MolView 1.1
(originally MacInPlot)

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by

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Smith, T. J. (1995) MolView: a program for analyzing and displaying atomic structures on the Macintosh personal computer. J. Mol. Graphics 13:122-125.

(available by anonymous FTP: rhino.bocklabs.wisc.edu [144.92.19.130])

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INTRODUCTION:
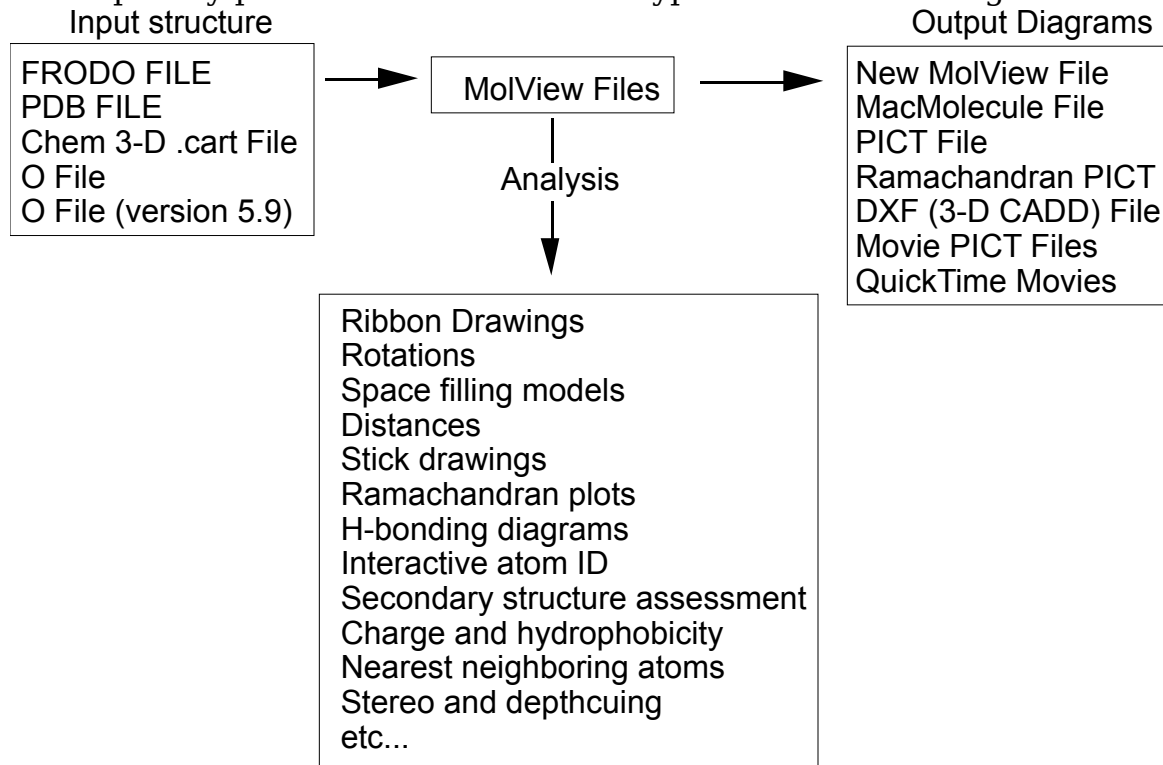
For copyright reasons, the name of the program has changed during the last major revision (someone else had apparently chosen the horrid name 'MacInPlot'). All old files work without any problems.

MolView (MacInPlot) started off as a simple way to plot crystallographic results but has turned into a life form of its own. It is now becoming a "poor man's" structural analysis and teaching tool. The basic premise is that MolView can read in several types of structure files, convert to my own "MolView" format, and allow you to examine and subsequently put out several different types of files and images:

Input structure   Output Diagrams

```
FRODO FILE                              New MolView File
PDB FILE            MolView Files       MacMolecule File
Chem 3-D .cart File      →              PICT File
O File                                  Ramachandran PICT
O File (version 5.9)                    DXF (3-D CADD) File
                      Analysis          Movie PICT Files
                         ↓              QuickTime Movies
```

```
Ribbon Drawings
Rotations
Space filling models
Distances
Stick drawings
Ramachandran plots
H-bonding diagrams
Interactive atom ID
Secondary structure assessment
Charge and hydrophobicity
Nearest neighboring atoms
Stereo and depthcuing
etc...
```

The program has changed a great deal over the past couple of years and can currently handle more atoms than is feasible to display on a Macintosh (I have examined proteins >13,000 atoms). All arrays are dynamic and therefore the more you allocate to the program, the more you can do. I recommend no less than 5 Mbytes.

File Input and Output:

With version 1.0.4, I finally bothered to take the time to read 'Inside Macintosh' to write routines to accept Apple Events (sorry it took so long). These routines now give MolView the following abilities:

Double clicking on the following MolView files will launch MolView and display the file. If MolView is already running, then the new file will replace the file being currently displayed.
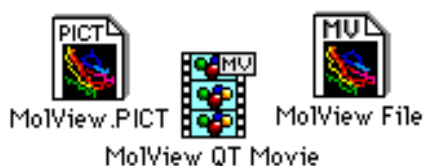
There is no restriction on the name being used for the various files. !!NOTE: to see these icons, you must rebuild your desktop after installing the program (especially users of version 1.0.3 or older).

The following MolView files are created, but have other functions are not read in this way:
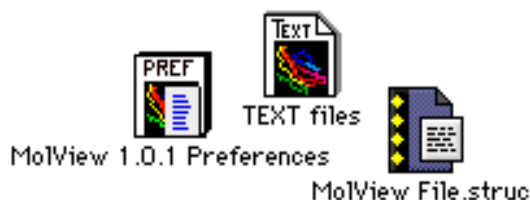
The Preference file can be deleted (it is normally found in the System Folder) without affecting the program -- only the preferences from the last run will be lost. Please do not alter the contents of this file. The '.struc' file is used in making ribbons and can be edited and saved as a TEXT file.

**NOTE for users of MolView 1.0.3 or older: the 'TEXT' icon will appear on your old MolView files. If double clicked, MolView 1.0.4 will read the file and automatically change the ICON to the new type. This is to help error trap in the future versions.

In System 7.5, one can 'Drag&Drop'. The user can use the mouse to slide the icon of a file onto the icon of an application to force the application to read the file. If the application is not currently running, then it will launch the program and force the file to be read. This allows you to take a file created by another program and make the application read it without using menu dialogs (MolView also has the menu options to do the same operations). Files that can be forced opened:

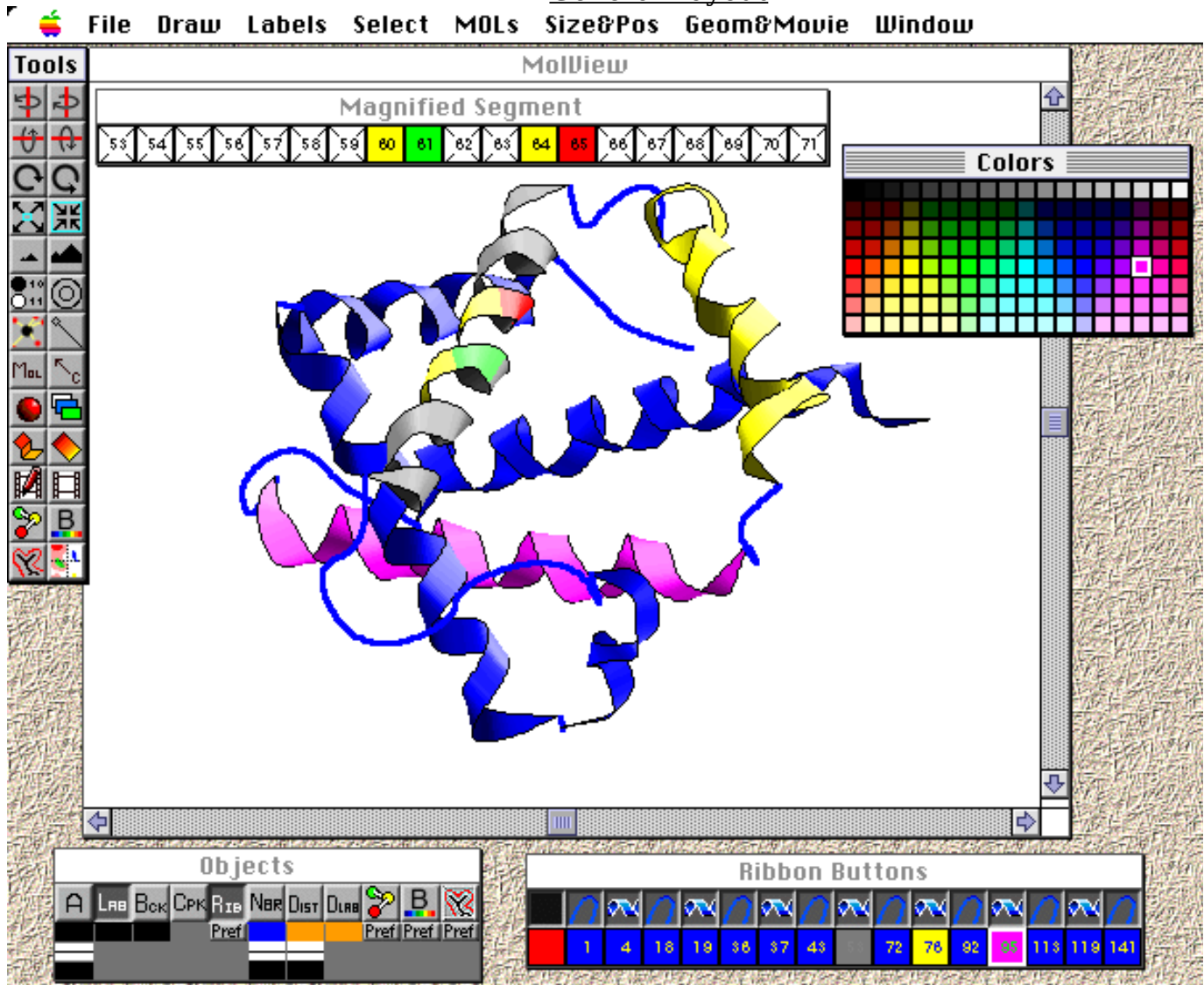protein.pdb   asp.space.MooV   MolView.PICT   protein.ent

1) TEXT files (also known as ASCII format), created by any program that contains the PDB formatted structures of molecules. **The name of the file MUST end with '.pdb', '.PDB', '.ent', or '.ENT'.** If it is a PDB file without this name, either change the name and then 'Drag&Drop', or

open the file within MolView. Upon reading the file, the user will be asked for an output MolView name.

2) QuickTime movie (type MooV) files. Up to two movies can be displayed at a time in MolView.

3) PICT files. In version 1.0.4, there is a 'PICT viewer'. Upon the 'Drag&Drop' of a PICT file, MolView will open a new window and display the PICT image. If the image is bigger than the screen, then it will proportionally scale the image to fit. Only one PICT image can be displayed at a time. PICT files can also be opened from the Menu. I may or may not add the buzzers and bells to this PICT window. There are other routines I am currently writing instead.

General Layout

File   Draw   Labels   Select   MOLs   Size&Pos   Geom&Movie   Window

Tools

MolView

Magnified Segment

| 53 | 54 | 55 | 56 | 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 | 71 |

Colors

Objects

A Lab Bck Cpk Rib Nbr Dist Dlab

Pref   Pref Pref Pref

Ribbon Buttons

| 1 | 4 | 18 | 19 | 36 | 37 | 43 | | 72 | 76 | 92 | 97 | 113 | 119 | 141 |

Color Palette

This palette controls the color of the various objects. Whenever you want to change the color of the object, first click on the color button of the object, and then the desired colored button on the color palette. The selected color and object buttons are highlighted by a white box.

Tool Palette

1,2: Y axis rotation
3,4: X axis rotation
5,6: Z axis rotation
7: Zoom In on an atom
8: Zoom Out on an atom
9: Decrease size to 75% of original
10: Scale up image by 150% of original
11: Pick atoms for labeling from a list of all atoms
12: Pick atoms for labeling with the mouse
13: Find the nearest neighbors to atoms and the distances
14: Measure the distance between only two atoms
15: Create a 'Mol' diagram - analysis properties of molecule
16: Center rotations about an atom - mouse selected
17: Change which atoms comprise CPK image
18: Sort lines and models from back to front
19: Make a ribbon diagram of a protein
20: Smooth the ribbon diagram
21: Create a QuickTime Movie
22: Play up to two movies at the same time
23: Create/Add to Ball and Stick model
24: Create/Add to model colored by B values (thermal factors
      to show mobility.
25. Create a 'Stipple file' to show molecular surfaces
26.   To create Ramachandran Plots, Edmunson wheels, hydrophobicity
     plots and to make distance plots.

More Details:

1-6 Rotations:

Rotations occur upon each mouse click. The rotation step is controlled by the 'Change Rotation Step Size' of the 'Preferences...' option of the Drawing menu.   The step size here is the same as the 'large step size' in the subsequent dialog box.

**If you hold the mouse button down on while the cursor is on any of the rotation buttons of the toolbox, the image will continue to rotate until you let up on the button or position the cursor off one of the six rotation buttons.

7 Zoom In:

You can 'Zoom In' on a particular atom in the atomic structure. This is handy for the 'Hand Pick' and 'Draw Distance Line' options. Note that you MUST select an atom to zoom in on. I need an atom for a reference point to calculate the offset and scale factors. Therefore, if your MolView file only contains Mol objects, this option will not work (nor will the 'Zoom Out' option work).   When this option is activated, the cursor changes to:

Simply click on an atom. The chosen atom will be placed in the center of the screen and the size of the objects will be increase by 1 1/2. Unlike FRODO, you do not have to have the atomic structure displayed at the time of selection, but you must have the atoms in the file.

8 Zoom Out:

Pretty much the same as Zoom In except the size of the objects are decrease by 75%. When this option is active, the cursor changes to:

Again, you need to select an atom, and the selected atom is centered in the middle of the screen.

9-10 Shrink, Enlarge :

This simply shrinks the image to 75% or increases the size of the image to 150%. Does not require mouse selection of an atom in the atomic model.

11: Pick atoms for labeling from a list of all atoms.

A window will appear with a list of ALL atoms in the atomic model. You can advance or go back in single pages of atoms on the list by big jumps. Click on the radio button to turn that particular atomic label off and on. Scroll to the next 10 atoms with 'Next Page' or back to the previous 10 atoms with 'Previous Page'.

The jump ahead and jump back jumps (# atoms)/10 each time the buttons are selected. This allows the user to quickly leap-frog to the right section. Will eventually put in a proper scroll bar, just too lazy to do it now...

12: Pick atoms for labeling with the mouse.

This option allows the user to use the mouse to hand pick the atoms to be labeled. After this menu is selected, the cursor changes to a

'bulls-eye'. The 'hot' pixel of this cursor is the center. Therefore, center the bulls-eye over the desired atom before clicking the mouse button. This cursor will hopefully help one to remember which interactive subroutine is currently active.

13: Find the nearest neighbors to atoms and the distances.

This option is for examining the atoms in proximity to a selected atom (distances, colors, and other parameters are set in the 'Preferences' item of the 'Draw' menu). Merely toggle this option on and click on an atom. Lines will be drawn to neighboring atoms and the distance will be marked in the middle (in Å).
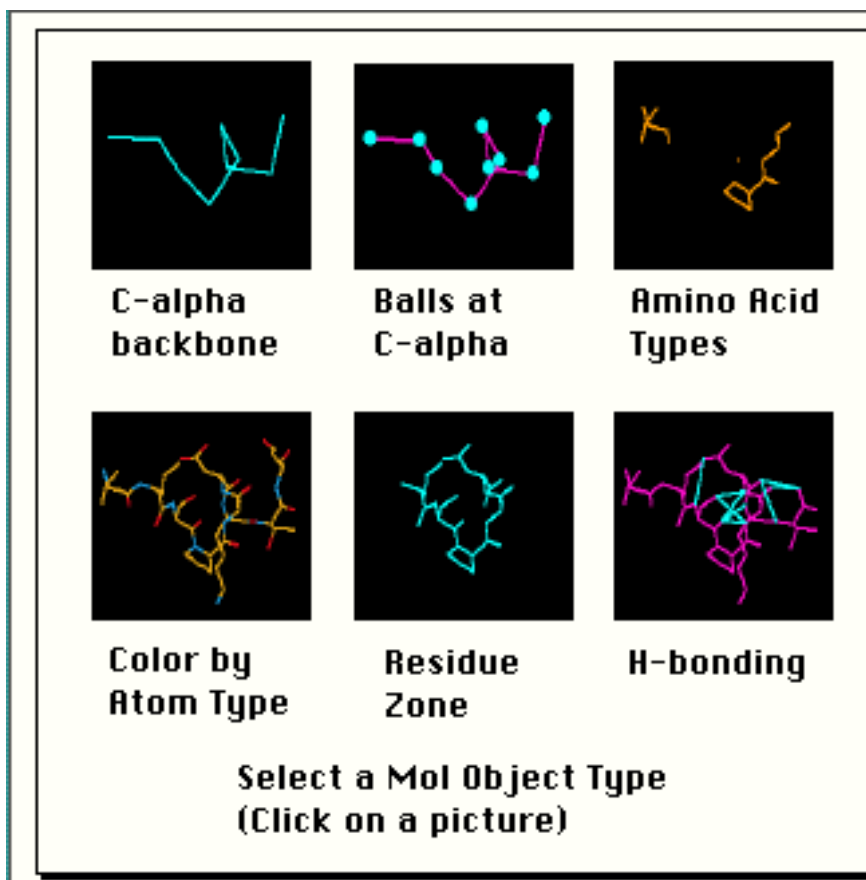
14: Measure distance between two atoms.

This option measures the distance between two atoms (not Mol objects), draws a line between them, and places a desired label in the middle of the line. When this menu item is chosen, the cursor changes to the following shape:

The 'hot' pixel of the cursor is in the center of the box in the upper right hand corner of the cursor. You can turn off this interactive menu item by selecting it again from the menu. To run this option, simply click on the first atom to label and you should see a box appear about the atom. Move the cursor to the second atom and click on it. A dialog box will then appear telling you the distance and asking you for a label. If you do not want a label, simply delete all of the default text found in the dialog box. ****Note, you are limited to 30 characters.** I felt that more than 30 was a bit verbose. The color and thickness of these lines can be changed as described under the 'Object Palette' description.

15: Create a 'Mol' diagram

C-alpha backbone   Balls at C-alpha   Amino Acid Types

Color by Atom Type   Residue Zone   H-bonding

Select a Mol Object Type
(Click on a picture)

There are several different types of MOL objects that you can create, but are limited to ten at this time. When you select this option, the following pictorial dialog box appears...

• C-α (Creates a C-α Backbone from your atomic coordinates)
• Balls at C-alpha (Draws a ball of desired diameter at each C-α position within the chosen zone).
• Color by residue type Residue Type (Displays desired amino acid types found   within a chosen zone).
• Color by Atom Type (each type of atom is represented by a different color- Note that each atom type is its own MOL object. Therefore you change the line attributes to what you want rather than what I make)
• Residue Zone (Displays all atoms within a desired Zone)
• H bonding (Draws a line between donor N and acceptor O for all possible atoms within the atomic model that lie within 2.8 and 3.2Å distance). When this item is selected, a dialog box appears and allows the user to change the default distance criteria.

Just follow the dialog boxes for the residue ranges and types. Remember that most files contain all uppercase letters.

16: Center rotations about an atom

This option allows the user to re-center the 3-D rotations about a particular atom. As with the other 'mouse' selections, only the atoms on the left side of a stereo pair are 'selectable'. After selecting this menu item, the cursor changes into a:

The 'hot' spot of this cursor is in the upper left hand corner (the arrow). Simply click on an atom and you might see the diagram shift slightly. Any future rotations are now performed with the chosen atom in the center.

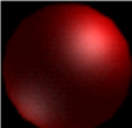## 17: Change which atoms comprise CPK image.

This option allows you to change/create space filling models with a single dialog box. Note: When you read in a MOLVIEW file, I automatically create a CPK model of all of the atoms. If you select 'CPK' from the 'Select' menu, you can see it. O are red, C are white, N are blue, S are yellow, and the rest are green and purple.
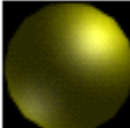
This dialog box is designed for speed... You can continue giving input until you hit the 'Quit' button. I did this since making a CPK model is relatively slow and you will probably want to make more than one selection. You will not be notified that your entry was made... you'll have to trust me...
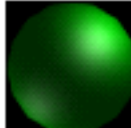
To change radii, edit the end of 'names.pdb' file*

Make Default CPK:

This turns on all of the atoms and assigns them default colors and radii as when the MOLVIEW was first read in.

Delete All CPK atoms:

This turns off all CPK atoms. Usually this is the first thing I hit when making a CPK diagram to make sure that all of the old colors and atoms are eliminated. You will not be notified that the atoms are deleted, but they will be --

this option is very fast.

Coloring residues....

The following is the flow of logic for coloring parts of the model at a time -- remember that you will not be notified that your input was entered, but it will be if you hit o.k. (this option is also very fast).

1)   Select the residue range to be colored

2)   Select a color for the residue range (click on a colored ball or its label)

3)   How do you want this subset of residues colored?
a)   **Using default colors**? All atoms will be colored according to atom type (N=blue, C=white, etc...)

b)   **Color all atoms in range**? If you chose, say, the red ball in #2, then all atoms in this residue range will become red, but the radii will be set according to the atom type

c)   **Color Atoms beginning with ___**? This use the color selected in step #2 to color this subset of atoms. For example, I have a peptide and I'd rather have the carbon atoms yellow instead of white (the default color). I would select the residue range, select the yellow ball, choose this option, type in the letter 'C' , hit the o.k. button, and then hit the quit button. All of the other atoms would remain the same color, but the Carbons will now be yellow. NOTE: only one letter is recognized in this option.

d)   **Color residues called ____**? This use the color selected in step #2 to color only residues with the name type in the text box. One might use this option several times to color all of the acidic residues red, the basic residues blue, etc... While you only color one residue type at a time, I set it up so that you can rapidly change many at once. Another example... I want all of the atoms to be colored yellow, but the acidic residues red. I open this dialog box, hit **Delete All CPK atoms,** type in the residue range for the protein, select the yellow ball, choose **Color all atoms in range,** hit o.k. Now all atoms are yellow. Now I color the acidic residues. Input the residue range for the protein, hit the red ball, choose **Color residues called ____,** type in ASP, and then hit o.k. Do the same for GLU. I then hit Quit, and I get a pretty picture with all atoms yellow except for the acidic residues.

e)   **Color by hydrophobicity** This option automatically colors the residues within the specified range according to their hydrophobic character. I used the colors and designation from the book Introduction to Protein Structure by C. Branden and J. Tooze since it is a very popular book to teach structure (Garland Publishing, Inc, New York, 1991). According to their tables of hydrophobic character (p. 210), the charged residues are red (glu, asp, arg, lys), the polar residues are blue (asn, gln, his, tyr, ser, thr, trp, cys), gly is yellow, and the hydrophobic residues are green (pro, ala, val, leu, ile, met, phe). I especially

wrote this to show the ampipathic nature of some α-helices.

4)   Do I want only the side chains visible in this residue range?
If you select this button and hit o.k., then the backbone atoms will be deleted for that particular residue range. I wrote this option to let people mix types of diagrams.

5)   If I want these things done, I hit 'O.K.' and the changes will be made.

6)   If I want these CPK models depth sorted with the line drawings and ribbon drawings, then I select the 'Sort with others' button.

7)   If I am now done, I hit 'Quit', and my CPK will appear on the screen.
****
****

18: Sort lines and models from back to front.

The Mac graphics 'paste' one line on top of the other rather than mixing the colors together. Therefore, often lines in the back get drawn on top. This makes for a confusing diagram. However, I found that the older Macs cannot keep up with the required vector sorting to get it right. Therefore, I suggest the following... Get the diagram you like and when you are all set for a final version (or if you have a Quadra) then hit this button and the atomic models, Mol objects, labels, distance lines, and electron density maps will be sorted together and drawn back to front. ***This does not include ribbon diagrams or CPK models. Those must be turned on separately. Again, the only reason for this is to take mercy on those with Mac LC's.   Eventually, as everyone gets power Macs, I will eliminate this confusion.

19: Create Ribbon diagram.

This option works in two stages: 1) read in or create a list of secondary structural elements or 2) create a crude ribbon diagram. Under the default mode, the program scans through the protein, calculates the psi-phi values of each protein and determines the closest residue that it may have a H-bond with via its main chain N and O atoms. It then uses this information to try to figure out where the helices, coils, and sheets may occur in the protein. It then writes these values out to a TEXT file which can be edited by the user later and read back in by the program. The name of this file is the same as the MolView file with an '.struc' appended to the name. This file is easily edited since the program just looks for key words. For example:

coil 1 4
sheet 5 10
coil 11 12
helix 13 20
..etc...

If you decide to read in your own TEXT file, the dialog box will allow you to do so. The ß-strands are depicted as arrows with the arrow head being on the COOH end of the strand, the random coils are depicted as thick lines, and the helices as tapered 'pig tails'.
       After the ribbon diagram is created, the default coloration is a color ramp from red -> orange -> yellow -> green -> blue as the ribbon goes from the N to C terminus. The residues must be in sequential order.
When reading in a Brookhaven PDB file, this structure information is in the header of the file. MolView, if it finds it, will write out a *.PDB.struc file based on this information.

20. Smooth Ribbon:

This option doubles the number of planes in the ribbon diagram, thereby 'smoothing' the image. The advantage of making the procedure completely automatic is that any protein can be displayed without any user input.**Note: Please only smooth a couple of times. Each time you smooth, the number of planes doubles and makes the Mac scream.

21: Create a QuickTime Movie.

This option avoids having to use any other program to make QuickTime movie. You can create 3 kinds of movies: rotation, 'chase a rainbow', or slabbing. Rotation will rotate the model during the movie. The user sets the number of degrees per frame and the number of frames in the movie. The 'chase the rainbow' option does fancy coloring of ribbon diagrams. The user sets the number of frames and displays a ribbon diagram. MolView then turns the entire ribbon gray, and then 'bleeds' in the color of the rainbow. e.g. I have a ribbon diagram of hemeglobin and set the number of frames to 20. Over 20 frames the colors of the rainbow appear in the ribbon starting with the N terminus (colored red) and ending with the C terminus (colored blue). This is a handy way to clearly show the fold of the protein. The third kind of movie is slab. You will be asked for the number of frames and then MolView creates a movie that slabs the front part away in pieces. e.g. I have a CPK model of Hemeglobin but want to show how the Heme group is buried in the heart of the protein. I input 20 frames. MolView then creates a QuickTIme movie that slabs most of the protein away (front to back) over the next 20 steps. In all cases, the user is asked for a frame rate. This rate is set in units of 1/600 seconds. Say I want a movie that displays 2 frames per second. Therefore I would input a frame rate of 300 ticks.

22: Play a QuickTime Movie.

Play up to two movies at the same time. This option allows the user to open up to two QuickTime type movies and play them. Be aware that when coming from another window, it may take a couple of mouse clicks to start the movie.

23: Create Ball & Stick Model.

This option will create a ball&stick object. This is where there is a ball representing the atom and a thick stick connecting them. In the Object Palette, you will be able to change the color and radii of the balls and sticks. If you have already created a Ball and Stick model, then you can either add to it or start over again. As you add on to the model, you can change the colors of the various segments.
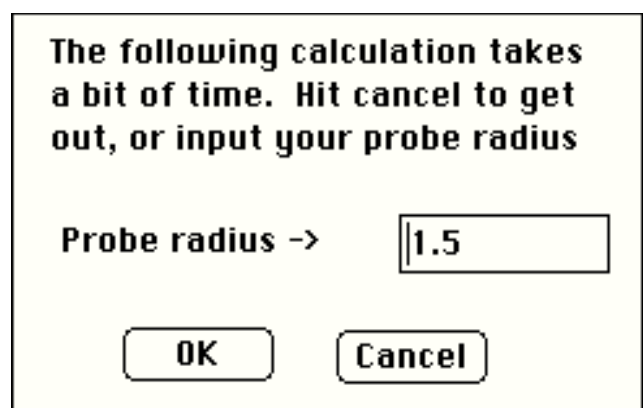
24: Create a B value (thermal factor) Model.

This option allows you to create or add to a stick model where the color ramps from red to blue as you go from the less to the more mobile part of the molecule. Be aware that it only works on PDB files, converted to MolView files, using this version of the pgm. Old MolView files work except for this option.

25: Create a 'Stippled' Molecular Envelope

This option allows you to create a molecular envelope about the atomic model. The inputted probe radii allows you to define what kind of envelope this is and the 'pref' buttons allows you to show the whole or a portion of the surface with various color cues.

> **The following calculation takes a bit of time. Hit cancel to get out, or input your probe radius**
>
> Probe radius -> `1.5`
>
> [OK]   [Cancel]

If you input a radius of 0.0, then the resulting molecular envelope will represent the molecular surface. If a radius of ~1.5Å is used, then the resulting envelope represents the water accessible surface area. When the surface has been calculated, you will be asked to write the 'stipples' out to a TEXT file. This allows you to read the stipples in again at a later time. BE AWARE that the stipples pertain to the atomic model at ONLY the currently displayed orientation. Therefore, be sure that if you rotated the model after initially opening it, that you write out the new MolView file before or after making the stipple file.

BE AWARE that this is a time-consuming option. A slow moving bar will show you

the progress of the calculation. BE PATIENT... For this option, 125,000 grid points are tested against each atom in the atomic model to see if it is within contact distance.
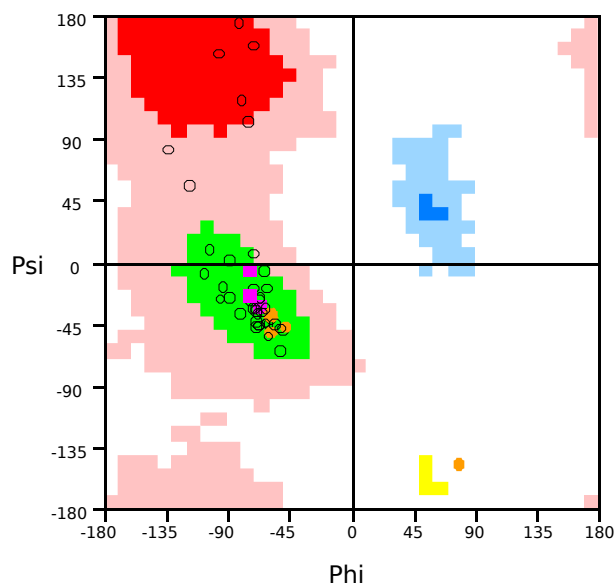
25: Create graphs to analyze your protein

This option allows you to create a four different graphs to analyze your protein: Ramachandran Plots, distance plots, Edmunson wheels, and hydrophobicity plots.->

1) Ramachandran Plots:

Ramachandran plots display the psi-phi backbone angles for proteins. The green region is the area of the graph that alpha helices are found, the deep red the region of beta-strands and the blue region is for sharp turns. Under the Geom&Movie menu, you can set this graph to B&W or color and turn on the option to select data points with the mouse (the residue number is displayed when clicked).

2) Edmunson Wheels
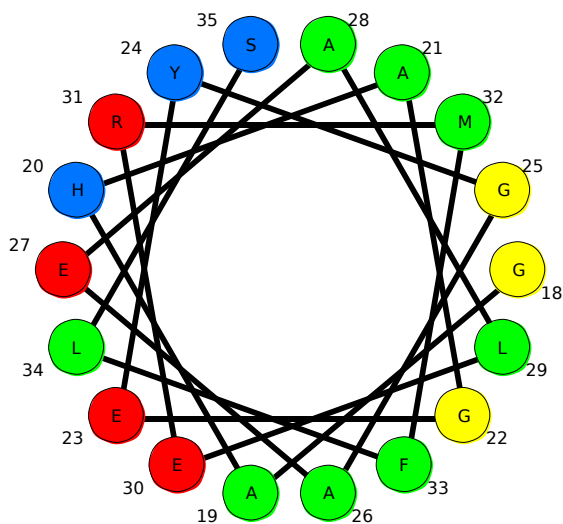
Edmunson wheels are a way of displaying amphipathic helices. This diagram is the 2-D display of a 3-D helix looking down one end of the helix. The colors represent hydrophobicity of the residues: green=hydrophobic, red=charged, blue=polar, and yellow=glycine. The residue type is represented by the single letter code in the center of the circles and the residue number is immediately adjacent to the circles.

3) Distance Plots
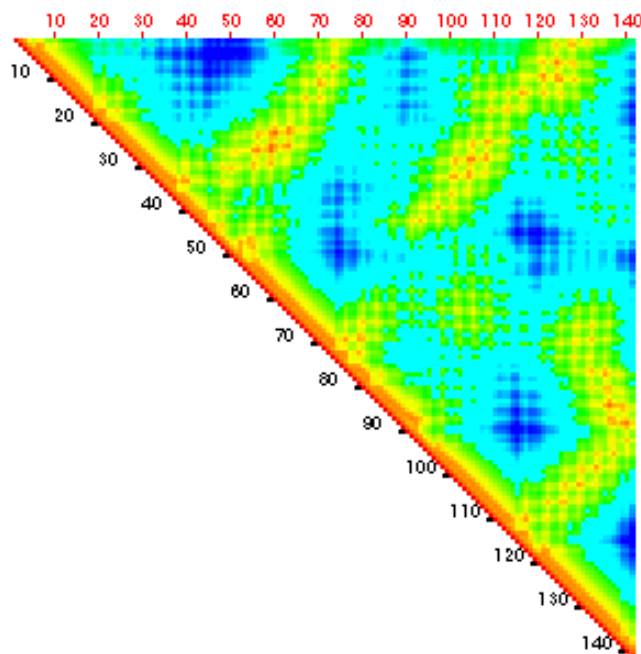
Distance plots, first described by Michael Rossmann, are a way to visualize domains and interactions within a protein. For these graphs, the distance between every C-alpha atom and every other C-alpha atom is measured. The colors range from red=shortest to blue=longest distances. The plot can also be displayed in B&W.

4) Hydrophobicity plots
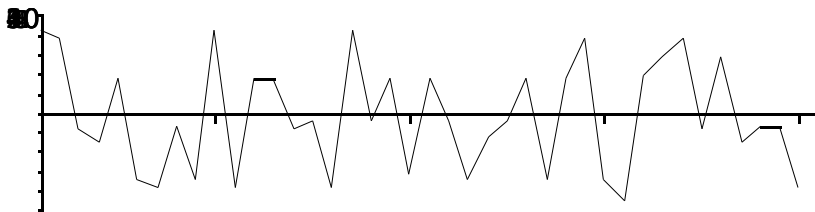
Hydrophobicity plots are the simplest way to display hydrophic cores or stretches of amino acids. The Y axis represents the Kyte & Doolittle hydophobic index (the more + the number, the more hydrophobic it is) and the X axis represents the residue number.

Object Palette
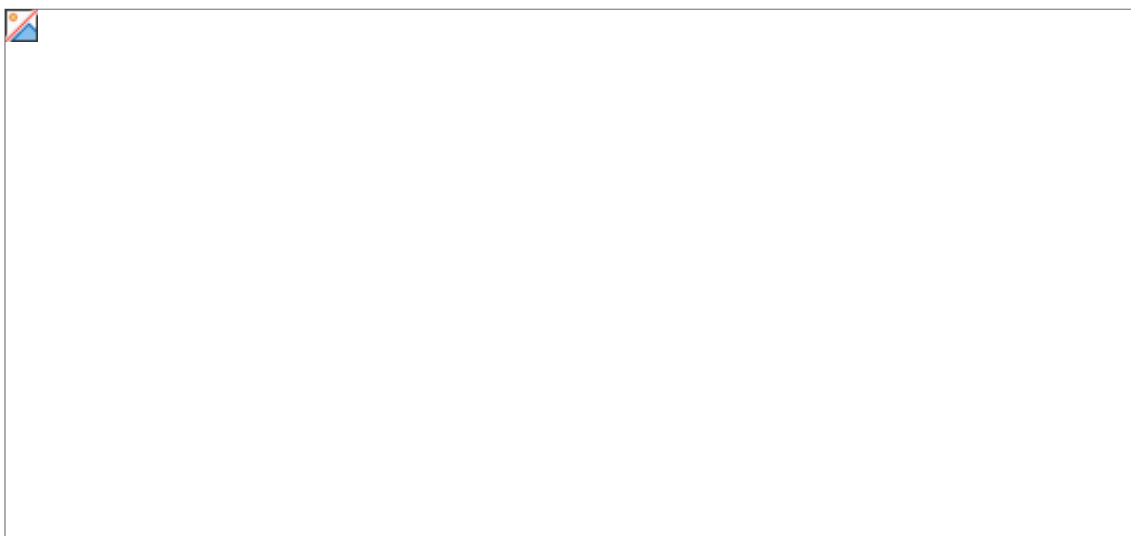
      The object palette is comprise of several columns of four (or less) buttons. The first button (when depressed) turns on the various objects. The second button (when selected with the mouse) lets you select the object to be colored (in conjunction with the Color Palette). This new color is reflected by the color of this button. The third button controls and displays the pen thickness for that particular object (the gray regions represent a 'nonsense' choice for that object and are inactive). The last button (on the very bottom) controls the pattern to be used by the pen when drawing the object. When selected, a small window appears and the user chooses the desired pen pattern.

      When a new object is created (MOL) or if the file contained electron density, additional buttons will appear M0 -> M9 and E1 -> E3, respectively. If a MOL object is deleted, then those buttons are eliminated and the palette shrinks to just the right size.

      The 'Pref' buttons set a wide variety of options all at once

Ribbon Preferences:
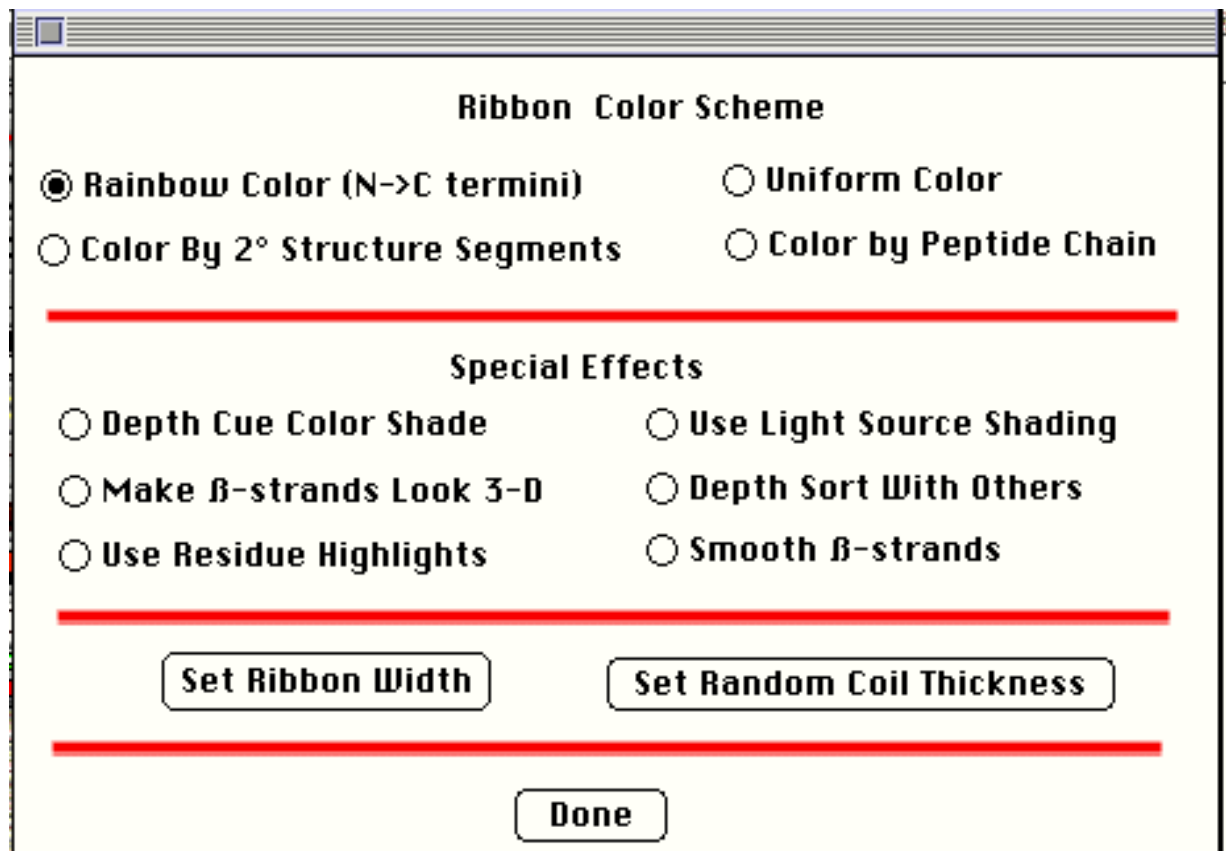
Ribbon Color Scheme:

Rainbow Color:
      This is the default color scheme when a ribbon is first drawn. The color ramps through the rainbow colors as the ribbons go from the first to last atom in the file. Selecting this color scheme turns off the next two.

Color by 2° Structure Segments
      When this is selected, a thin bar opens up (and can be moved around the screen, put behind the main window, or closed) and allows you to change the color of each segment and turn it off and on. As described above, in order to make these color changes, you need to work in the 'ribbon button window' . This menu item just toggles this color scheme on.

Color by Peptide Chain:
      Again, described above. Allows the user to use the colors chosen in the ribbon button window to color the protein according to polypeptide chains.

Uniform Color:
      As the name suggests, this makes all the ribbons the same color. When this is selected, a color wheel appears displaying the current color setting and the user can change it if desired. This option looks best in conjunction with the depth cue

shading.

Some Highlight Options:

The next 3 options only act via residue highlights (therefore can be toggled off and on).

Color by Charge:
ASP and GLU are colored red, HIS,ARG,and LYS are colored blue. The rest remain uncolored (highlights get turned off).

Color per Branden and Tooze:
This option colors charged=red, polar=blue, glycine=yellow, and hydrophobic=green.

Reset all residue highlights:
Resets the colors for all residue highlights (to clear).

**NOTE: The above color schemes can be changed via the stipple dialog box - the colors used here are the same as used for the color schemes for the stippling.

Special Effects:

Depth Cue Shade:
This toggles off/on a shading routine where the ribbons fade into the background color to enhance the depth perception.

Use Light Source:
Here I use the normal to the planes to determine the 'reflectivity' of the sheets and helices. For example the side of the helix facing you fades to white, and the back fades to black. This enhances the 3-D feel of the diagram. Future versions will allow you to move the light source.

Make ß-strands 3-D:
Turning this on will give the ß-strands a 'thickness' rather than having them look like thin sheets of paper.

Depth Sort With Others:
I do not automatically include the ribbon model into the depth sorting routine that is in the 'Drawing' Menu. I felt that there may be occasions where the user might want the other objects 'pasted' onto the ribbons. When you select this item, the ribbons are included in the depth sorting. For example... I make a diagram of hemoglobin. The diagram has ribbons for the protein chain, and colored atom mol objects for the heme. The 'Depth Sort (SLOW)' option will not automatically include the ribbons into the sorting process. Therefore, the hemes will look like they were pasted onto the ribbons. If I then select this option, the heme looks like it is nestled in the heart of the protein ribbons. NOTE: if you turn this option on, it automatically turns on the 'Depth Sort (SLOW)' for logical reasons.

Use Residue Highlights:
As described below, you can color residues in the ribbon model to highlight particular amino acids. This toggles these highlight colors off and on. **NOTE: These highlight colors override the other color schemes for these selected residues.

Smooth ß-strands
There are two ways to make a ß-strand: to follow the carbonyl backbone precisely or to interpolate between the planes. When this is off, the ribbons will

have the 'pleated' look that the strand actually has. When this is on, this will give a more esthetically pleasing straight arrow for the strand. This latter strand will follow the general contours but will not show the pleated nature. **** The ribbon must be redrawn from scratch again after this is selected to show the change since the routine alters how the first planes are calculated****

Thickness Controls:

Ribbon Width:
When the user chooses this option, a dialog box appears and asks the user for the new ribbon width (in Å). This allows the user to make the ribbons wider and thinner. After it is selected, the ribbon is redrawn. You may want to re-smooth it.

Random Coil Thickness:
When the user chooses this option, a dialog box appears and asks the user for the new random coil width (in Å).

Ball&Stick Preferences

Ball and Stick thickness

○ **Use uniform ball and stick thickness**

Balls -> `0.50` Å   Sticks -> `0.15` Å

◉ **Make Balls proportional to atomic radii**

Balls -> `33` %   Sticks -> `0.15` Å

Ball & Stick Color

○ **Use overall color**

[Set Color]

◉ **Use Original Color**

○ **Use Color based on Atom Type**

[Done]   [Cancel]

**Note: Changes in Ball and Stick thicknesses will ONLY be made if one of the first two radio buttons have been pushed. e.g. the example shown above is set to 'Make Balls proportional to atomic radii" and the Balls will be 33% of the radii and the sticks will be 0.15 Å thick.

Use uniform ball and stick thickness:
      This allows you to make the Balls and Sticks different thicknesses if you do not like the default settings (shown in the window). Changes will only take place if you click on the radio button entitled 'Change ball radius and stick thickness'. Then, when leaving the dialog box, the inputted numbers will be used.

Make Balls proportional to atomic radii:
      This options reads the 'CPK_radii' section at the end of the 'names.pdb' file to figure out the radii for the various atoms. If you do not like my settings, feel free to edit the TEXT file. This option sets the radii of the balls to be proportional to this CPK radii. In the above example, the balls will be 33% of the listed CPK radii (a good setting). If it cannot find a radii for a particular atom type, the radius of the unknown atom is set to 1.5Å. Changes and this option will only be activated if you click on the radio button. The default setting is for a uniform radii and not this setting.

Ball and Stick Color:

    1) Use overall color: you can set all balls and sticks to be the same color and define this color by clicking on the button.

2) To use the color of the segments as inputted (as you created it) just click on the radio button.

3) Click on the radio button to have the balls colored based on the atom type (i.e. red for O, and blue for N....)

B-Value Object Preferences

B-Value Object Preferences

⦿ Show All Atoms

○ Show only C-Alpha Backbone

Set Pen Thickness

Done
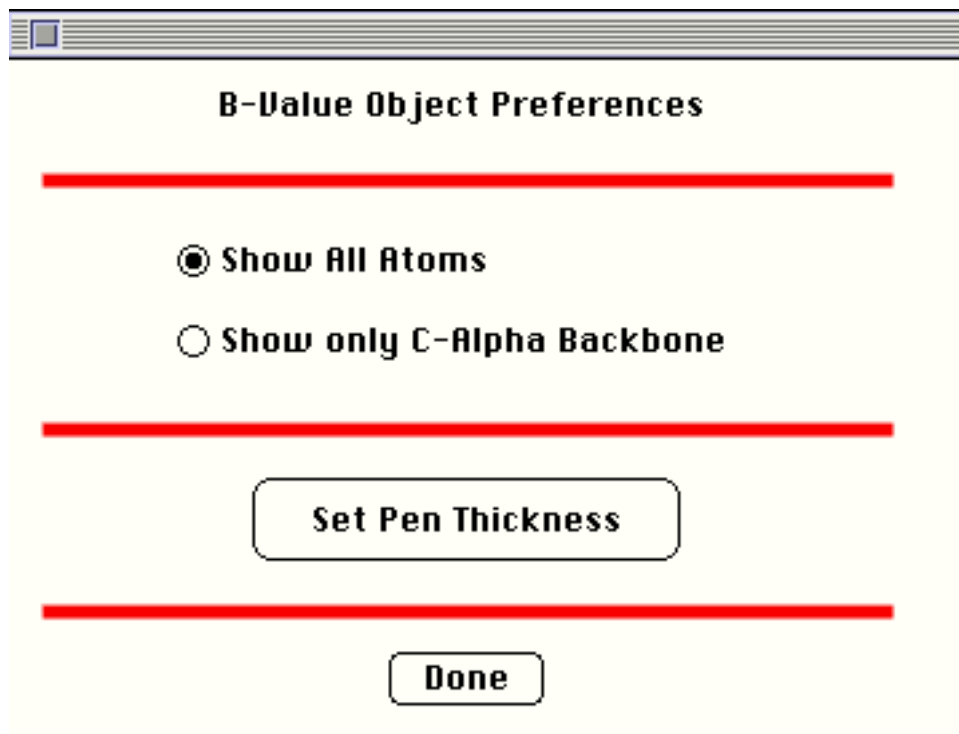
Show all Atoms: Represent all atoms with colored sticks
Show only C-alpha Backbone: Only trace the protein backbone and ignore all other atoms.
Set Pen Thickness: Change the line thickness.

Molecular Surface Stippling Preferences

○ **Color by atom type**

○ **Color by charge**   [Change Scheme]

○ **Color per Branden&Tooze book**   [Change Scheme]

Stipple thickness ->   [1]

───────────────

Display surface only about a residue:

   Residue # ->   [1]

   Display Radius (Å) ->   [5.0]

[Select Subset]   [Display all]

───────────────

[All Done]

Color by Atom Type: Colors the molecular envelope according to the nearest atom type: e.g. N=blue, O=red, C=yellow, S=green, H=grey, others=purple.

Color by Charge: Colors the molecular envelope according to the charge of the nearest residue e.g. red=acidic, blue=basic, and grey=neither.

Color as per Brandis and Toose book: Colors the molecular envelope according to the nearest atom type: e.g. hydrophobic=green, glycine=yellow, charged=red, and polar=blue.

Stipple Thickness: Allows you to change the thickness of the 'dots' comprising the stippling.

Display surface about a residue: You can first input a residue number about which the surface is to be selected, and then input the radius for the cutoff. When ready, hit 'select subset'. This is a very fast option, and will be finished in a flash.

Display All: Removes all of the selection used previously and shows all of the surface.

All Done: When done, hit this button.

Ribbon Button Window

On/off button for entire
polypeptide segment

Secondary Structure
Elements (on/off buttons)

Color of entire
polypeptide segment

Color of individual elements
and residue number of start
of that element.
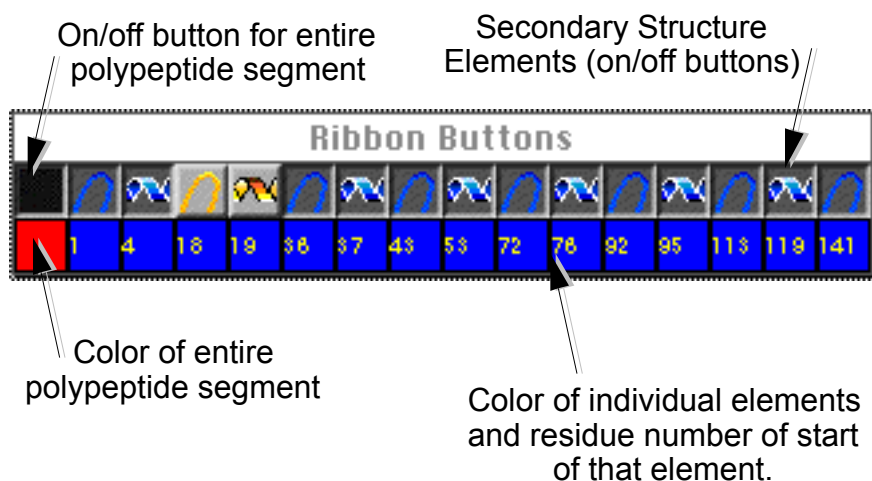
MolView can create ribbon diagrams for proteins: thick lines for random coils, arrows for ß-strands, and 'pig tails' for α-helices.   There are several ways MolView can color the ribbon diagrams: the whole thing is one color, each polypeptide is a different color, the diagram's color spans the rainbow going from the N to the C termini, and finally where each secondary structural element can have its own color. **The choice for the color scheme is in the Menu Item 'Ribbon' and not in this palette. If you choose to color the ribbon diagram according to polypeptide chain, the a click on the red button (in this case) will allow you to change the color of that protein (in conjunction with the Color Palette). The selected color is reflected in the button color. By clicking on the button directly above it, the entire protein is turned off and on. These two buttons precede each polypeptide chain.   The subsequent buttons turn each separate element off and on (the type of secondary structure is reflected by the picture on the button) and the button beneath it displays the residue number of the first amino acid of that structural element and its color (only if the user has chosen the 'color by segments' option from the ribbon menu.

These diagrams are different than other programs in that I do not 'smooth' the secondary elements to make them more esoterically pleasing. The only reason I do this is so that the user can accurately pick regions of the diagram for labeling and examination. This results in a kind of funny looking 'wavy-ness' to the ß strands.

NEW OPTION:

If you hold down the '⚘' button while clicking on the colored, numbered button, an new Window will appear that allows you to color each residue independently...

Segment Magnification Window
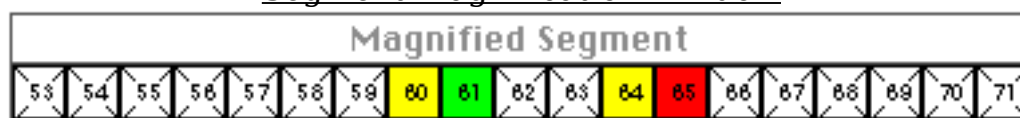
Here we '⚘-clicked' on the colored button labelled with the number 53 from the above Ribbon Button Window. This is a magnification of that window. The buttons that have an X in the background show that those residues have not been given a highlight color. By clicking on one of these buttons, then selecting a color from the palette, you can highlight

a particular residue in this segment. Simply close to window to work on another segment. If you '⚠-click' on one of the colored buttons, the color highlight for that residue goes away.

**NOTE: To see the highlight colors, you must have selected the 'Use Residue Highlight' button in the 'Ribbon Preferences' Dialog box (see above). This also allows you to toggle all of the colored highlights off and on.

Notes about the 'names.pdb' file
        MolView reads a file called "names.pdb". This file should be in the same folder as the MolView program. If it is not found there, the program will make you look for it.

        The 'names.pdb' contains several pieces of information needed to run MolView. I have made this file a TEXT file so that you can edit and change it as your needs change. The major sections are:

<div align="center">

RESIDUES
ATOMS
CPK_Radii
Bond_Distances

</div>

The section "RESIDUES" contains the names of possible types of 'residues' (e.g. amino acid or nucleotide names).
The section "ATOMS" contains the names of possible atom types (e.g. CA, N, CB, OT, O, etc.)
If you open a MolView file, and the name of an atom is ???, then this means that the name of this particular atom is not found in the 'names.pdb' list. YOU SHOULD add this name to the list and
start MolView up again to make sure that all of the options are read properly.
The section "CPK_Radii" is for the radii of the various atoms. These values are used to define the ball radii used in the Ball&Stick options and the ball radi used in the CPK models. The program only reads the first two letters in the atom name (try to keep the the double letter atoms towards the end of the list: e.g. put NI after N).
The section "Bond_Distances" is for the minimum and maximum distances to be used for bond distances. This is the closest I want to come to an atomic dictionary. While this is not as robust as the dictionaries used by other programs, it is simple enough for the most naive user to edit while lending a great deal of flexibility to the program.

Example input line:
C N 1.2 1.99
This means that the bond between C and N atoms must be > 1.2Å and < 1.99Å to be drawn as a bond. Again, only the first two letters are read by MolView, and keep the double letters towards the end of the list. If not found in the list, the default bond distance is very generous.

GETTING STARTED

1) Install the MolView program onto your hard drive. I distributing the file as an 'auto-decompressing' file. Just double click on it and it will expand itself. As with other programs, there are icons associated with the various files. You may need to rebuild your desktop after copying the files to your hard drive (hold down the 'option' and ⚠ buttons while the Mac is starting up).

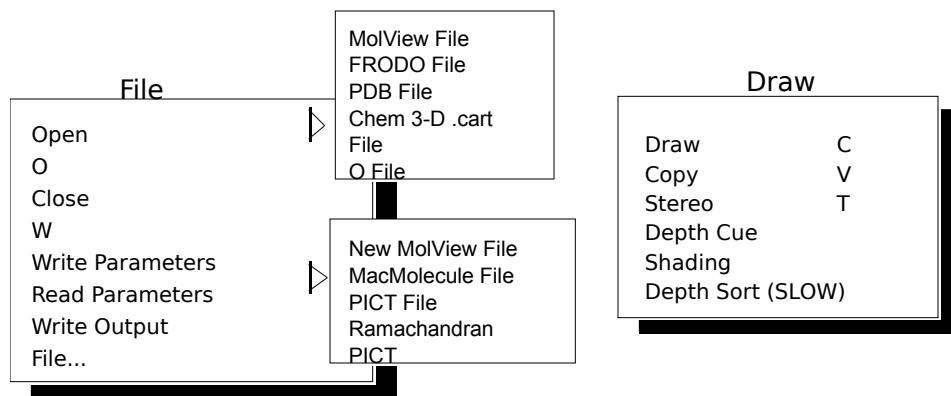2) Get the FRODO plot, PDB, or Chem Draw 3-D files from the network.
      All letters in the files must be UPPER CASE

3) Start MolView.

4) Convert PDB or FRODO files to a MolView file.

5) Open the new MolView file and have fun.

MolView Quick Reference Quide

File

Open
O
Close
W
Write Parameters
Read Parameters
Write Output
File...

MolView File
FRODO File
PDB File
Chem 3-D .cart
File
O File

New MolView File
MacMolecule File
PICT File
Ramachandran
PICT

Draw

Draw	C
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Stereo	T
Depth Cue
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Labels

Delete all labels
Move a Label

Keep Label
Change
Discard Change
Global Offset   G
Reset Label Offset R
Create Labels
Font
Style

MOLs

Delete Mol Object
Clip MOL Object w/At. Model

Size&Pos

Rotate
Stereo Separation
Change Scale
Original Size&Pos.
Slab...
Reset Slab
PICT Size = window size

Geom&Movies

Rama Plot
Pick Rama Points
Plot Preferences...
See Movie
Make Movie PICTS

Windows

Main Window
Tools
Objects
Ramachandran Plot
Movie 1
Movie 2
Ribbon Buttons
Magnified Segment
Color Palette

*Note:

'⛰-mouse click' on the Color Palette to change a particular color.

'Control-mouse click' on the Color Palette to return to the default color pattern.

'⛰-mouse click' on a color button in the Ribbon Button Palette to display a magnified view of that secondary structure element (for coloring individual amino acids.

'⛰-mouse click' on the Magnified Ribbon Button Palette to remove the coloring that particular amino acid in the ribbon drawing.
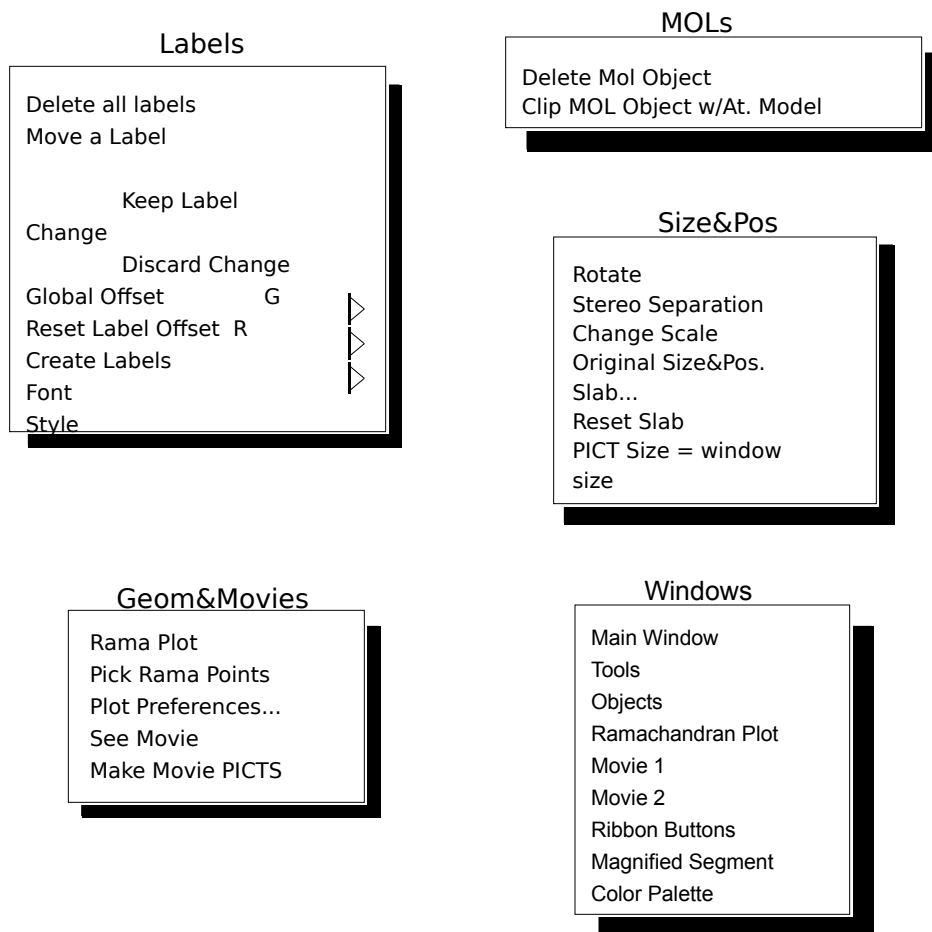
MENU: FILE

Open:
      This pop-up menu now directs the user as to which input file he has. After the files have been converted to a MolView file (in the case of PDB, O, FRODO, and .cart files), the structures are automatically displayed. Upon selecting this menu item with the mouse, a pop-up menu appears, and the user selects the file type...

   MolView File:
            All other structure files are first converted to this format and then opened. For example, I have a file called 'Fred.pdb'. The first time I look at this structure, I open it as a PDB file (see below). During the read, I am asked to save it as a 'MolView' file. Being unoriginal, I save it as 'Fred.MV'. The next day, I open 'Fred.MV' as a MolView File rather than going back to scratch with the PDB file.

   FRODO File:
            User is asked to open a FRODO plot file. This file must be in the same directory as the MolView application. If the file contains electron density, then the user can strip away electron density that is not within the cutoff distance to the atomic model. Note that only the atomic model is used and not Mol objects. The resulting file is a MolView format input file. Be aware that if you have a large electron density and decide to use the clip option to remove the unwanted density, it will take some time (curl up to a good book or get some coffee). For normal files, the files are read and converted in a few seconds.

   PDB File:
            User can open a PDB format file and create a MolView file. **Be sure that the header information is removed from the file (i.e. the first line should begin with the word 'ATOM'). Am just now getting back to fixing this bad bit of code. The user can make bond connections according to the order in which they appear in the list (Link) or according to the distance between the atoms (NoLink). In the case of NoLink, each atom is checked with the next # of atoms for whether or not a possible bond exists. The # of atoms searched through is determined by the 'bond search #' set in the preferences of the Draw menu.
            If there is a chain identifier, 1000 will be added to the residue number. For example, 'A 201' becomes residue '201', whereas 'B 201' becomes '1201', and so on.
            If the file contains helix and sheet information, this routine will write out a *.PDB.struc file to be used in creating a ribbon diagram. This will probably be more accurate than the current algorithm for secondary structure determination.
   Chem 3-D .cart File:
            This allows the user to read in the TEXT file produced by ChemDraw 3-D called Cartesian Coordinates 1 and produce a MolView File.

   O File (before version 5.9):

This option allows the user to convert the ASCII plot files generated by Alwyn Jones's graphics program called 'O'. It should be noted that these plot files do not have atomic coordinates in them, therefore many of MolView object creation routines will not work. They should not even be tried. Each object, whether it came from electron density or the atomic model, is read in as a MOL object. The labels are kept, but are fixed - they can only be turned off and on but not changed. What you had on the screen should be what you get on the Mac. You can still rotate, color, and

change pen thickness (etc.), but just cannot do as many things on the Mac as you can with PDB or FRODO plot files. By default, MOLVIEW files created by 'O' plot files will open with all objects turned on.

O File (after version 5.9):

Alwyn Jones changed his O program such that MolView cannot read the new versions of his plot files anymore. This option can read in the new format (not the old). **!!! Be aware that one can now append PDB coordinates to all O plot files!!!** In this way, O plot files can do every thing that FRODO plot files can do. With atomic coordinates appended to the file, the user can finally use all the options in MOLVIEW. To use this new option, have your PDB file (corresponding to the O plot file) on the Mac. You will be prompted with a dialog box asking if you want to append a PDB file to your O plot file and where the file is to be located.

Close (⌘-W):

User can close this MolView File and open another. Many of the parameters are kept from the previous run of the program.

Write Parameters:

User can write out many of the parameters defining the currently displayed diagram; the colors of all objects, the pen thicknesses of all objects, stereo off/on, which objects are off/on, label colors, and label styles. **Note, I do not keep label offsets and which atom labels are turned on.** I did this purposely so that one parameter file could pertain to any MolView file.

Read Parameters:

User can open the parameter files created above and instantly set the colors and various parameters to the user had at the time of the file creation.

Write Output File...:

This pop-up menu directs the user to select which kind of output file they would like to write...

New MolView File:

The current coordinates are written out to a new MolView file. The coordinates saved correspond to those displayed on the screen. For example, say a PDB file was used to make a MolView with the previous option. The user might then read in the new MolView file and perform rotations and maybe create Mol objects. The new orientation and Mol objects are saved to the new MolView file.

MacMolecule File:

An interesting shareware program called MacMolecule can pretty nice space filling and ball+stick models. However, software does not come with a program to convert normal atomic files to the input necessary for the program. This option takes the atomic model displayed and writes out the required file. The user can write out a file where the atoms are bonded according to the order that they appear in the list of atomic coordinates, or according to a

distance cutoff. This version specially handles H, Fe, and Mo atoms. The inputted distance cutoff is ignored and uses more reasonable values to make the connections. I have created this output file with a resource fork so that the moment it is written, it will have a MacMolecule Icon, and therefore MacMolecule will be launched when the file is 'double-clicked'.

PICT File:

This option writes out the chosen objects to a file of universal PICT format. Two types of PICT files are written (transparent to the user). If space filling models (CPK) have been drawn, then the PICT file will be binary and limited to the resolution of the screen. The second type of PICT file is when there is not any CPK models displayed. This PICT file can be opened by all programs and is object oriented. This means that each line can be individually picked by other graphic programs, and the resolution is not limited by the screen.

Rama PICT File:

This option writes out the Ramachandran plot to an object oriented PICT file. You must have created a Ramachandran plot first (see Geom&Movie menu).

DXF File:

This is a fairly new option, that will be expanded in the future. DXF files are ASCII files that can be read by many 3-D CAD programs. At the moment, this option writes out a DXF file for desired C-α residues within a specified range and/or grabs a user-specified Mol object and turns it into a DXF object. We then take this file and read it into Macromodel to make very pretty 3-D rendered tubes and sheets. These models, in turn, can be made into movies with Macromind's '3-D' program. I have included a PICT file to show you an example of a rendered PICT file using this procedure.

Quit (⌘-Q):

Kind of obvious.

MENU: Draw

Draw (⌘-V):
> Clears the screen then draws the objects that are turned on. This just displays to the screen and does not write to the Clipboard.

Copy (⌘-C):
> Draws all of the objects that you have turned on to the Clipboard. E.g. Get the diagram that you like, select copy, then go to another drawing application and hit 'Paste'. If there are a lot of vectors, the clipboard may run out of memory. In these cases, write out a PICT file instead (see 'Write output file' option in the 'File' menu).

Stereo (⌘-T):
> The user can toggle on/off the stereo image.

Depth Cue Shading:
> When this item is selected, all objects fade to whatever the background color is currently set to. If the background color option is turned off, then the objects fade to white. This option is 'toggled' off and on.

Depth Sort (SLOW):
> This option sorts the vectors for Mol objects, distance lines, ED maps, and the atomic model. Albeit slow, the lines that are supposed to be in front are drawn last and do appear to be in front. This is significantly slower than normal. I suggest that you get the objects and views that you want and then hit this option just before making your final diagram or movie. While it is slow, it is worth it in the end for a high quality diagram with proper depth cueing.

Preferences…:
> I put some of the more obscure menu items into a preference file such as stereo and such. The first time the program is launched, it assigns default values. Upon quitting, it writes out a preference file to the system folder. The user has the option to write out their own preference file in a separate location if they wish to. When this item is selected, the following dialog box appears…

Preferences

Stereo:
- ○ Cross-eyed Stereo
- ◉ Wall-eyed Stereo

FRODO MOL Dot Color:
- ◉ FRODO Color Scheme
- ○ User Defined Color Scheme

[Read Preference File]
[Write Preference File]

- ◉ Idiot Input Dialogs
- ○ Expert Input Dialogs
- ○ Refresh Always (SLOW)

Change Rotation Step Size ->   [O.K.]

Change FRODO MOL Dot Size -> | 2 | Pixel

Bond Search # -> | 25 | [Set PICT Type]

Depth Sorting bins | 50 | #Slab Steps | 20 |

Neighbors:
- Font Size: | 9 |
- Color-> [Set Color]
- ○ Label Neighbors

Min Distance | 2.2999 |
Max Distance | 3.7999 |

[Done]

To explain each item...

Walleyed Stereo:
When a stereo pair is drawn, it will be with a +6° rotation about the screen's Y axis. This is the 'standard' stereo pair that can be viewed with stereo glasses, or with Marty Feldman's eyes.

Cross-eye Stereo:
The stereo pair will be drawn with a -6° rotation about the Y axis. This is not the 'standard' stereo image, cannot be properly viewed with stereo glasses, but I can see easily.

Dot Color:
FRODO can simulate the surface of a molecule by placing 'dots' at a given radius about the atoms. This is done by creating a 'MOL' object and using the 'SURF' option within the MOL menu. I have tried to duplicate these colors when I read the dots in from the FRODO plot file. The carbon atoms have yellow dots about them, the oxygen's have red and the nitrogen's have blue. The default for this pop-up menu is the above 'original color scheme'. However, I thought that the user might not like this color scheme, and since these dots are in a MOL object, I allow the user to change the color scheme with this menu by selecting the 'New color' choice of this pop-up menu. If this

latter menu item is selected, then all of the dot colors will be changed to the color of that particular MOL object.

Dot Size:
      The size of the dots can be changed with this pop-up menu. The default size is 2 pixels in diameter. The previous selection is marked with a check mark.

Read Preference File:
Write Preference File:
      As described above, all of this information (and more in the future) is stored in a file called 'MOLVIEW Preferences'. Normally it is written to and read from the System Folder without the user knowing about it. However, for machines where the System Folder is protected, or for community machines, this may not be advisable. Therefor the user may use the following 'Write Preference File' to create the MOLVIEW Preference file in another directory. Subsequently, the user can use this option to read in their own personal preference file.

Change Rot. Step Size:
      The user can change the step sizes used in the 'Interactive Rotation' option to be described in the 'Misc' menu. A dialog box appears, and the user inputs the new value(s). Hit O.K. when you are done.

Bond Search #:
      This option allows you to 'search' through more or less atoms when models are created. In the Read PDB, Create Mols, and Write MM file, the distance between atoms is used as the only criterea as to whether atoms are to be bonded together. I have made special dispensation for H, Mo, and Fe atoms so that proper bonds are made. The default and initial value is 30. This means that when you, for example, 'Read PDB', the 30 atoms following each atom is checked as to whether they might be in bonding distance to the first. For a protein, this value of 30 is usually sufficient. However, for AMP, for example, you need a value of ~40 since there are so many atoms within a single 'residue'. The smaller the number, the faster the program can create the objects. If you find that certain bonds are not being made as you read PDB files, Create Mol Objects, or Write MM File, try increasing this number first and then try your action again.

Set PICT Type
      When I write out a PICT file, I can make its 'creator' anything that I want. If this button is clicked, then the user can force the output PICT file to be read by other graphics programs. For example, if I set the 'Creator' to be Adobe Photoshop, then a PICT file is created that has the Adobe icon. If I then 'double click' this file, Adobe Photoshop automatically launches and opens the MolView file. Be aware that some programs are better to read the PICT files than other. For example, if you do not include a CPK model, then I recommend either Canvas or MacDraw Pro since these programs will keep the lines as objects rather than converting to a bit image. If you have CPK models included, I recommend Photoshop or PixelPaint Pro.

Number of Bins for Depth Sorting:
      In the option 'Depth Sort (SLOW)' in the 'Drawing' menu, the total depth (Z distance) of the objects are divided into bins. The vectors in these bins are

then draw from back to front. For small diagrams, MolView will work fast and correctly with a few bins (say about 10). For larger diagrams, more bins may be needed (say 30-50). The more bins, the slower the program, but more accurate the depth perception.

Idiot Dialog boxes:
Expert Dialog boxes:

This is the beginning of further changes. This allows a naive user to not know anything and get a drawing. For now, selecting 'Idiot Dialog Boxes' allows a user to read in a PDB file and not answer any questions. I determine the number of atoms in the file and set everything else for a 'typical' conversion. Gets rid of all of the dialog boxes in this option. Will be expanding this option to the Mol creating options as well.

Refresh Always:

When this is selected, the screen is refreshed after each menu selection. This option allows a person on an LC to not have to wait so much, or a person on a Quadra to get what they want immediately.

 # Slab Steps:

This allows the user to change the number of 'slices' used to slab away the structure. The more steps, the finer the slabbing routine. This is the only parameter not saved in the preference file. If this is badly set, the next user may think that something is seriously wrong with their file or MolView. Therefore, to save e-mail responses, it is not saved for the next user.

Neighbors:

Neighbor is an option found in the Geom&Movies menu. After selecting this item neighboring atoms are identified, lines drawn to them, and distances marked on the lines. This option allows you to define how this is to be done...

Font Size: Font size of the distance label on the lines
Color: Color of the lines and labels.
Min, Max distances: minimum and maximum distances defining a neighbor
Label Neighbors: Labels the atoms neighboring the selected atom.

MENU: Labels:

Delete All Labels:

This deletes all labels. This is helpful if you've labeled too many atoms and want to start from scratch.

Move A Label:

This option allows the user to move individual labels to increase diagram clarity. After this menu is selected, the cursor changes to a

The 'hot' area of this cursor is the upper left corner. In other words, get the box in the upper left corner of the cursor over an atom before clicking the mouse. Again, I have tried to prevent unusual behavior by shutting this option off at the appropriate times. To activate a particular label, just click on the corresponding atom. If that atom was not previously labeled, it will be now. Move the mouse to where you want it to be, and click again. Do not 'click and drag', just click. You can keep moving the label around with mouse clicks. After you have selected an atom, the next two items on the menu('Keep Label Change' and 'Discard Label Change') go from gray to black and can now be selected. If you like the new position of the label, just select 'Keep Label Change', if you do not, hit 'Discard Label Change'. You will stay in this interactive mode until you select the 'Move a Label' menu item again, or another of the interactive menu items such as 'Hand Pick Atoms', 'Zoom In', or "Zoom Out'. These adjustments to the label positions are discarded once you go to any of the rotation functions since I felt that such adjustments would be useless in another orientation. Be aware that the label movement 'erases' bits of the model as it passes over it. This is because I did not refresh the screen after each label movement - I found that it slowed the Mac down too much. The adjustments to the label position are multiplied by a scale factor such that the distance you offset the label at one scale factor is proportionally the same at a different scale factor.

Keep Label Change:
Discard Label Change:
These two items are used in conjunction with the 'Move a Label' option and are ONLY active once a label has been selected and the user has started the moving process. These functions are discussed above.

Global Offset (⌘-G):
Simple routine. Allows the user to offset all of the labels in the X and Y directions. Just input the offset (in pixels) in the dialog box and hit O.K. As with other label offsets, these adjustments are cleared after any rotations are performed.

Reset Label Offsets (⌘-R):

Erases all label offsets. After selection the labels are moved to right of the atoms.

Create Labels:

Allows the user to create the exact type of label to be applied to the atoms. Each atom has a residue type, residue number, and atom type identifier. To create a type of label, just select them in the order you wish them to appear. You do not have to use all three atom identifiers for the labels. To help you, I have changed the buttons over the various labels upon selection. For example, say that you decided that the residue type is the first thing to appear in the label. You click on the button above the label saying 'Residue Type' and the button will change to read 'Item #1'. If you make a mistake, just hit the "Start over" button and do it again. Every time you enter this routine, I have to purge the memory that these labels reside in. Therefore, each time you enter this subroutine, you loose the label that you chose before. However, the atoms that you selected are still flagged for being labeled with the new label.

Font:

The program goes to the System file and finds all available Fonts. These fonts are displayed as a pop-menu. The selected font will be used for all subsequent labeling.

Style:

The user is allowed to change the style of all labeling with this pop-up menu. Each menu item is drawn with that particular style.

Size:

The user can change the label font size to one of the standard sizes shown in the pop-up menu or some other size by selecting 'other...'.

MENU: MOLs

Delete Mol Object:

When the cursor is dragged over this item, a pop-up menu appears and the user is able to choose which MOL object is to be deleted. The MOL objects that appear after the deleted object are shuffled up one. i.e. if you have 3 objects and delete the second one, the third object now becomes the second object and there is no longer a third object. All of the menus are updated to show the change. To conserve as much memory as possible, I create a scratch area of RAM, write the objects to that area, and reallocate exactly as much memory is needed after the deletion. Therefore, the memory usage is maximized (I also use Handles instead of fixed pointers during the moves). **Note, in this latest version, the pen pattern and colors are still associated with a particular Mol object even though the # designation has changed. e.g. Mol object #3 is red. I delete Mol object #2. Mol object #3 becomes Mol object #2. However, this object is still red and not the color of the previous Mol object #2. **Note, in the last version, if the Mol object was empty, you could not delete it (a C problem). I programmed around this problem, and you can now delete empty Mol objects.

Clip Mol Object w/ At. model:

This is a rather odd routine to fix a bug in O (version 5.9). O, a program for the larger graphics machines, does not properly clip the electron density in the plot files. This fixes that. Read in the O plot file and append the PDB file while reading it in and follow dialog box instructions.

Menu: Size & Pos

Rotate:
Allows the user to rotate all objects by inputting rotation angles about the x, y, and z axes (x axis is horizontal, y is vertical, and z is towards the screen). If you have a color Mac, a multicolored diagram appears in the dialog box to show you the directions of the various rotations. When you are happy with your input, hit 'O.K.'. Wait a minute and the screen will clear and the new diagram will appear.

Stereo Separation:
The user can change the separation (in pixels) between the stereo pairs. Adjustments to the scale factor also adjust this stereo separation. Say the user is at a scale factor of 100. If he chooses a scale factor of 200, then the stereo separation will double as well. I did this to try to fit the most of the objects into the screen and prevent the stereo pairs from overlapping.

Change Scale:
Allows the user to change the scale factor applied to the models. A dialog box appears, displays the old value, and asks the user for a new value.

Original size & position:
This option resets the images back to the size and position on the screen as when the MOLVIEW file was first opened. Helpful when you get completely lost...

Slab...:
This menu option allows the user to 'slab' or to trim the image on the front, back, top, bottom, left, and right sides. A window appears with + and - buttons next to the words front, back, top, bottom, left and right. For example, if the user selects the ⊟ button next to the word top, then the image gets trimmed down on the top. If he had selected the ⊞ , then the image would have gotten larger at the top. Some notes about this procedure. 1) The image gets trimmed down by 5% of the maximum width of the image for each press of the button, and 2) the slab is with respect to the screen coordinate system. Therefore, as a slabbed image is rotated, you will see different vectors appear and disappear. This is the same idea as used in FRODO, except FRODO only uses a uniform slab in the front and back of the image. 3) When you copy this image to the Clipboard or to a PICT file, the vectors which have been slabbed away, will not appear in these files. 4) I cheated. FRODO will trim each vector where MolView either keeps or deletes entire vectors. This was done for the sake of speed and memory. Sorry, this may make smaller images look a little ragged around the edges. Smaller Macs could not handle what I would have to do if I were to do it properly.

Reset Slab:
This option resets all of the slabs to get back to the original image.

PICT size = window size

When making a PICT file, you need to define the size of the PICT image. In the case where there are no CPK models, this area is actually much larger than the visible screen to make sure that all vectors are transported. This is a pain when making movies -- the

background is inordinately large. This option fixes the background size to equal the window size

PICT size = Real Size

This option allows the user to restore the original background and clip size. By default, I have made the 'Clipping' region very large to encompass all of the vectors of the more unusually shaped diagrams.

Menu: Geom & Movies

Rama Plot:

When this is selected, the user is asked for a residue range of the protein. A window then opens and a Ramachandran plot is displayed with the various Phi-Psi values plotted. The GLY residues are orange dots and the PRO residues are purple boxes. If a Ramachandran window is already open when this option is selected, then the plot is simply redrawn. To do a different zone, you need to close the Rama window first and select this option (close window by hitting the small box in the upper left corner of the widow). This window can be re-sized by dragging the box in the lower right hand corner. !!The font selected by the Labeling menu is used for this diagram as well.

Pick Rama Points:

This option displays the residue number of each point on the Ramachandran plot when selected by the mouse. Couple of things to note: If this option is toggled on, then you are not allowed to put the other window in front or to work on the atomic model window. You need to toggle this option off and then work on the other window (or select some of the other options on the other window like 'Hand Pick Atoms'). Also, the numerical values are not saved on the plot. You can clear the numbers by selecting the 'Rama Plot' option again.

Plot Preferences:

This option opens a window that displays the current settings of the Ramachandran plot routine and allows the user to change them. It allows the user to display the boundaries of the allowable zones and allows the user to switch between color and B&W diagrams. For B&W diagrams, GLY residues become filled black circles and PRO residues become square, gray blocks.

See Movie:

This is a fairly useless option, but was only a couple of lines of code--so what the heck. When you select this option, you are given the same dialog box found in the 'Rotate' option. You can input the rotation you wish each step of the movie to be. After this, the objects that are currently selected begin to rotate. To stop the movie, just click the mouse within the window.

Make Movie PICTS:

This is the same as the last option except that for each rotation, a PICT file is written out. The process continues until the mouse is clicked on the image. The files are created in the local directory and start with the name 'Frame0' and numbered sequentially after that. We have used this option to readily create a movie using MacroMind Director. Remember to use the 'User Set Back and Clip' option (under the 'Misc.' menu) to draw the size and shape background you would like for the movies. This latter option is really essential for making movies.

Menu: Windows

This Menu brings the desired window, if it exists, to the foreground. Select the various window to activate it.

Main Window: The main drawing window
Tools
Objects:
Ramachandran: The Ramachandran plot window
Movie 1: QuickTime Movie #1
Movie 2: QuickTime Movie #2
Ribbon Buttons:
Magnified Segment:
Color Palette:
Edmunson wheel:
Distance Plot:
Hydrophobicity plot:

Example:

Making a ribbon drawing of hemoglobin with the CPK model of the Heme nestled in the middle (MOLVIEW file included).

1) Open MOLVIEW file
2) Turn off Atomic model (Select menu)
3) Make Ribbon drawing (**Ribbon Button** on **Tool Palette**)
4) Smooth (**Ribbon Button Smooth Button** on **Tool Palette**)
5) Depth sort with others (**'Pref' button beneath "Ribbon Button' on 'Object Window'**)
6) Change CPK (**'CPK Button'** on**Tool Palette**)
7) Do the following in the Change CPK dialog box:
      a)   Hit 'Delete all CPK atoms' button
      b)   Enter 300 to 300 for residue range
      c)   Hit the 'Default Colors' radio button
      d)   Hit the o.k. button
      e)   Hit the 'Sort with others' button
      f)   Hit the 'Quit' button

That's all!!

EXAMPLE:

1) While working with FRODO 6.6, I have a view that I like and hit 'Plot' on the menu.
2) Using a program like 'Fetch' or 'Kermit' I ship the 'FRODO plot file' to the Mac.
3) I put the plot file into the MolView directory and launch MolView.

4) I go to **'File'** menu and choose **'Open'** and select **'Frodo File'** from the pop-up menu. After a few seconds, the file is read in, and I am asked to input a new file name. This file contains an electron image and I get asked if I want to clip the electron density. I hit the yes button and the electron density gets clipped to include only those vectors near atoms in the atomic structure section.

5) The file is read in, as the menu goes from gray to black. By default, the atomic model is displayed in mono.

6) I want to see stereo so I go to the **'Drawing** 'menu and choose **'Stereo'**, then go back to the **'Drawing'** menu and choose **'Draw'**. I now see a stereo pair on the screen.

7) Since I have slightly crossed-eyes, I do not like the stereo on the screen (the default is 'wall-eyed stereo') so I go back '**Drawing**' to and choose **'Preferences'** and select **'Cross-eyed Stereo'** from the dialog box.

8) I now want to see my electron density so I go back to the **'Object'** window and choose the item labeled **'ED1'**. The map should now appear.

9) I now would like to label some of the atoms. I first go to the **'Labels'** menu and select my desired Font, Size and style. I then go to the **'Labels'** window and choose the **'Create Labels'** option. A widow opens up and I can now create the type of label that I want. I want to have the Residue number followed by the residue type, so I click on the 'Residue number' button, then the 'Residue type' button and then select O.K. I am now ready to label my model.

10) I want to hand pick the atoms like in FRODO, so I now select the **'Hand Pick Atoms'** icon from the **Tool palette** (the bulls-eye). The mouse cursor is a 'bulls-eye' and stays so until I select this menu option again or some of the other ones. I click on the left hand image of the stereo pairs and the appropriate labels appear.

12) I chose the wrong atom by accident, so I go back to the **Tool Palette** menu and choose **'Pick From List'** icon (two circles with letters next to them). I scroll through the list until I find the mistake and 'de-select' it by clicking on the radio button next to it.

13) I now would like to change the colors of the atomic model so I go to the **Object Tool Palette** and select the colored box beneath the **'A'** button. A color window appears and the color of the wheel is black. I use the mouse to move the slide bar on the right hand side all the way to the top. Now all of the colors of the rainbow appear. I use the mouse to click on a blue color and then select O.K. The windows update for me.

14) I am not satisfied with the image position so I click on the **'Interactive Rotation buttons'** on the **'Tool Palette'** and rotate about the X, Y, and Z axes.

15) I would like to have a colored background. I select **'BCK'** button from the **'Object Palette'** and then click on the colored beneath it to change the color of the background.

17) I like the image a lot so I select **' PICT File'** from the pop-up menu of the **'Output File'** from the **File** menu. I get asked for the file name and then hit o.k. This file can be read by every commercial Mac program including MS Word, MacDraw, and Canvas.

Special Hint

1) With Laser printers, having the electron density maps set to a pixel size of ~0.2-0.5 and the atomic model set to a size of ~2 makes for a nice diagram. However, my program can only do integer value pen thicknesses. For these diagrams I have the ED map and atomic model displayed together I select 'Copy' from the 'Drawing' menu and transfer, via the clipboard, to MacDraw Pro (for example). I hit paste in that program and all of the vectors are drawn to the MacDraw Pro window. While all of the vectors are selected, I hit 'Group' in the MacDraw Pro program. I then go to 'Pens...', create a pensize of 0.25 in the menu, and then select that size for the selected diagram. All of the vectors are now 0.25 pixels. I then window back to MolView II, de-select the ED map in the 'Select' menu, Clear the image in the 'Draw' menu, and then hit 'Copy' in the 'Draw' menu. Now, only the atomic model is drawn. I transfer this image over to MacDraw Pro, hit paste, and group these vectors together as a second object in the MacDraw file. I change the pensize to ~2 within MacDraw Pro. I then carefully position the atomic model (with a pensize of 2) over the appropriate lines of the ED+atomic model object that has a pen size of 0.25. I included the atomic model in the ED map in the first group to align the thicker, atomic model object. Now, when the diagram is printed, the ED map is very nice, fine lines that do not occlude the atomic model, yet clearly display the electron envelope.

2) Be sure to use the new **'User Set Back and Clip'** option under the **'Misc**.' menu before making PICT files or movies to make an identical background for each image.

Input Files:

      The MolView file is a normal ASCII file that is read as free format. The input values are read in the following order.

MolView File:

xmin, xmax, ymin, ymax, zmin, zmax [all floating points]
(the min and max values for the x, y, and z coordinates)

number of atoms, number of vectors in atomic model, number of Mol objects [all integers]

number of vectors in each Mol Object [integers]
(one value per line, one value per Mol object)

X, Y, Z, residue number, residue type, atom type [3 floating point, 1 integer]
(for i=0 to i<number of atoms)

X, Y, Z, action [3 floating point, 1 integer]
(for i=0 to i< number of vectors in atomic model
action =0 for MOVE, and action=1 for DRAW)

X, Y, Z, action [3 floating point, 1 integer]
(for i=0 to i< number of vectors in each Mol Object--
Mol Objects are one right after another)

Number of electron density maps [integer]

Number of electron density vectors [integer]
(for i=0 to i< number of electron density maps
one value per line)

X, Y, Z, action [3 floating point, 1 integer]
(for i=0 to i< number of vectors in each electron density map--
electron density maps are one right after another)

INPUT ChemDraw 3-D files

These files are read in as free format. The only things my program needs are as follows.

natoms (integer value)
atomtype atomnumber x y z (for natoms)

That's all!

Future Plans (?)

1) I have now switched to Metroworks Codewarrior for compiling my program. This alone has fixed most of the PowerMac bugs. I also switched because they promise to support IBM compilation by early 1995. So... those stubborn people that have never tried a Mac (i.e. IBM users) may get MolView sometime this summer.

2) Will soon write options to display crystallographically and non-crystallographically related atoms.

3) May write a 'Movie Script' subroutine to automatically make fancy movies.

4) Will write a routine to compare and structurally align different proteins with similar structural motifs.

5) May write a routine to automatically draw 2-D motif and H-bonding patterns--e.g. to show that a protein has a 'Greek Key' motif and the H-bonding distances drawn out.

6) Will incorporate the new Mac 3-D graphics for surface rendering and to increase speed.