pink boxes indicate the positions of the selected atoms in the Display Area (including the side chain atoms). After the selection was made, the cursor was placed over a sequence letter in the selection and right-clicked to bring up the cascading menus for choosing the color of the selection.

You can make and modify selections by left-clicking and dragging the cursor over the sequence letters. When a selection is activated, right-clicking with the cursor directly on a residue character in the selection will bring up a menu of actions to be applied to that selection. This menu provides an alternative to the object & selections list for altering representations of selections (See Figure X.18 and Figure X.19).

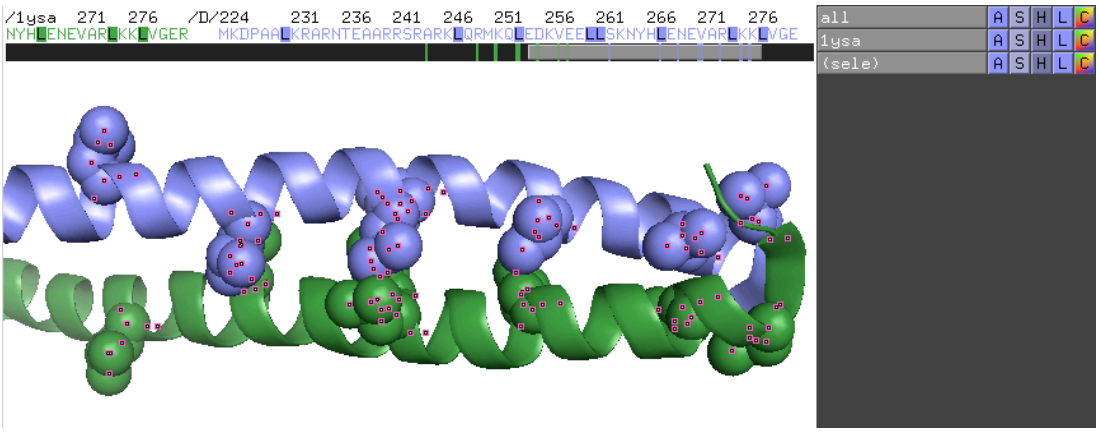


Figure X.19 After the color **blue / slate** was applied to chain D in Figure X.18, the chain was deselected. Chain C was selected, colored **green / forest,** and deselected. Leucines (Ls) were selected by left-clicking on all the Ls in the sequence viewer, as you see here. The leucine side chains were shown as spheres. The recipe for showing only the side chain atom as spheres, and not the main chain atoms, is to **S** show **/ spheres** and **H** hide **/ main chain** of the selection. Choosing **Show as / cartoon** again for **1ysa** then restores the dropped pieces of the main chain. These operations can be done in the pop-up menus next to **(sele)** in the object & selections list, or by right-clicking on one of the Ls in the sequence viewer to get a pop-up menu.

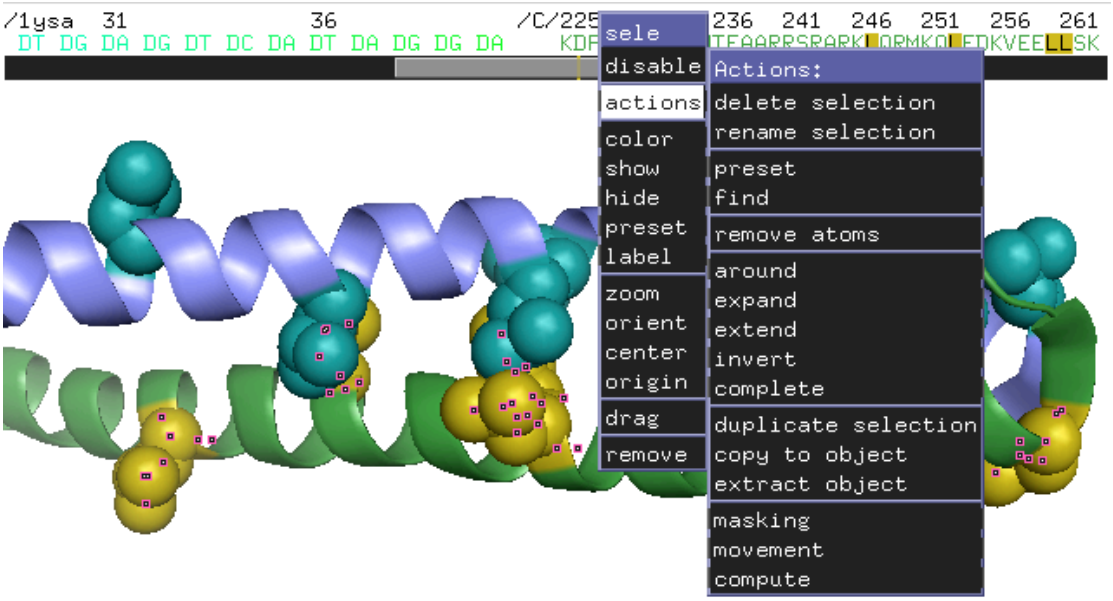


Figure X.20 Starting from Figure X.19, right-clicking on a selected L popped-up cascading menus. **C** Color **/ cyans / deep teal** was chosen for the L side chains. Left-clicking on the selected Ls in chain D deselected them. Then **C** Color **/ orange / olive** was selected for the L side chains in chain C. Right-clicking again with the cursor over one of the selected L's popped-up cascading menus. Note that one of the available options is to rename the selection to save it for later use.

To repeat, left-clicking and dragging the cursor over the sequence display makes the selection. Right-clicking with the cursor over a letter in the selection pops up a menu for representing it. If you right-click on an unselected residue in the sequence viewer, then a different menu will appear. This menu is titled with identifying information for the residue you right-clicked on, and enables you to perform various actions, such as changing colors or altering representations for the residue — without creating a selection.

Besides selecting and changing representations by clicking the mouse with the cursor over letters in the sequence display, you can change your view of the molecule. Middle-clicking with the cursor over any letter in the sequence will center that residue in the display. Pressing Control (CTRL) on your keyboard and middle-clicking will center the display on the residue and zoom in on it.

Changing representations by clicking in the Display Area

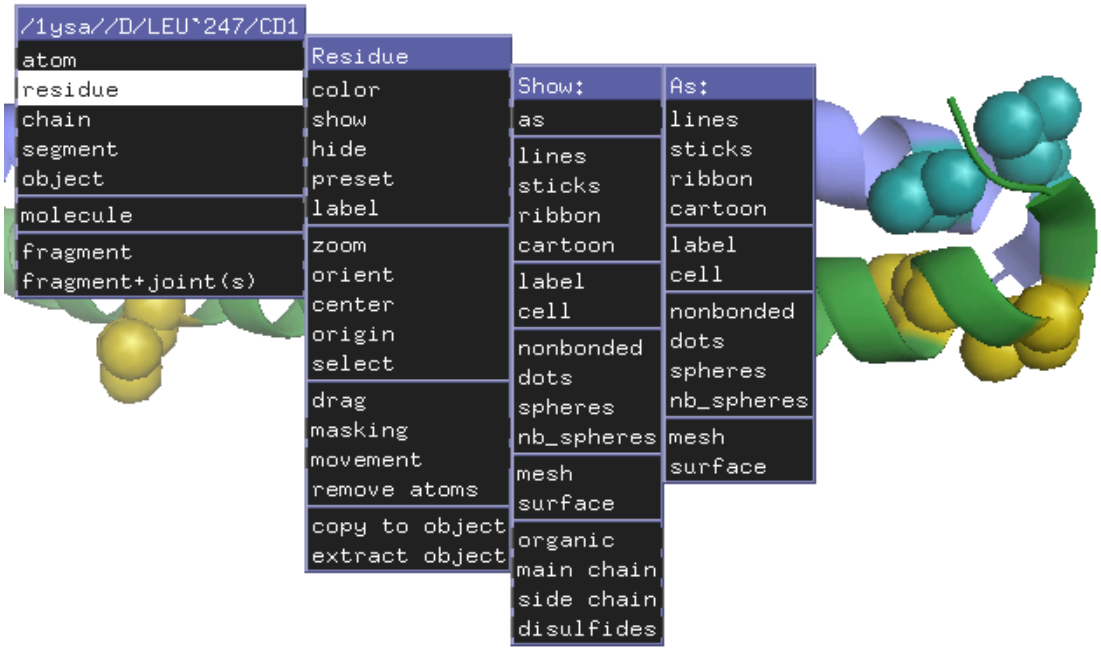


Figure X.21 Right-clicking over an unselected atom in the Display Area brings up a menu of choices for representing the groups of atoms to which the right-clicked atom belongs — without creating a selection. (The grouping is chosen by toggling through the list of groupings next to **Selecting**, near the bottom of the mouse control matrix to the right of the Display Area).

As you have seen, left-clicking with the cursor positioned over an atom in the Display Area selects the atom and the group to which it belongs, according to the mouse options

you have chosen. Right-clicking over a selected atom in the Display Area gives you the same cascading menus as in Figures X.18 and X.20. However, when you right-click with the cursor over an unselected atom in the Display Area (See Figure X.21), or over an unselected residue letter in the sequence display, a different cascading menu pops-up, headed by an identification of the atom (or residue, etc.) that was right-clicked. This menu gives you the options of applying actions to the atom (or residue, etc.) without creating a selection.

Save as You Go

The many ways to save

During a PyMOL session you may create program states (called sessions), scenes, shows, images, molecules, logs, views, and images that you need to save. Here we introduce the ways to save sessions, scenes, shows, and images. Chapters XY and Z discuss logs, views, and molecules.

Saving and restoring sessions

You can save a PyMOL session file at any point during a PyMOL work session. The session file will contain all the structures that are loaded in PyMOL at that point, and all the information for displaying the structures, including colors, representations, and camera views. When you reopen a session file, you can continue your work from the point you left off. *Be sure to save a session file when you are done with a PyMOL session, just as you would save a document in a word processor to avoid losing your work.* To save a PyMOL session in a new session file, choose **Save Session As...** from the **File** menu, choose a suitable location and type the name for the file, and then left-click Save. To update an existing session file, choose **Save Session**. PyMOL session files are given a ".pse" filename extension so that PyMOL can recognize them to open them again. On Windows PCs and Macs, you can open session files by double-clicking on the session file icon. Or if PyMOL is already open, you can choose **Open...** from the **File** menu.

Using session files in place of undo Presently, there is no “undo” function in PyMOL. To keep the amount of backtracking tolerable, it is important to save your PyMOL session before you deviate from a satisfactory session state. Act defensively against mistakes by saving session files often. Then you can return to a previous state without hav-

ing to start over from scratch. *It's a good habit to save session files every five minutes when using PyMOL for extended tasks.*

Creating, viewing and manipulating scenes

Creating Scenes PyMOL can store a series of molecular views in Scenes, each with its own colors, representations, camera positions, and annotations. Scenes are organized in sequence, like the slides in a PowerPoint™ presentation. Even when you aren't preparing a presentation, storing your work as a series of Scenes is useful for your own documentation and reference.

First, choose **Buttons**, under the **Scene** menu. This activates a display of Scene names at the lower left of the Display Area in the order they will be presented. When you have a representation in the Display Area that you want to save, create a Scene by choosing **Append** from the **Scene** menu (Choose **Append** for the first representation even though you are not literally appending to anything). PyMOL stores the representation in the Display Area as a **Scene**, and automatically assigns a name to it (*e. g.* "001"). The assigned name will appear in the diagnostics display area above the upper command line and in the stack at the lower left of the Display Area.

Manipulating scenes You can then change the view and choose new representations to **Append** as additional scenes in your presentation. Once you have appended two or more scenes, use the **Next** and **Previous** options in the **Scene** menu to display the scenes.

More conveniently, you can use the Page Down (PGDN) and Page Up (PGUP) keys on your keyboard to move through your scenes. You can also insert new scenes using these keys. Press CTRL and PGDN simultaneously on your keyboard to insert the existing display as a new Scene after the current one. Pressing CTRL and PGUP simultaneously will insert the existing display as a new scene before the current one.

It is also easy to navigate through existing scenes by clicking on the Scene names in the stack at the lower left of the Display Area. Clicking on a Scene name activates the scene in the Display Area.

The last scene displayed can be updated by choosing **Update** in the **Scene** menu. You can also add a note to the current scene by typing in the command line, as in

```
PyMOL> scene auto, update, Some annotation information
```

(and return, or enter) will display "Some annotation information" on the screen the next time the current Scene is recalled.

When you save a PyMOL Session, all the Scenes you have defined will be saved as well. Other PyMOL users can open the Session file and view the sequence of Scenes you have defined.

Saving shows

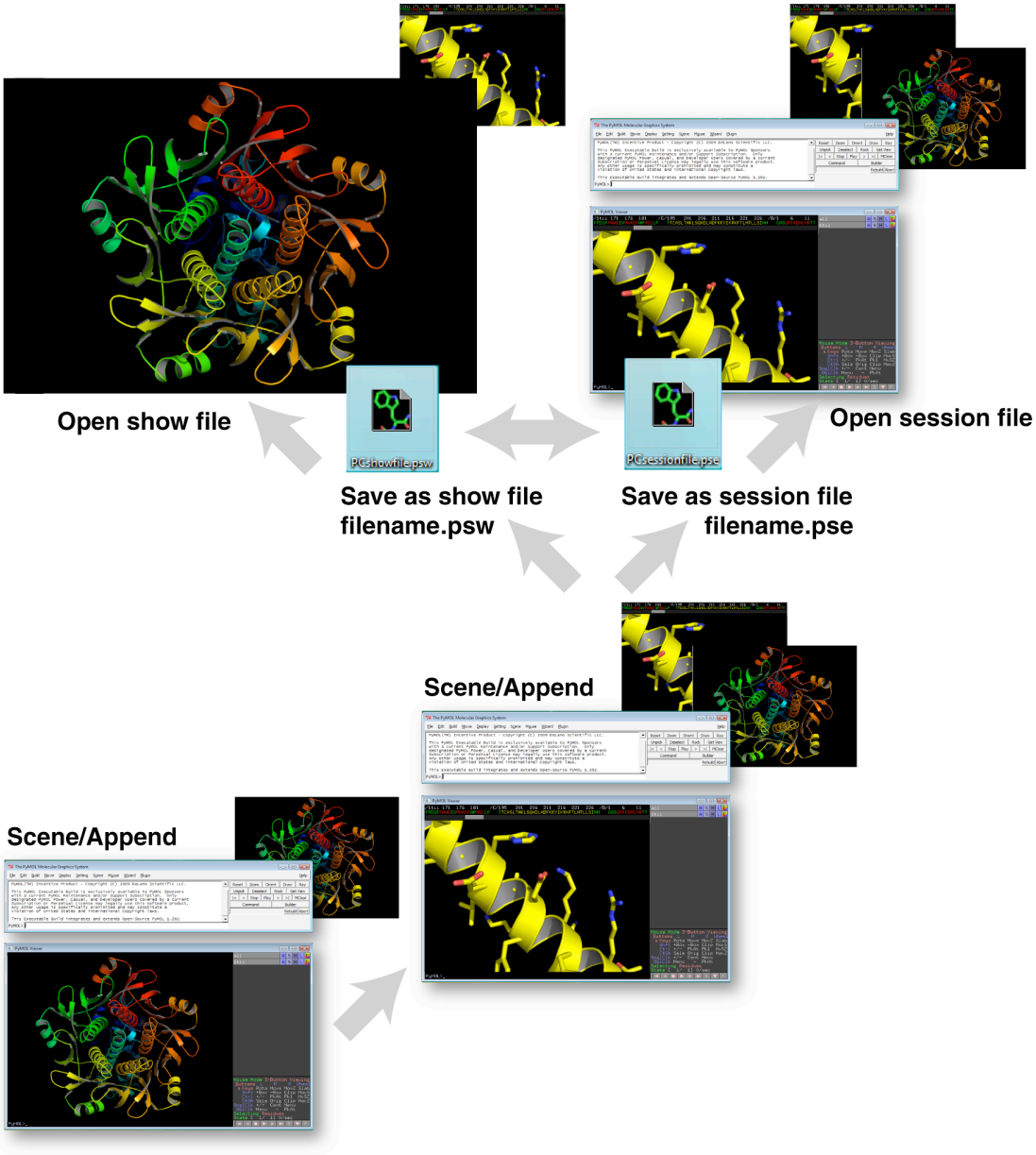


Figure X.22 PyMOL Session and Show files contain the same information, with one exception. They contain different instructions to the operating system on how they are to be displayed. Here, we show two Scenes being appended in PyMOL's memory. The same information is saved as a PyMOL Show file (with .psw file name extension) and a PyMOL Session file (with .pse file name extension). The Show file opens with a full-screen image. The Session file opens with the PyMOL user interface. Show and Session files are interconverted by changing their file name extensions.

A Show file is simply a PyMOL Session file that contains one or more scenes, and is saved with a ".psw" file name extension instead of ".pse." When a ".psw" file is opened, PyMOL automatically enters full-screen mode, and begins with the first scene in the sequence (See Figure X.22). To see how a PyMOL Show works, double-click the "demo_show.psw" file in the PyMOL Tutorial Folder, and use the PGDN and PGUP keys to step through the presentation. When playing back scenes, PyMOL animates the camera view to pan and zoom between the scenes. This gives a 3-dimensional sense of flying around the molecule. You can manipulate the view using the mouse without corrupting the presentation. Press the Escape (ESC) key to return to the desktop.

Interconverting shows and sessions To convert a PyMOL file from a Session to a Show, change the ".pse" file name extension to ".psw". To convert a PyMOL show back to a session, change the ".psw" back to ".pse." If you are using Microsoft Windows™ and cannot see the file extension, open the "Folder Options..." from the "Tools" menu of the Windows folder containing your file. Under the "View" tab, make sure that the "Hide extensions for known file types" option is not checked.

Saving images

You can save images from the PyMOL Display Area for presentations or publications by creating Portable Network Graphics (PNG) files. PNG files can be read by PowerPoint, Microsoft Word™, Keynote™, Pages™, and many other common programs. Once you have the image you want in the Display Area, choose **Save Image...** from the **File** menu, and enter a suitable destination and name for the file. You can import the saved image into PowerPoint by using the PowerPoint "Insert" menu, selecting "Picture" and "From File..." More conveniently, you can directly copy and paste images from PyMOL on a Windows PC or Mac. On a Windows PC, choose **Copy Image to Clipboard** in the **Edit** menu. On a Mac, choose **Edit / Copy** or type Command−C. The Paste command depends on your destination program and operating system. Most programs have Paste functions in their Edit menus.

Ray-tracing images PyMOL has a built-in renderer for ray-tracing. Ray-tracing and rendering eliminate rough edges and generate better lighting effects, including shadows. The result is a photorealistic image (see Figure X.23). Once an image is ray-traced, it is displayed in the PyMOL Display Area. Then you can save the image with all its photo-realistic effects in a PNG file. Rendering can be rather time consuming, depending upon the complexity of the image, sometimes requiring several minutes. Rendering progress is indicated in a bar below the top bank of control buttons. On a Windows PC, you can abort a ray-trace process by left-clicking on the abort button in the right bank of buttons of the Tk window.

To render a representation in the Display Area, left-click on the **Ray** button in the top bank of control buttons. Then, to save the photorealistic image, before clicking in the image area again, choose **Scene / Append** or **File / Save image as / PNG**. A progress indicator should appear if the Save takes a long time.

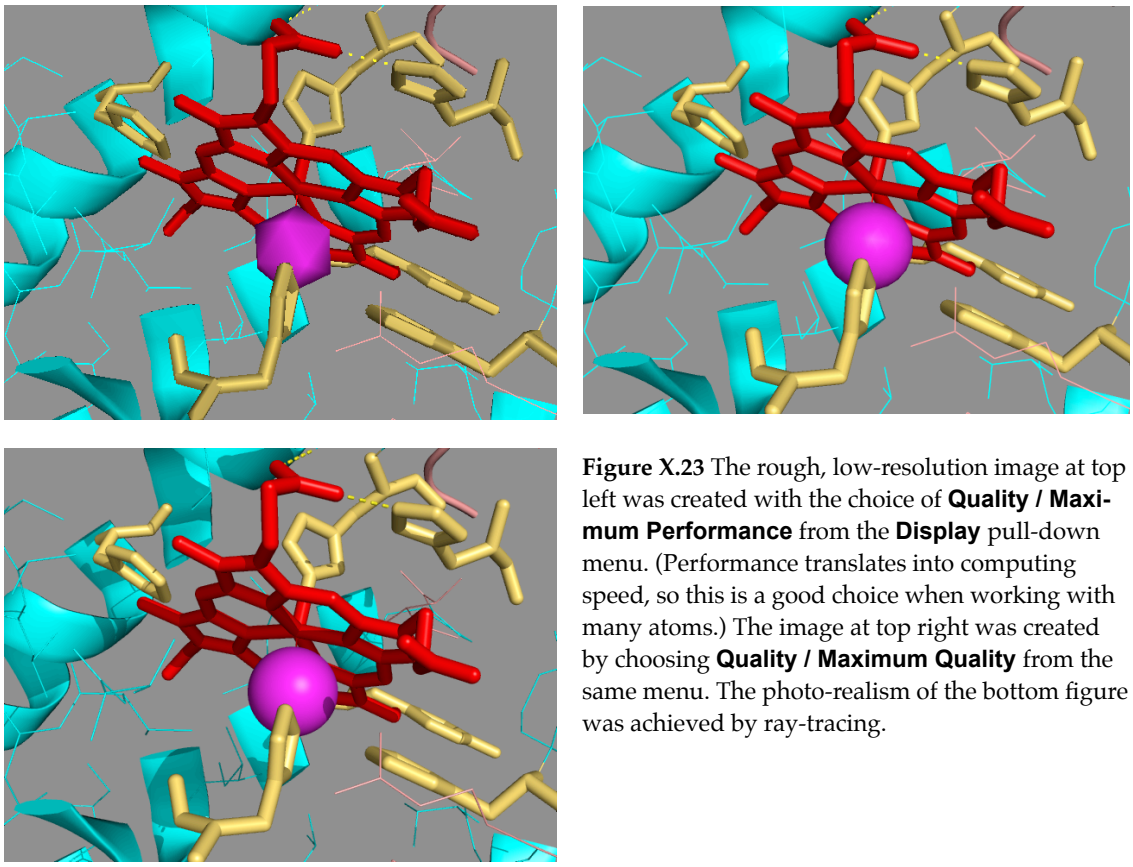


Figure X.23 The rough, low-resolution image at top left was created with the choice of **Quality / Maximum Performance** from the **Display** pull-down menu. (Performance translates into computing speed, so this is a good choice when working with many atoms.) The image at top right was created by choosing **Quality / Maximum Quality** from the same menu. The photo-realism of the bottom figure was achieved by ray-tracing.

Controlling Image Resolution

By default, PyMOL saves images at the current size and resolution of the Display Area. There are two ways to save images at higher resolutions. You can expand the size of the Display Area by dragging on the lower right corner of the window. Or, for greater control, set the number of pixels in the width and height of the image by typing **draw** or **ray** commands with the width and height as arguments:

```
PyMOL> draw 1200, 900
```

```
PyMOL> ray 1200, 900
```

These commands each generate a 4 inch × 3 inch image at 300 dots per inch (1200 pixels × 900 pixels). If you like the shape (aspect ratio) of the Display Area, but need to change its size, you can specify only the width, and the aspect ratio will be maintained.