Viewer's Guide to the Chime 2 Menu Biochemistry I Carnegie Mellon Univ.

A. The **Main** Menu Choices

File **Save Molecule as . . .** save the PDB file to your disk.

Edit **Copy** the image to the clipboard. (Paste it into a File.doc.)
Copy Chime Script to the clipboard. (Paste it into a File.txt.)
Clear the PDB file from the display. (Reload to see it again.)

2D Rendering Flattens the structure of small (<256 atoms) molecules.

Animation Available if the page contains an (file.xyz) animation.

Rotation √Toggle on/off

Display **Wireframe**: atoms connected by thin "bonds".
Sticks: atoms connected by thicker "bonds".
Ball & Stick: atoms are small equal-sized balls.
Spacefill: atoms are balls with van der Waals radii.
Backbone: α-carbons are connected by straight segments.
Ribbons: α- and β-segments are smooth wide surfaces.
Strands: α- and β-segments are five smooth curves.
Cartoons: thicker than Ribbons, and β-strands have arrowheads.

Options √Toggle the following:
Display Hydrogens | **Display Hetero Atom Groups** | **Display Hydrogen Bonds** | Display Disulfide Bridges | **Display Wireframe Double Bonds** | **Dot Surface** | **Slab Mode** | **Specular** | **Shadows** | **Labels** | **Sprout Hydrogens** | **Stereo Display**

Color **Monochrome** | **CPK** | **Amino Acid** | **Shapely** | **Group** | **Chain** | **Temperature** | **Structure** | **User**

Select See below for the **Select** menu choices.
General point: "Selecting" any portion of the model does not change the display, coloring, *etc.* These changes occur only after they are specified for the portion selected.

Mouse 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 **Slab Mode** has been selected in the **Options** 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.

On the Web:
CMU Chime 2 Tutorial: `http://stingray.bio.cmu.edu/~rule/chime_tut/chime.html`

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