

# MolViewX v2.0

## Installation:

Much to my chagrin, there is still an issue with where MolViewX is installed. I recommend moving the MolViewX folder to your home directory. There also may be issues with unusual directory names (e.g. dashes, special characters, or spaces). Keeping MolViewX in your home directory and your files in simply named directories seems to be the most stable thing to do at this time. I am using standard ANSI C directory path addressing for the files and it is not quite right. There seems to be a disconnect between the name of the path and being able to directly get to it using C calls. I am working to fix this.

## General instruction:

MolViewX has its own file format so that it can include object (MOL) figures. You simply read in a PDB format file or a plot file from the graphical program 'O' and the program writes out a MolViewX file. The 'Tool' palette on the left is a series of 'instructions' as to how to analyze and display the structure and the 'object' palette on the bottom controls the display and details of the various objects.

## Menus:

### File

#### Open

MolView	Read in a MolView formatted file
PDB File	Read in a PDB formatted file
O Plot File	Read in a 'plot' file from the program 'O'
MOL File	Read in a 'MOL' object file from MolViewX
Second MolView File	Read in a second MolView file to compare structure
Stipple file	Read in a surface 'stipple' file created by MolViewX

#### Write

MolView File	Write out current file with MOL objects
Main Window PICT	Make a PICT file of the main window image
Ramachandran PICT	Make a PICT file of the Ramachandran plot
Edmunson Wheel PICT	Make a PICT file of the Edmunson Wheel
MOL file	Write out a MolViewX file of the MOL objects
B Value Graph PICT	Write out a PICT file of the B value graph
PDB file	Write out a PDB file of the rotated structure
VRML file	Write out a VRML file for rendering
POV-ray file	Write out a POV-ray file for image rendering

## Draw

Draw	Refresh the main image window
Stereo	Toggle the split screen stereo on and off
Depth Cue Shading	Turn on 'fog' or depth cue shading
Delete Symmetry atoms	Remove the symmetry related atoms (see below)

## Labels

Delete all labels	Remove all of the labels on the atoms
Create labels	Make your own style of labels

## MOL's

Clip MOL object w/At. Model	Trim electron density plot files made by 'O'
Delete all distance lines	Remove all of the distance lines

## View

Rotate	Rotate the image with a dialog box
Stereo Preference	Change the stereo separation and type of stereo
Change Scale	Dialog to change the size of the image
Slab	Clip the object along all three axes

## Geometry

Rama Plot	Redisplay the Ramachandran plot
Pick Rama Points	Allow the user to ID residues on the Rama Plot

## Window

Main	Move the Main window to the front
Tools	Move the Tool window to the front
Objects	Move the Object window to the front
Color Palette	Move the Color Palette to the front
Ribbon Buttons	Move the Ribbon buttons window to the front
Magnified Ribbon	Move the Magnified Ribbone window to the front
Ramachandran	Move the Ramachandran window to the front
Edmunson Wheel	Move the Edmunson Wheel window to the front
Hydrophathy Plot	Move the Hydrophathy Plot window to the front



### Tool Palette:

- 1-6: Rotates the structure about the x, y, and z axes.
- 7: Zoom in on an atom by using the mouse to click on it.
- 8: Zoom out on an atom by using the mouse to click on it.
- 9: Scale the image down (mouse click anywhere on the window).
- 10: Scale the image up (mouse click anywhere on the window).
- 11: Pick which atom to label from a scrolling list of all of the atoms in the MolView file.
- 12: With this turned on, pick which atom to label with the mouse.
- 13: Neighboring atoms: with this turned on, you click on an atom and it will draw vectors to neighboring atoms and display the distance.
- 14: Measure the distance between two atoms. Turn this on, click on the first atom and then click on the second. A line and associated distance will appear.
- 15: Click on this and a dialog box will appear to let you create 8 different kinds of MOL objects (described below).
- 16: This is to remove MOL objects from the Object Window. Click on this and then click on the MOL object to be removed from the Object Palette.
- 17: Click on this to make CPK models (spheres the size of the atomic radi).
- 18: Sort the lines according to the Z direction to fix the depth perception. Can be a bit slow for larger diagrams.
- 19: Make a ribbon diagram from a file parsed out from the PDB file, one that the user made, or one created by MolViewX.
- 20: Smooth out the ribbon diagram by increasing the number of planes by 2x.
- 21: Make ball and stick models.
- 22: Make a stick model that is colored according to their mobility (B values).
- 23: Make a solvent accessibility plot as represented by a series of dots around the protein surface.
- 24: Examine the protein structure using Ramachandran, Edmunson Wheels, hydrophathy, and B value plots.
- 25: Pick up a color with the eyedropper (the color is stored in the bottom left box of the color palette).
- 26: Drop down the eyedropper color onto the object palette.
- 27: Select this and rotate the protein by holding down the mouse button and dragging the mouse around the main window.
- 28: Align the two structures that were read into MolViewX. Go to the 'File' menu and say open MolView file. Then go back and 'Open Second MolViewX file'. You now have two proteins in memory. Click on this option and MolViewX will help to do a 3D alignment of the proteins. You will need to know a section(s) of the two proteins (and

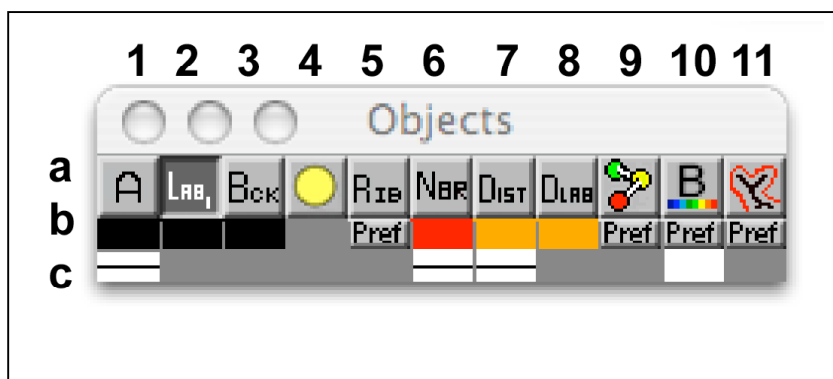
the associated amino acids numbers) that you think have homologous structures to start the alignment process. There is a brief tutorial in the MolViewX directory.

29: Click on this to make a ribbon along the phosphate backbone of DNA/RNA.

30: Click on this to fill in bases of RNA/DNA with colored planes. The definitions and colors for this process are read in by MolViewX from the file "DNA\_RNA.script" found in the same directory as MolViewX. You can modify this to fill in other kinds of ring structures as well.

31: Make symmetry related molecules (either crystallographic or non-crystallographic). There are two examples of how to do this in the MolViewX directory. In essence, MolViewX applies symmetry to your atoms to expand the number of atoms in memory to see how proteins are packed in a crystal cell ("Crystal symmetry example") or in a large oligomeric structure such as a virus ("Non-cryst symm example"). To use this option (and a similar option in the MOL option), you need to read in the symmetry relationships. For crystallographic symmetry, the line starting with the word 'CELL' lists the length of the a, b, and c axes and the three angles ( $\alpha$ ,  $\beta$ ,  $\gamma$ ). This is followed by a number telling MolViewX how many symmetry matrices are to follow. In the case of non-crystallographic symmetry, the CELL line is followed by 1, 1, 1, 90, 90, 90, to let MolViewX know that the symmetry is to be directly applied.

32: Center the rotations on one atom selected using the mouse. Click on this button and then click on a particular atom and all rotations will be performed about this atom. This can also be useful when exporting to POV-ray files.



Object Palette:

Row:

- a) Turn object type off and on.
- b) If the button is a solid color, you can set the color by clicking on it and then click on a color from the color palette. If the button says 'Pref' then click on the button and a dialog window will open and you will be able to set a number of different parameters.
- c) If there is a button (white button with a line through it) clicking on this button will open up a dialog box so that you can change the pen thickness.

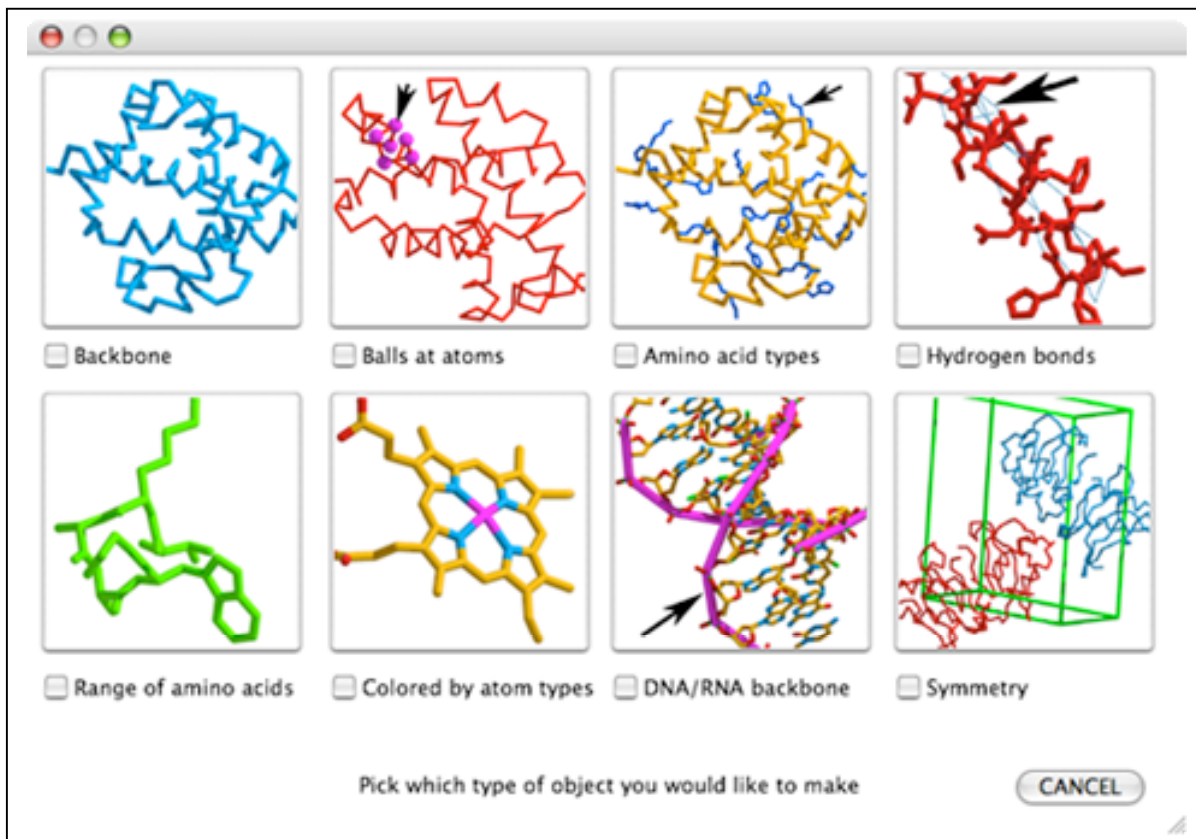
Column:

- 1) Atomic model. When you open a MolView file, a backbone image will appear. These buttons control that display.
- 2) Labels. This allows you to toggle the labels off and on and change the color. If you open a second MolView file, a second line of buttons will appear in the next columns and will be called A2 and Lab2.
- 3) Background. Turn a background off and on and change the color.
- 4) CPK. This turns the CPK model off and on.
- 5) Ribbons. Turns the ribbon diagram off and on and sets the various preferences.
- 6) Nearest neighbor. See Tool Palette. This turns the nearest neighbors off and on and allows you to change the color.
- 7) Distance lines. Turns the distance lines off and on, controls color, and thickness.
- 8) Controls the labels for the distance lines.
- 9) Ball and Stick. This toggles the Ball and Stick models and controls various drawing parameters.
- 10) Bvalue model. This controls the model colored according to mobility, associated preferences, and line thickness.
- 11) Stipple image preferences. This controls the display and coloring of the surface rendering.

For each MOL object created, a new column of buttons will appear much that for the atomic model.

Some details about the more complex options:

Making MOL objects:



When you click on the 'MOL' tool button, the following dialog box will open. To select one, just click on the picture or the check box. For each type of MOL object created, buttons will be added to the 'Object' button palette so you can control color and line thickness. Specifically:

- 1) Backbone. You can create a backbone structure for some or all of the protein. It should be noted that when you open a MolViewX file, this is how the protein is initially drawn. However, this initial backbone (the 'A' button in the object palette) is not written out when making POV-ray or VRML rendering files.
- 2) Balls at atoms: This is a great way to highlight positions of amino acids on a protein backbone. I use this to note the locations of mutations and critical residues. You have complete control over the color and size of these balls.
- 3) Amino acid types: Here you can instantly make a 'MOL' object showing only particular types of amino acids. This is a great way to show all of the, say, PHE amino acids without having to find them all from the list and creating MOL objects one by one.

- 4) Hydrogen bonds. This option will help you make a MOL object showing all possible H bonds between backbone atoms and/or sidechain atoms. Good way to show students the difference between helices and  $\beta$ - sheets.
- 5) Range of amino acids. This is mainly to make a single colored MOL object for a linear section of the protein.
- 6) Colored by atom types. This makes a MOL object for each type of atom (e.g. O, N, C, S) with the default colors of O=red, N=blue, C=yellow, S=green, and metal=mauve. You can change these colors however you wish after they are created. You can create these objects as a linear stretch of amino acids or as a 'box' of atoms around a particular amino acid. You can also eliminate the main chain atoms and only show the side chains (as with options 3 and 5).
- 7) DNA/RNA backbone: this is a kind of simple option that makes a stick backbone for DNA and RNA so that you can output to a rendering file.
- 8) Symmetry. This allows you to make MOL objects that demonstrate the symmetry of the protein. This is similar to the 'symmetry' option in the toolbox except it does not expand your atoms in memory it only creates MOL objects. It also makes a pretty box showing your unit cell if you are showing crystallographic symmetry.

#### Deleting MOL objects:

This is much simpler than in previous versions. Simply click on this button from the toolbox and then click on the MOL object in the Object button window to delete a particular object. Helps keep things tidy.



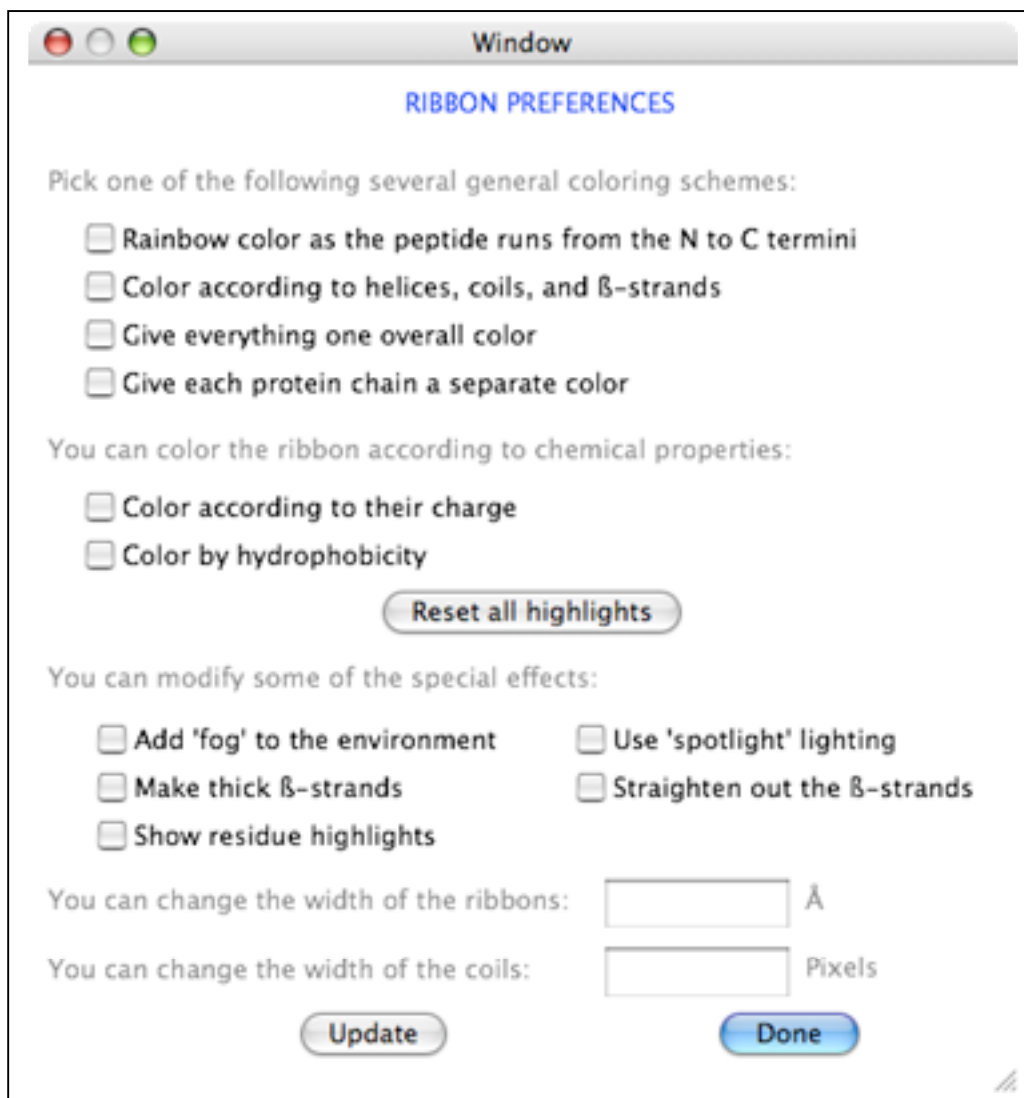
Ribbons:

This can be the most complicated of the options in MolViewX since I wanted to give the user a lot of ways to color the ribbon diagrams.

When reading in a PDB file, MolViewX reads the header information and tries to figure out where the secondary structures are located. MolViewX then silently writes out a \*.struc file in the same location as your new MolViewX file. Usually, it does a good job with this but occasionally messes up. Therefore, if you get a funky ribbon diagram, you may need to quickly edit the \*.struc text file. The errors are usually obvious in that you should have a word (coil, helix, sheet) followed by two numbers – the first and last amino acid for that secondary structural element.

To create a Ribbon, click on the 'Rib' button in the tool box. You will then be asked to either read in a \*.struc or to make one on the fly. Normally, the \*.struc file made by reading in the PDB file works the best. If the PDB file does not have this information, you can have MolViewX try to figure it out for you. As with most programs that do this, the better the structure, the more accurate the \*.struc file. It is based on backbone angles and hydrogen bonding patterns.

Once you create you Ribbon figure, you can change the coloring scheme using the 'Pref' button under the 'Rib' button on the object button palette.



There are four general coloring schemes:

- 1) Rainbow color. Here the color ramps from red to blue as the chain is traced from the first to last residue.
- 2) Color by secondary structural elements. Here you can select individual segments for coloring.
- 3) Give the whole ribbon one color. This is useful if you want to highlight residues or bound chemicals
- 4) Give each protein a separate color. If you have a protein that is composed of more than one peptide chain, then you can give each their own color.

There are two 'highlight' coloring schemes. These ignore the above four options and color individual amino acids according to their chemical properties. You will notice that when these are chosen, that the 'Show residue highlights' button below is checked. This is because you are essentially using this option to highlight each amino acid. If you click on that button after using these two options, you will notice that you toggle these color schemes off and on.

- 1) Color by charge: the uncharged residues are colored grey, the acids red, and the bases blue.
- 2) Color by hydrophobicity. Here the charged residues are red, the polar blue, glycine yellow, and hydrophobic green

There are a few 'special effects':

- 1) You can add 'fog' or shade the ribbons according to their depth. This gives it a bit of a 3D effect.
- 2) You can make the  $\beta$ -strands look a bit thicker rather than as thin sheets of paper.
- 3) You can highlight residues. This is activated by the two options above or here. If you turn this on, you can color individual amino acids using the 'Ribbon button window' as described below.
- 4) Straighten out the  $\beta$ -strands. Normally the strands have a 'wavy' appearance since that is how they actually look. If you select this, you need to hit the 'Rib' button again, reread the \*struc file and recreate the ribbon diagram. This will make the arrow for the strands look a bit smoother.

Ribbon Button Window (see diagram below):

When you create a ribbon diagram, you can go to the 'Window' menu and select the Ribbon Button Window. There are several sets of buttons here. At the beginning of every polypeptide chain, there are a set of buttons of type 'A' and 'B'. Button 'A' will turn the entire polypeptide chain off and on. Button 'B' will allow you to change the color of that polypeptide chain. Click on this button and then go to the color palette and click on a color. BE AWARE that this color choice will only show up if you have turn on 'Color by polypeptide chain' from the 'Pref' dialog for the 'Rib' button from the Object button window. For every secondary structure element, you have a button of type 'C' that shows a picture of the type of secondary structure element that it is (loop for a coil, arrow for a sheet, and helix for a helix). If you click on button 'C' that element will turn off and on. Below that button is butt 'D' that shows what residue that element starts at and what color that element is when the 'Color by secondary structure element' is

turned on from the Ribbon 'Pref' dialog. If you click on button 'D' and then click on the color palette, the color will change. If you hold down the 'apple' key and click on button 'D', the 'Magnified segment' window will open up. This will show a button and the associated color for each amino acid in that secondary structure element. An 'X' means that there is not color assigned to that amino acid. You can change the color as described above. BE AWARE that these colors will only show up if you have chosen 'Highlight amino acids' option from the 'Rib' 'Pref' dialog.

