

## A. The Main Menu Choices

<b>File</b>	<b>Save Molecule as . . .</b> save the PDB file to your disk.
<b>Edit</b>	<b>Copy</b> the image to the clipboard. (Paste it into a File.doc.) <b>Copy Chime Script</b> to the clipboard. (Paste it into a File.txt.) <b>Clear</b> the PDB file from the display. (Reload to see it again.)
<b>2D Rendering</b>	Flattens the structure of small (<256 atoms) molecules.
<b>Animation</b>	Available if the page contains an (file.xyz) animation.
<b>Rotation</b>	√ Toggle on/off
<b>Display</b>	<b>Wireframe:</b> atoms connected by thin "bonds". <b>Sticks:</b> atoms connected by thicker "bonds". <b>Ball &amp; Stick:</b> atoms are small equal-sized balls. <b>Spacefill:</b> atoms are balls with van der Waals radii. <b>Backbone:</b> $\alpha$ -carbons are connected by straight segments. <b>Ribbons:</b> $\alpha$ - and $\beta$ - segments are smooth wide surfaces. <b>Strands:</b> $\alpha$ - and $\beta$ - segments are five smooth curves. <b>Cartoons:</b> thicker than Ribbons, and $\beta$ - strands have arrowheads.
<b>Options</b>	√ Toggle the following: <b>Display Hydrogens</b>   <b>Display Hetero Atom Groups</b>   <b>Display Hydrogen Bonds</b>   <b>Display Disulfide Bridges</b>   <b>Display Wireframe Double Bonds</b>   <b>Dot Surface</b>   <b>Slab Mode</b>   <b>Specular</b>   <b>Shadows</b>   <b>Labels</b>   <b>Sprout Hydrogens</b>   <b>Stereo Display</b>
<b>Color</b>	<b>Monochrome</b>   <b>CPK</b>   <b>Amino Acid</b>   <b>Shapely</b>   <b>Group</b>   <b>Chain</b>   <b>Temperature</b>   <b>Structure</b>   <b>User</b>
<b>Select</b>	See below for the <b>Select</b> menu choices. General point: "Selecting" any portion of the model does not change the display, coloring, <i>etc.</i> These changes occur only after they are specified for the portion selected.
<b>Mouse</b>	New window with the following information:
	Windows      Macintosh      Result
	Left          None              Rotate about X or Y axes
	Ctrl-Right    Command        Translate in X or Y direction
	Shift-Right   Shift-Command   Rotate about Z axis
	Shift-Left    Shift             Zoom in or out
	Ctrl-Left     Control          Slab in and out
	(Applies if <b>Slab Mode</b> has been selected in the <b>Options</b> menu.)

## B. The Select Menu Choices

**Select All** The entire model is selected.

**Mouse Click Action** (√ indicates the current mode.)

**None**

**Identify** picked atom shown in the status bar. *e.g.* Atom: CA 12 Group: ALA 2

**Distance** between two picked atoms in the status bar.

**Angle** between three picked atoms in the status bar.

**Torsion** between four picked atoms (*i.e.* two planes) in the status bar.

**Toggle Distance Monitor:** shown in the image. (Clear by repicking.)

**Toggle Atom Label:** shown in the image. (Clear by repicking.)

**Pick Center of Rotation:** then zoom a little to center the atom.

**Toggle Atom's Selected State** selected portion is orange; next, pick an atom.

**Toggle Residue's Selected State** selected portion is orange; pick a residue.

**Toggle Chain's Selected State** selected portion is orange; pick a chain.

**Highlight Selection** √ Toggles the orange coloring of the **Selected States** above.

**Invert Selection** swaps the orange coloring between selected and non-selected.

**Hide Hide Selected** removes selected portions from view.

**Hide Not Selected** removes unselected portions from view.

**Change Color To:** 13 colors to choose from.

**Modify Selection Mode** : resulting selected state (& RasMol equivalent)

**Replace Selection:** new selection (select x)

**Add to Selection:** addition to selection (select selected *or* x)

**Add Common to Selection:** intersection (select selected *and* x)

**Subtract from Selection:** reduced selection (select selected *and* not x)

**Mutual exclusion [XOR]:** reciprocal selection (select not selected *and* x)

[In the above, "x" is the next item selected after modifying the selection mode. The italicized words above are the Boolean *or* (union) and *and* (intersection).

Caution: The last three of these modes are much more easily handled using the RasMol program. Keeping track of the selected status in Chime after choosing the any of the last three modes requires a Boolean genius with a very good memory!]

**Model:** Available if the page contains more than one model, *e.g.* an NMR file.

**Chain:** Available if there is more than one subunit, *e.g.* hemoglobin.

**Residue:** Select from the list of the residues in the PDB file.

**Atom:** Select from the list of the atoms in the PDB file.

**Hydrogen:** can be selected in NMR or small molecule structure files.

**Non Hydrogen:** complement of the above.

**Hetero Hetero** are all of the waters, ligands and ions.

**Solvent:** *i.e.* water, only.

**Non Solvent:** Ions and Ligands, only.

**Water:** same as solvent.

**Ions:** *e.g.*  $M^{2+}$ ,  $SO_4^{2-}$ , *etc.*

**Ligand:** *e.g.* substrate, inhibitor, *etc.*

**Protein:** (Choices are based on the RasMol categories of the amino acids.)

**Protein | Amino**

Size categories: **Large | Medium | Small**

Structure categories: **Alpha Carbon | Backbone | Bonded | Buried | Helix | Sheet | Sidechain | Surface | Turn**

Characteristics categories: **Acidic | Acyclic | Aliphatic | Aromatic | Basic | Charged | Cyclic | Cystine | Hydrophobic | Neutral | Polar**

**Nucleic:** (Choices are based on standard components of nucleic acids.)

**Nucleic | DNA | Backbone | AT | CG | Purine | Pyrimidine**

**Display List**

**surface\_1** (if it has previously been created)

**Create Molecular Surface** (white "shrink-wrap" of selected portions)

**Toggle Visability** of one of the previously created molecular surfaces.

**Toggle Transparency** of one of the molecular surfaces.

**Delete Selected Lists** (removes the selected surface)

**Color**

**Electrostatic Potential:** Two choices

**Lipophilic Potential:** Two choices

13 colors to choose from.

