

Section I – Using Jmol as a Computer Visualization Tool

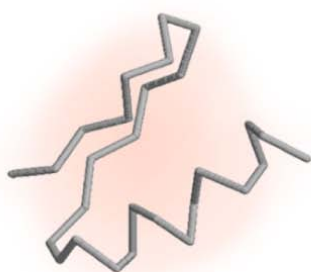
Jmol is a free open source molecular visualization program used by students, educators and researchers to explore protein structure. Section I of this Jmol Training Guide is designed to introduce you to this software. This program is a simple, yet powerful tool, which enables you to visualize a molecule in 3-dimensional space. As you actively manipulate the computer mouse to rotate the molecule, you will develop a sense of the 3-dimensional nature of a protein. Through the Jmol command line, you can also change the display format of the molecule to display different features of the molecule.

At the MSOE Center for BioMolecular Modeling (CBM), we believe that physical models of proteins are powerful tools that can be used synergistically with computer visualization tools to explore protein structure and function. Recent advances in 3-D printing technology make it possible to generate a physical model of any virtual image of a protein generated in the computer environment of Jmol. Therefore, as you learn to generate different images of proteins in Jmol, you will also be designing a physical model of that protein. Welcome to the amazing world of proteins --- and the fascinating stories that each one can tell!

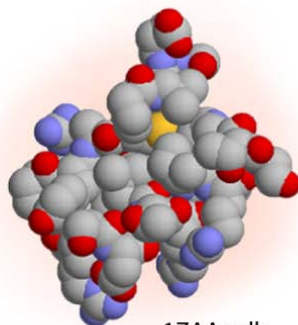
At the end of this section, you should be familiar with how to use Jmol as a computer visualization tool. We will introduce you to the basic features of Jmol, including:

Section 1: Using Jmol as a Computer Visualization Tool

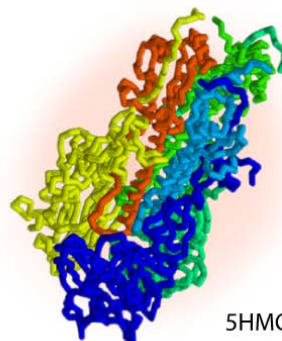
- 1-1 - Downloading Jmol
- 1-2 - Protein Data Bank (PDB) Files
- 1-3 - Launching Jmol and Opening a PDB File
- 1-4 - The Command Line and Common Display Formats and Display Colors
- 1-5 - The Select Command
- 1-6 - Boolean Operators
- 1-7 - Exporting Images
- 1-8 - Saving Your Work and Organizing Files



1ZAA.pdb



1ZAA.pdb



5HMG.pdb

1-1 - Downloading Jmol

- **About Jmol** – Jmol runs on a Java platform and therefore functions equally well in a PC or Mac environment. Because Jmol is freeware and an open source program, it can be obtained from many locations. For total functionality in designing a structure to be built on a 3-D printer, you must use the version 12.0.14 that is available on our website.
- **Downloading Jmol** - We suggest that you download Jmol directly from the CBM website to ensure you are using the correct version for creating physical models.
 - <http://cbm.msoc.edu/stupro/smart/resources.html>
- **Unzipping Jmol** - The program Jmol should download as one zipped folder that will need to be unzipped. Most computers running Microsoft Windows will automatically do this using the program WinZip. If your computer does not have WinZip, you may download the free unzipping software **CAM UnZip**, available at:
 - <http://www.camunzip.com/>
- **Unzipping for Mac** - If you are using a Mac that does not have an unzipping program, you may download the free unzipping software MacZip, available at:
 - http://download.cnet.com/MacZip/3000-2250_4-10025248.html
- **Jmol File Location** – The Jmol folder contains all the files your computer needs to run Jmol, and they need to be kept together in the same folder. You may save this folder in any convenient location on your computer. Jmol does not need to be "installed", so once these files are in place on your computer, the program will be ready to use.

★ When first launching Jmol, you will need to click the "Jmol.jar" file (this will be discussed in more detail in section 1-3). For convenience, it is a good idea to create a shortcut to this "Jmol.jar" file on your desktop as well as in each of your working folders so you can easily launch Jmol. In Windows, right click on the Jmol.jar file and select 'create shortcut'. Drag and drop the shortcut to your desktop.

★ On some PCs, the Jmol.jar file is seen by the computer as a zipped folder. If your computer shows the Jmol.jar file as a zipped file, you can open Jmol by clicking on the Jmol.bat file. Similarly, you can create a shortcut to the Jmol.bat file and save it on your desktop.

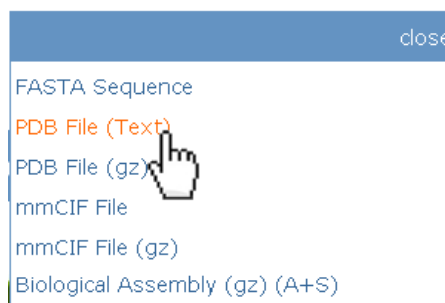
1-2 - Protein Data Bank (PDB) Files

- Molecular structures can be determined through the use of X-ray Crystallography, Nuclear Magnetic Resonance (NMR), or computer algorithm-based calculations.
- Once a structure has been determined, each atom in the structure is assigned an (X,Y,Z) coordinate to mark its location in 3-dimensional space. These coordinates are then stored in a file called a Protein Data Bank (PDB) file.
- Molecular visualization software, such as Jmol, can then use the coordinates stored in a PDB file to create an interactive 3-dimensional visualization of a molecular structure.
- **Downloading PDB Files** - The most common source of free PDB files of macromolecules is the RCSB Protein Data Bank website at <http://www.pdb.org>. For the first section of this Training Guide, we will be using Jmol to view the PDB file 1qys.pdb which contains the atomic coordinates for a single molecule of the protein "Top 7". To download this file from the Protein Data Bank:

- Go to the website <http://www.pdb.org>.
- In the top right corner of the website there is a search bar similar to the image below. Type in the four number/letter file name "1qys" and click the "Search" button.



- This should bring you to the page for "1qys.pdb - Top 7". Just below the search box on the right should be a list of four options similar to the image shown below left. Click "Download Files" and you will see an expanded menu similar to the image shown on the right below.



- Click "**PDB File (Text)**" to begin the download of the PDB file containing the coordinates for Top 7. This file, named "1qys.pdb", can be saved to the location of your choosing on your computer.

★ Note: It is a good idea to create a new folder for each molecule you work on to organize all PDB files, images, and other related work. (See section 1.8 for more information.)

- More detailed information about the Protein Data Bank and PDB files will be discussed within the Jmol Training Guide Part II.

1-3 - Launching Jmol and Opening a PDB File

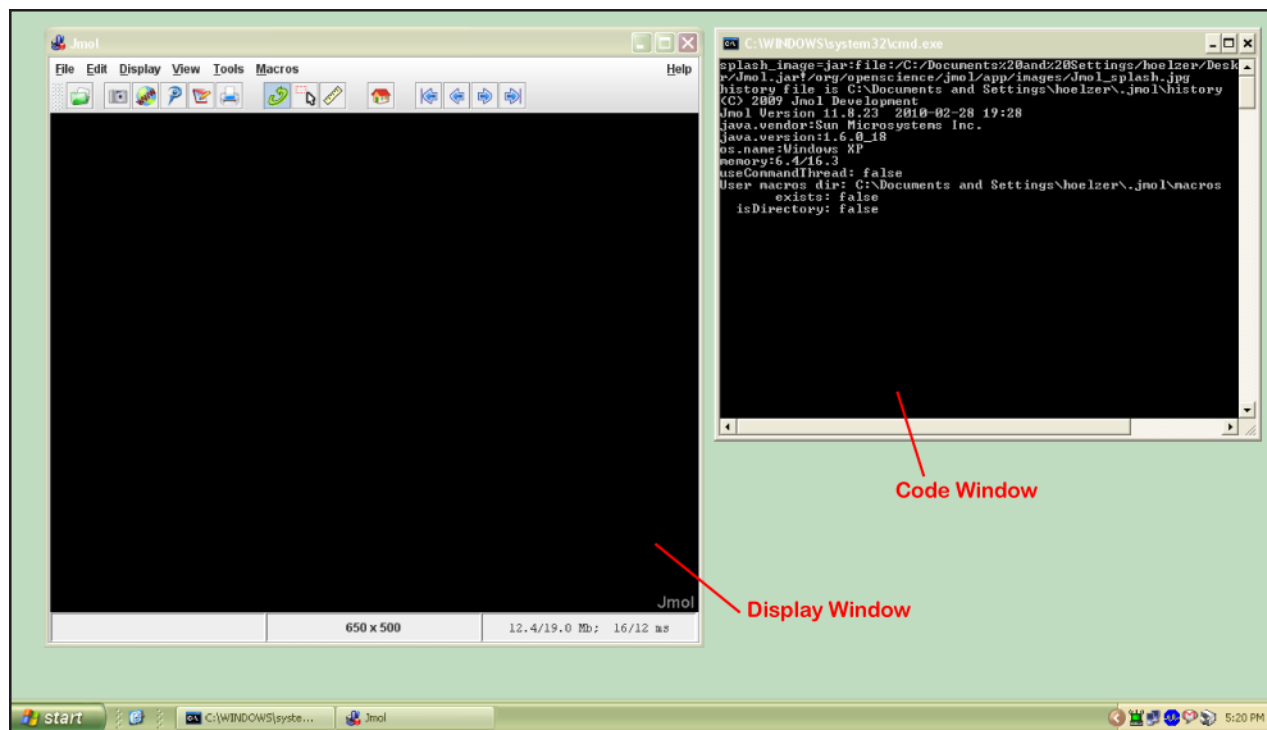
- **Launching Jmol** - To launch Jmol, open the Jmol folder you downloaded and unzipped earlier. In that folder, select the file "Jmol.jar". Note: it should have an icon similar to the image just to the right for PC and far to the right for Mac.



★ When first launching Jmol, you will need to click the "Jmol.jar" file. For convenience, it is a good idea to create a shortcut to this "Jmol.jar" file on your desktop as well as in each of your working folders so you can easily launch Jmol. In Windows, right click on the Jmol.jar file and select 'create shortcut'. Drag and drop the shortcut to your desktop.

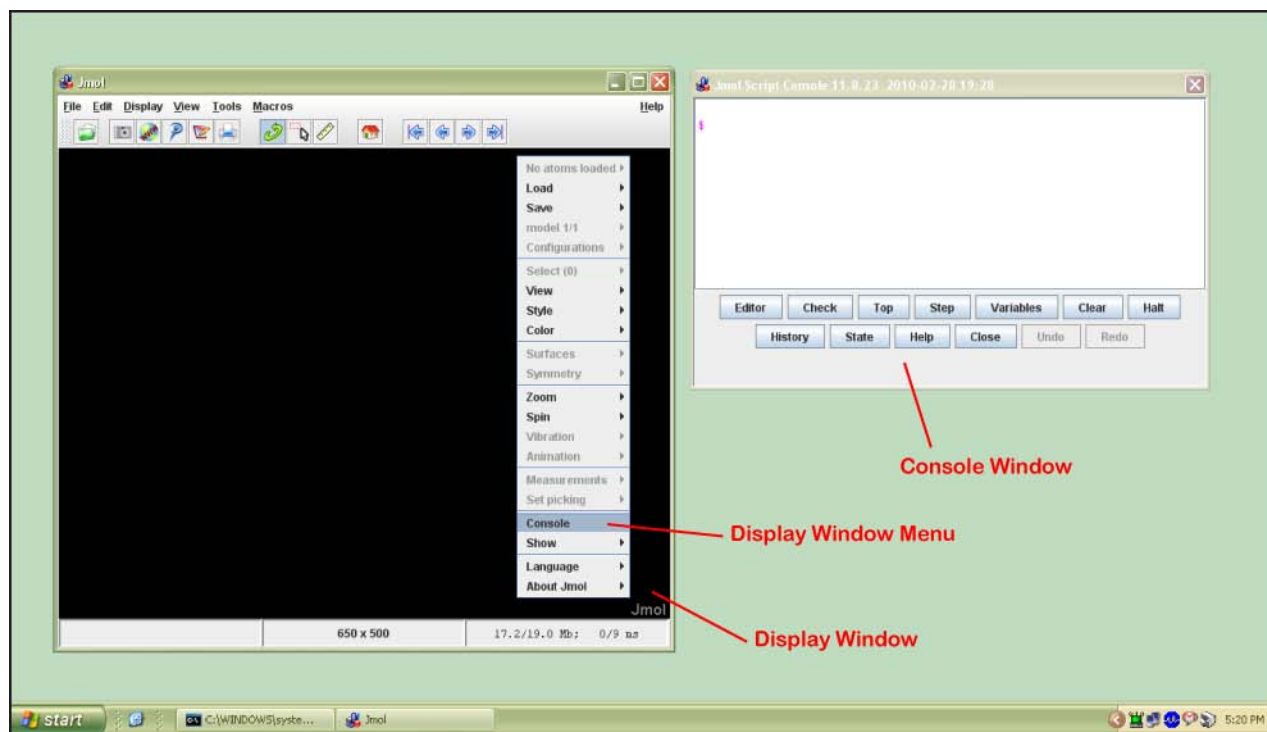
★ On some PCs, the Jmol.jar file is seen by the computer as a zipped folder. If your computer shows the Jmol.jar file as a zipped file, you can open Jmol by clicking on the Jmol.bat file. Similarly, you can create a shortcut to the Jmol.bat file and save it on your desktop.

- **Two Windows** - Once launched, Jmol will display two windows. The Display Window (below, left) is used to view your 3-dimensional images. The Code Window (below right) will not be used in this section of the Training Guide and can be minimized.



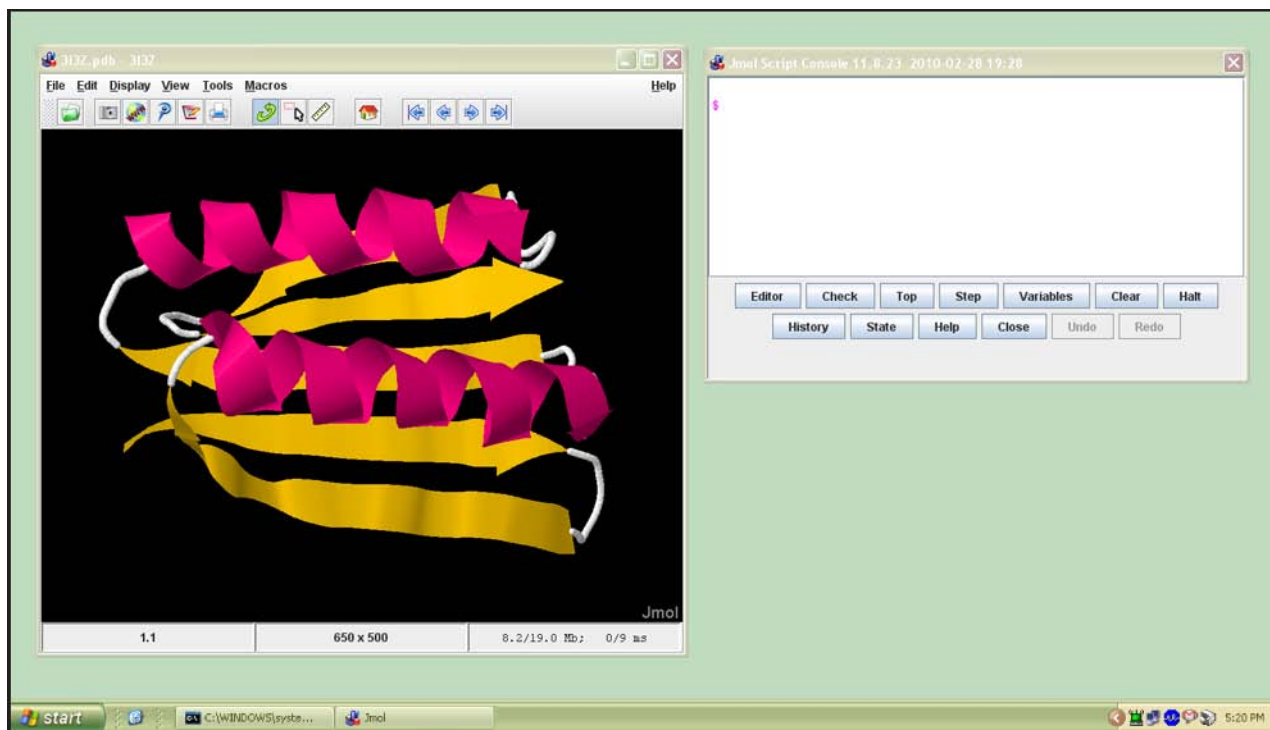
- **The Console** – Right click anywhere in the Display Window to bring up the Display Window Menu. In this menu, click on the button "Console" which will open a new window called the Console Window.

★ Because the Console and Display Windows will almost always be used in unison, arrange the windows so that they do not overlap and both fit comfortably on your screen.

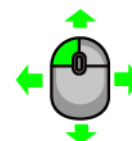


- **Opening a PDB File** - Click on the "File" button located at the top left of the Display Window. From the File Menu, click on the "Open" button.
 - The Jmol Open Menu will appear. For the remainder of this section, the Training Guide will use the protein Top 7 based on the PDB file 1qys.pdb that was downloaded in Section 1.2.
 - Locate the file 1qys.pdb, select it in the Jmol Open Menu, and click the "Open" button in the bottom right corner of the Jmol Open Menu.
 - The default Display Format for a protein opened in Jmol is cartoon format colored by secondary structure. Ligands are displayed with a spacefill and a wireframe while ions or individual water molecules are displayed in full spacefill format.

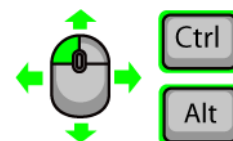
- **Interacting With The Display Window** - Your Jmol Display Window should now display the molecule similar to the image below. You can now rotate, relocate or zoom in on the molecule in the Display Window.



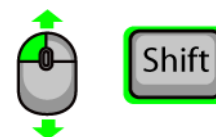
- **Rotating the Molecule** - To rotate the molecule within the X-Y axes on the computer screen, place the mouse cursor in the Display Window, hold down the left mouse button, and move the mouse.



- **Relocate the Molecule** - To relocate the molecule, place the mouse cursor in the Display Window, hold the left mouse button along with CTRL and ALT, and move the mouse.



- **Zoom** - To zoom in or out, place the mouse cursor in the Display Window, hold the left mouse button along with SHIFT, and move the mouse up or down. If the mouse you are using has a center rolling wheel, you can also zoom in and out using this wheel.



- **Barrel Roll** - To barrel roll (rotate the molecule on the Z axis), hold the left mouse button along with SHIFT as if you were going to zoom, but move your mouse left or right instead of up or down.



1-4 - The Command Line and Common Display Formats and Display Colors

- **The Command Line** - If you click in the white area of the Console Window, you will enter the Command Line. This area, highlighted by a magenta dollar sign (\$), is where text commands are entered. After typing a command and hitting enter, the 3-dimensional image of your molecule in the Display Window will change.

★ If you have typed a command incorrectly or the command is not recognized by Jmol, the text in the command line that is normally black will turn red.

- **Different Display Formats** - The first text commands we will explore are the Display Formats. These key terms, when typed into the command line, will let you change the way your molecule is displayed. Below is a description of each of the common Display Formats along with an image of how the Top 7 from 1qys.pdb looks when this command is entered.

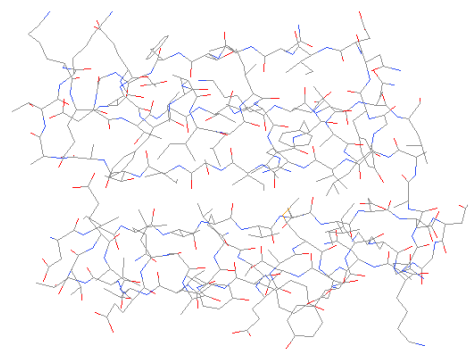
★ To reset the image so your display will match the images below, enter the following commands:

- `color cpk`
- `cartoon off`
- `spacefill off`

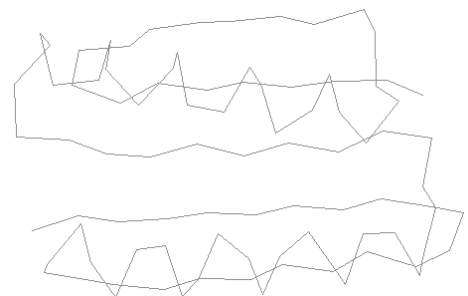
At this point, you should have a blank display window.

- **Wireframe** - The thin wire represents the bonds between atoms and the ends of the wires represent the locations of the atoms. The advantage of the wireframe is that all of the atoms are displayed. However, it is difficult to distinguish secondary structures in this format.

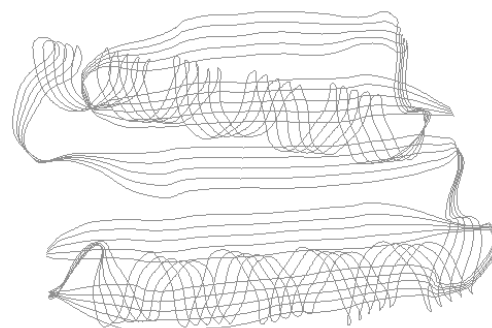
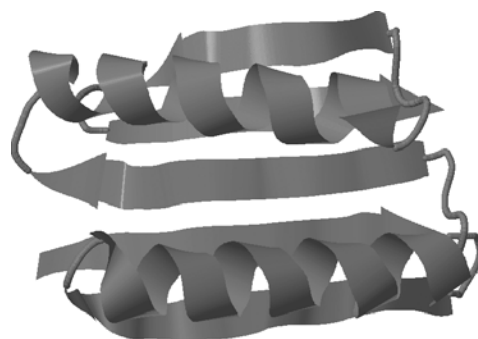
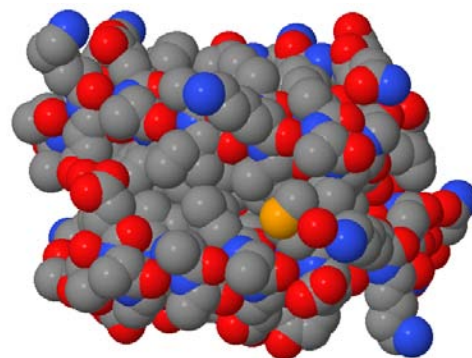
- To turn this format on, type `wireframe on`
- To turn this format off, type `wireframe off`



- **Backbone** - The alpha carbon backbone format only displays the position of the alpha carbon in each amino acid by a bend in the backbone. All of the other atoms within the amino acid are not displayed. The advantage of this display format is that it clearly illustrates the secondary structures within a molecule.



- To turn this format on, type **backbone on**
 - To turn this format off, type **backbone off**
- **Spacefill** - In this format, each atom is displayed as a sphere representing the volume that atom occupies in space. For example, hydrogen atoms are smaller than carbon atoms, which are smaller than sulfur atoms. This format best represents the volume and three-dimensional shape of a molecule. However, identifying the secondary structures or any internal atoms in this display format is challenging.
- To turn this format on, type **spacefill on**
 - To turn this format off, type **spacefill off**
- **Cartoon** - This format shows the molecule as if it were traced with a ribbon. This version may be familiar as it is often seen in textbooks. Secondary structures are easily identified within this format with the alpha helix represented as a coiled structure and the beta strand represented as a pleated structure. The direction of the protein chain can also be identified by arrows at the ends of beta strands.
- To turn this format on, type **cartoon on**
 - To turn this format off, type **cartoon off**
- **Strands** - This format is similar to Cartoon, except that rather than displaying a solid ribbon, there are several “strands” or thin lines that make up the model.
- To turn this format on, type **strands on**
 - To turn this format off, type **strands off**

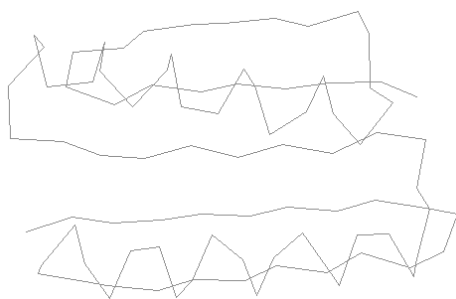


- **Advantages and Disadvantages** - Each of these display options will render your molecule in a different format. Some of these options will look new to you and some of them will look very familiar. Different formats are used for different purposes. Which option you choose to display your molecule depends on the story you wish to tell. The advantage of using Jmol within the classroom is that it enables you to represent the model in a variety of ways, thus illustrating different aspects of the molecule. A summary of the advantages and disadvantages of each format is provided below.

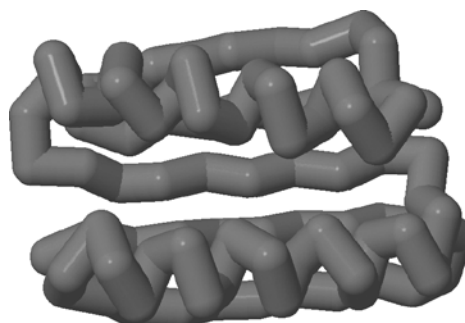
Format	Advantage	Disadvantage
Wireframe	Displays all atoms	Difficult to see secondary structures
Backbone	Secondary structures clearly seen	Detail of amino acids is lost
Spacefill	Represent 3D volume and shape	Cannot identify secondary structures
Ribbons and Strands	Secondary structures are easily visualized	No structural details

★ Note: Ribbons and strands are not used in designing models to be built using 3-D printing. Typically, backbone, wireframe and spacefill formats are used in combination to design a pleasing and informative model for 3-D printing.

- **Altering the Thickness of a Display Format** - Many of the display formats can be further altered by changing the thickness. To do this, simply add a number after any display format typed into the Command Line and then hit ENTER.



backbone on



backbone 1.5

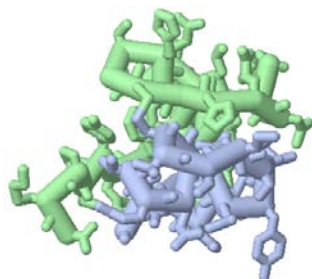
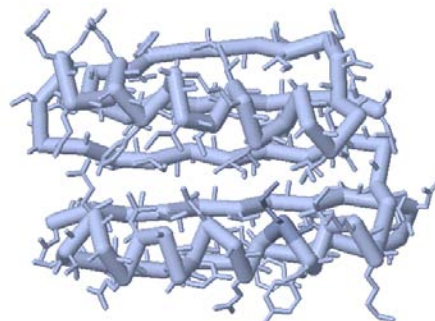
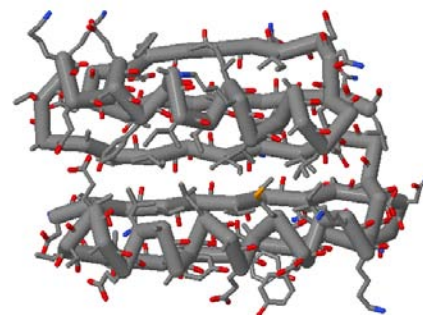
★ Note: The number added after the Display Format must include a decimal. For example, you will need to enter **backbone 1.5** and not simply **backbone 1**. This number represents the thickness you want in Ångströms (1×10^{-10} meters). So if you enter **backbone 1.0**, you will be showing a Display Format with a one Ångström diameter backbone.

★ Note: The standard scale for designing models for 3D printing is **backbone 1.5**.

- **The Different Display Colors** - Jmol has several common Display Color options to make your model look visually pleasing or to indicate specific features of the molecule. Below is a description of each of the Display Colors along with an image of how the Top 7 protein from 1qys.pdb will look with that color scheme.

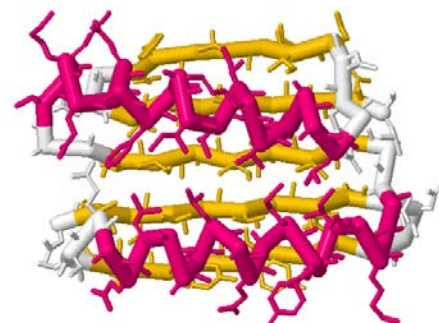
★ To reset the image so your display will match the images below, enter the following commands:

- **backbone 1.0**
- **wireframe 1.0**
- **CPK** - This is the default color scheme used in Jmol and was developed by **C**orey and **P**auling and later improved by **K**ultin. In CPK Color, carbon is gray, hydrogen is white, oxygen is red, nitrogen is blue and sulfur is yellow. This is the standard color code utilized in many textbooks.
 - To turn this color on, type **color CPK**
- **Chain** - If a PDB file has multiple chains (also known as polypeptides), this color option will color each chain a different color.
 - To turn this color on, type **color chain**



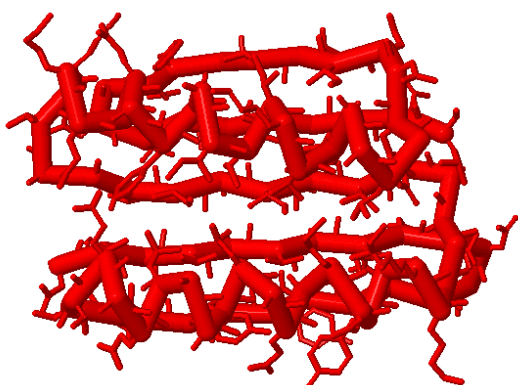
★ Note: The Top 7 protein has only one polypeptide chain and therefore is colored one color when the "color chain" command is used. Many proteins have more than one polypeptide chain and will therefore have more than one color. For example, a molecule of human insulin from the file 3i3z.pdb has two chains and therefore would have two colors.

- **Structure** - This option will color the secondary structures different colors. Magenta is used to highlight helices, yellow to indicate beta sheets, and white for non-structured regions.

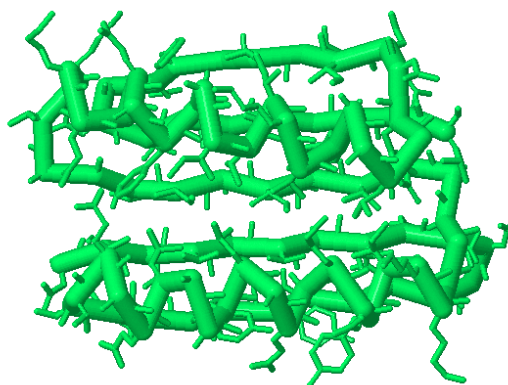


- To turn this color on, type `color structure`

- **Any Color** - This option allows you to color your molecule any solid color. Jmol recognizes a wide range of colors (for specific colors, visit: <http://Jmol.sourceforge.net/jscolors/>), or you can use RGB color codes entered between brackets and separated by commas [R,G,B] to specify a more specific color.

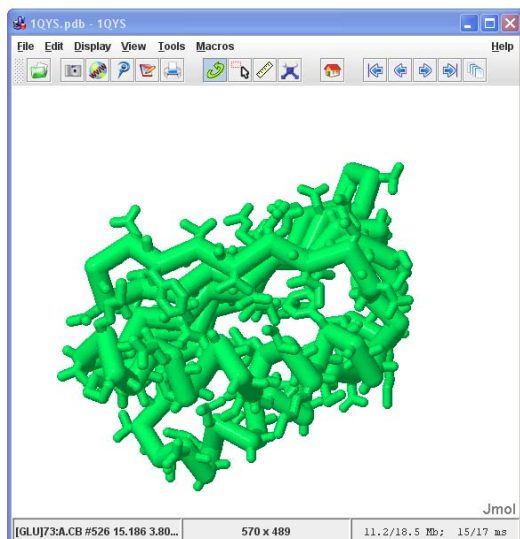


`color red`

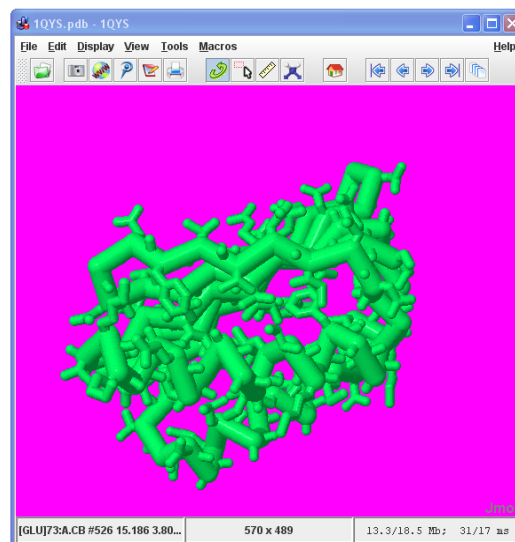


`color [0,255,100]`

- **Background Color of the Display Window** - The default color for the background of the Display Window will be black. This can be modified by using the color background command followed by the color you wish to change the background to.



color background white

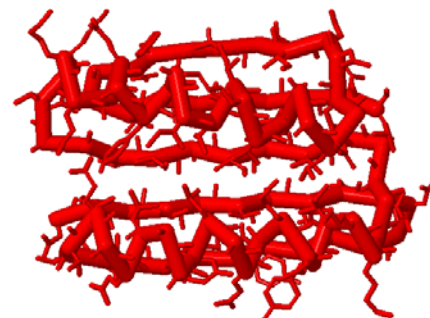


color background magenta

★ Note: We recommend that you avoid the red/green color combination in case you, or others, have problems with color blindness. Bright background colors from a computer monitor are also often hard on the eyes and therefore make it more difficult to focus on the protein. When creating an image for use on a poster, it is best to use a white background.

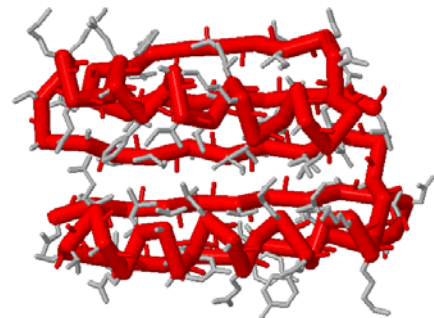
1-5 - The Select Command

- **The Select Command** - Thus far, every command we have typed into the Command Line has affected the entire protein. However, we can specify specific parts of a protein or molecule that we want to have future commands affect by using the Select command. Below is a description of each of the Select Commands along with an image of how the Top 7 from 1qys.pdb will look with the selected area colored red.
 - **All** - Select all is the default Jmol selection. With select all, every atom contained in a PDB file is selected and will be affected by future commands.
 - To select every atom, type `select all`
 - To color this selection green, type `color red`



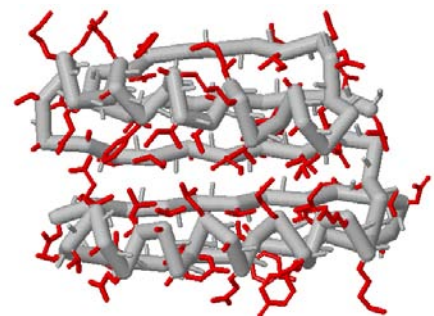
★ Note: The images of Top 7 shown below have been reset for each set of commands. To do this, use the `select all` command followed by `color gray`.

- **Backbone** - With select backbone, only the backbone atoms will be affected by future commands.
 - To select the backbone, type `select backbone`
 - To color this selection red, type `color red`

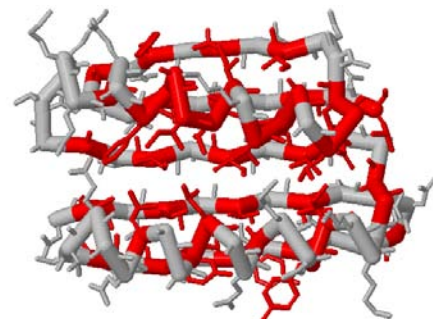


★ Note: The sidechains are not colored red.

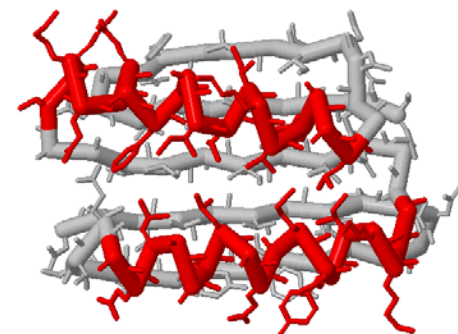
- **Sidechain**- With select sidechain, only the atoms that are part of sidechains in a protein will be affected by future commands.
 - To select the sidechains, type `select sidechain`
 - To color this selection red, type `color red`



- **Hydrophobic** - With select hydrophobic, only the hydrophobic amino acids in a protein will be affected by future commands.
 - To select hydrophobic, type `select hydrophobic`
 - To color this selection red, type `color red`



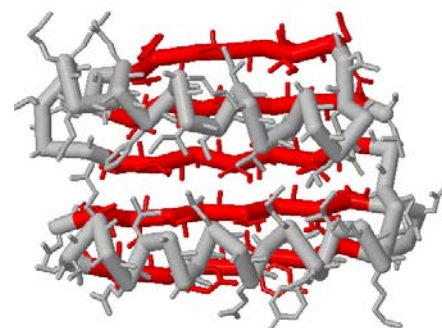
- **Helix** - With select helix, all atoms that are part of alpha helices will be affected by future commands.
 - To select helices, type `select helix`
 - To color this selection red, type `color red`



★ Note: Jmol does not recognize "helices" (plural) but only "helix" (singular).

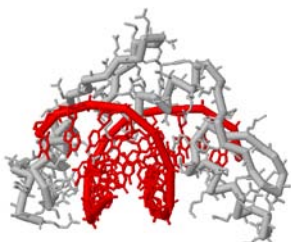
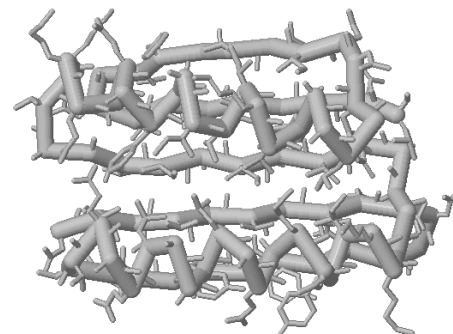
- **Sheet** - With select sheet, all atoms that are part of beta pleated sheets will be affected by future commands.

- To select beta pleated sheets, type `select sheet`
- To color this selection red, type `color red`



- **Nucleic**- With select nucleic, all atoms that are part of nucleic acids (DNA, RNA) will be affected by future commands.

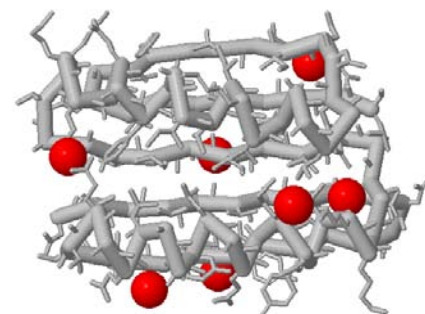
- To select nucleic acids, type `select nucleic`
- To color this selection red, type `color red`



★ Note: The Top 7 protein does not contain any nucleic acids and therefore nothing is colored when the "select nucleic" command is used. A zinc finger protein based on the file 1zaa.pdb does contain nucleic acids and therefore will have areas colored red.

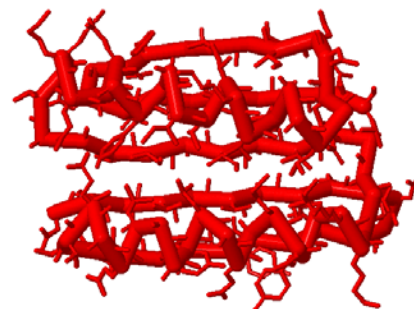
- **Water**- With select water, all water molecules will be affected by future commands.

- To select water molecules, type `select water`
- To display water molecules, type `spacefill`
- To color this selection red, type `color red`

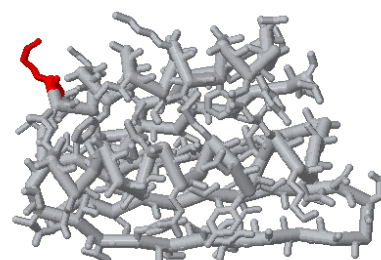


★ Note: Hydrogen atoms are not displayed in pdb files that are obtained via X-ray crystallography. Therefore water molecules appear as a single oxygen atom. Since the oxygen is not visually bonded to another atom, the only way water molecules can be displayed is in spacefill format.

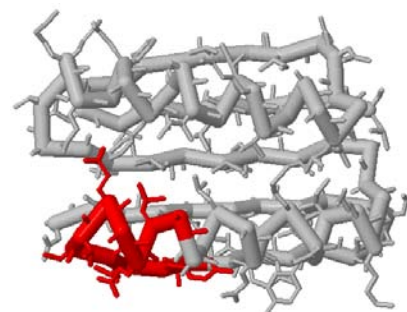
- **Chain-** With select chain * followed by the letter of the chain you would like to select, only the chain you select will be affected by future commands.
 - To select chain A, type `select *a`
 - To color this selection red, type `color red`



- **Residue Number-** With the Residue Number select command, you can select a specific amino acid or a range of amino acids that all future commands will affect.
 - To select residue number 58, type `select 58`
 - To color this selection red, type `color red`

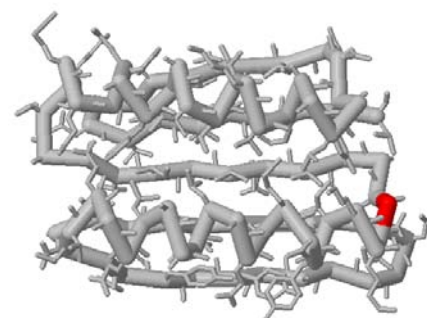


- To select residues 20 through 30, type `select 10-20`
- To color this selection red, type `color red`



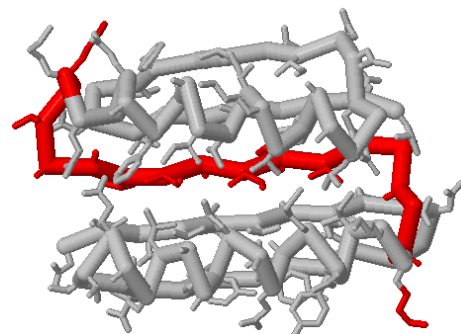
★ Note: You can also select an amino acid by its three letter abbreviation followed by the Residue Number. For example, instead of `select 58` as shown above, you could also use `select lys58` because the amino acid at Residue Number 58 in the Top 7 protein is a Lysine.

- **Atom Number-** With the Atom Number select command, you can select a specific atom number or range of atoms that all future commands will affect.
 - To select atom number 317, type `select atomno=317`
 - To color this selection green, type `color red`



- **Atom Number Range**- With an alteration to the Atom Number select command, you can select a range of atoms that all future commands will affect.

- To select atom number 303-410, type `select atomno>= 303 and atomno<= 410`
- To color this selection green, type `color red`



★ Note: If you do not know the Residue Number, Chain, Amino Acid Type, or the Atom Number you want to select, you can click on the residue in the Display Window. Clicking on an atom will result in information about that atom appearing in the Console Window. The image below explains this information in more detail:

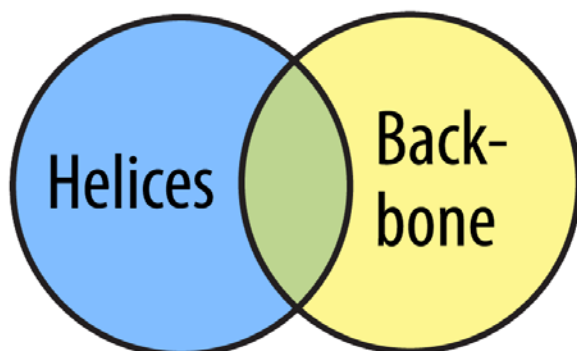
Tyrosine 14

[TYR]14:A:CA#92 - 3.55 - 21.94 - 5.889

- This is the three letter abbreviation for the amino acid residue clicked - in this case, TYR for Tyrosine.
- This is the residue number that will be used with the select command - in this case, 14.
- This letter identifies what chain the clicked residue is on - in this case, A.
- These letters identify what atom type has been clicked - in this case, CA for "Carbon Alpha".
- This number identifies the atom number that has been clicked - in this case, 92.
- These remaining three numbers identify the X,Y,Z coordinates for the atom that has been clicked.

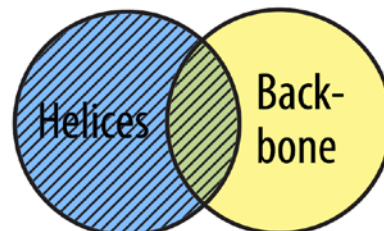
1-6 - Boolean Operators

- Once you are comfortable using the Select Command, you can begin to link together selections by using Boolean Operators. Imagine you are working with two predefined sets, for example, **helix** and **backbone** which are illustrated in the Venn diagram below.



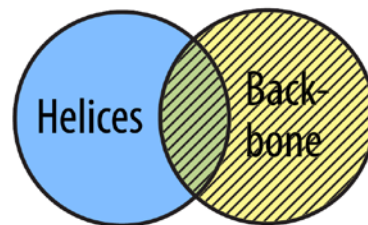
- You can select just the helices. This set includes all the alpha helices (including any backbone atoms that happen to be in alpha helices). The area with the hatched lines represents what is selected.

- `select helix`



- You can also select backbone. This set includes all the atoms that are part of the backbone (including any backbone atoms that also happen to be located in alpha helices).

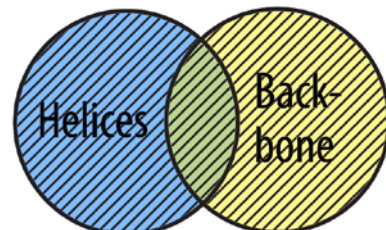
- `select backbone`



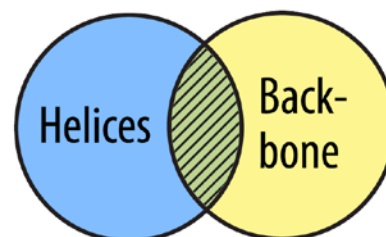
- You can use the **or** Boolean Operator to select all the amino acids that are either part of alpha helices or the atoms that are part of the backbone.

- `select helix or backbone`

- The phrase 'select helix or backbone' means 'select all atoms that are either a helix or in the backbone (or both)'.

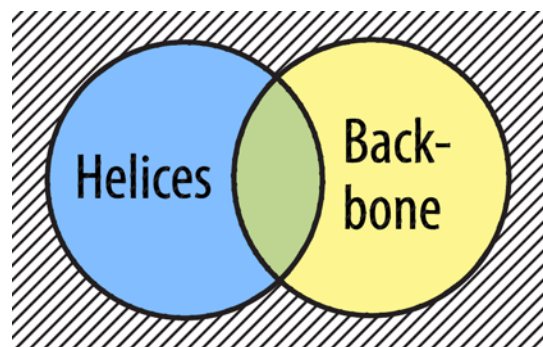


- You can use the **and** Boolean Operator to select all the amino acids that are both backbone amino acids as well as amino acids in alpha helices.



- select helix and backbone**
- The phrase 'select helix and backbone' means 'select all atoms that are both part of a helix AND part of the backbone'.

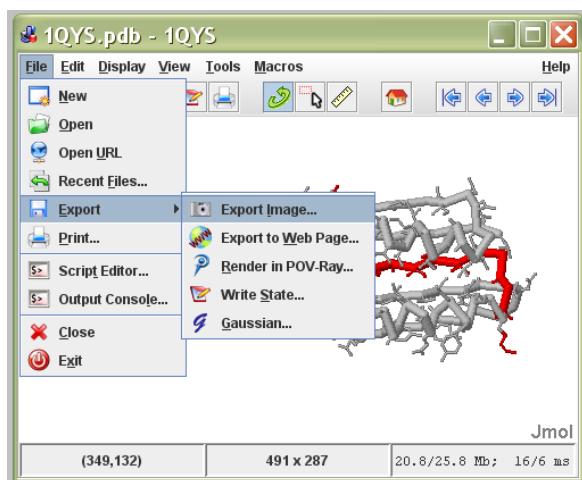
- You can use the **not** Boolean Operator to select only the atoms that are not part of helices and not part of the backbone.



- select not helices and not backbone**
- The phrase 'select not helices and not backbone' means 'select all atoms that are neither a helix nor part of the backbone'.

1-7 - Exporting Images

- Exporting an Image from Jmol** - If you want to create a JPEG image of your molecule from Jmol (to use in a poster, for example), click the "File" menu located on the top left of the Display Window. In the file menu, select "Export" and then "Export Image...".



it

★ Note: It is often a good idea to change your default black background to white to save cost in printing and for a better appearance.

★ Note: Your JPEG image will appear exactly as is displayed in the Jmol Display Window on your screen. The larger the size of your Display Window on the screen, the larger will be the dimensions of the JPEG that is exported.

1-8 - Saving Your Work and Organizing Your Files

- **Saving Your Work** - If you would like to save your work while working in Jmol, you simply export a JPEG file following the exact same directions shown in section 1-7. These JPEG files, even though they appear to be regular images, also contain information on what PDB file you have used and what commands you have entered. We recommend that you save your work frequently using sequential numbers
 - For example: Filename1.jpg
Filename2.jpg
Filename3.jpg

- **Organizing Files** - We recommend that you create a folder for each molecule you are designing. In this folder, place the following files:
 - Shortcut to Jmol
 - PDB file being used
 - All exported JPEG files

★ Note: We recommend the folder organization shown above because, in order for your saved work from your JPEG to load properly, you must have the PDB file and the JPEG file located in the same folder on your computer. When exporting a JPEG to save your work, save your file to this same folder.

- **Loading Your Saved Work** - To load your saved work from the JPEG that you have created, simply drag the JPG from the folder onto the Display Window. This will bring your saved work back up in Jmol.
- **Sending Your Saved Work** - When you are ready to send your saved model design for review or 3D Printing, attach the exported JPEG file to an e-mail. If the PDB file that was used to generate the model design and JPEG is not a standard PDB file available from www.pdb.org, the PDB file will need to be sent as an e-mail attachment as well.