

# Changing Colors and Display Formats

Part of the Jmol Training Guide from the MSOE Center for BioMolecular Modeling

Interactive version available at <http://cbm.msoe.edu/teachingResources/jmol/jmolTraining/colors.html>

## Introduction

One of the most powerful features of Jmol is the ability to completely **customize how your structure is displayed**. Every protein or molecular structure can be visualized in an endless variety of ways, each highlighting different features of the structure. Editing how your structure looks to best represent what you want to communicate is incredibly powerful.

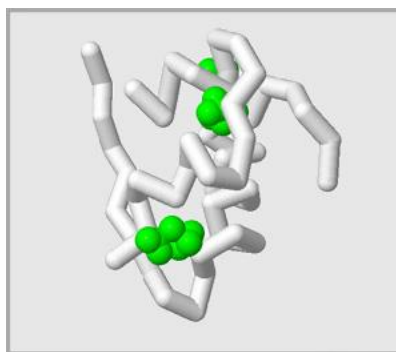
## Examples of Customized Representations in Jmol

Jmol allows users to rotate proteins and molecular structures in a fully interactive 3-dimensional display. Click on the images below to display an **Insulin Protein** in three different ways, each highlighting a different feature of the structure.

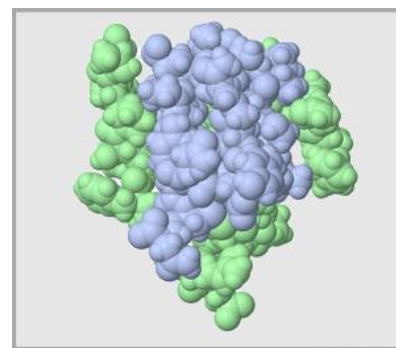
All three of these visualizations are based on the same .pdb file and 3D atomic coordinates, but are very different visually. This is the power of Jmol and molecular visualization!



**Ribbon Format with Secondary Structures** highlights the overall trace and the secondary structures (alpha helices and beta sheets).



**Backbone Format with Cysteine Amino Acids Colored** highlights the three disulfide bonds composed of six cysteine amino acids.



**Spacefill Format with Chains Colored** highlights the overall globular shape of insulin and the interaction of its two protein chains.

## The Console and the Command Line

### The Console

Once launched, Jmol will display two windows. The Jmol **Display Window** is used to view your 3-dimensional protein or molecular structure, and the Jmol **Console** contains the **Command Line**, which will be used to input commands that can alter your display.

**Note** that if you are running Jmol on your desktop and the Jmol Console does not pop up when you open Jmol, 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 the Jmol Console.

If you type a command incorrectly into the command line or the command is not recognized by Jmol, the text in the command line will be **red**. When a correct command is entered, the text will turn **black**.

**Note** that unless otherwise indicated, this section of the Jmol Training Guide uses the protein "**Top 7**" based on the .pdb file [1qys.pdb](#). Please see the "**Getting Started in Jmol**" section of the Jmol Training Guide for information on how to download and open .pdb files.

## Basic Display Formats

The first text commands we will explore are the **Display Formats**. These key commands, when typed into the command line, will change the way the molecule is displayed. Below is a description of each of the common display formats along with a Jmol button to demonstrate the commands using the Jmol display window shown to the right.

All Jmol commands discussed in this Jmol Training Guide will be **shown in orange font**.

## Wireframe Format

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

To turn wireframe on:

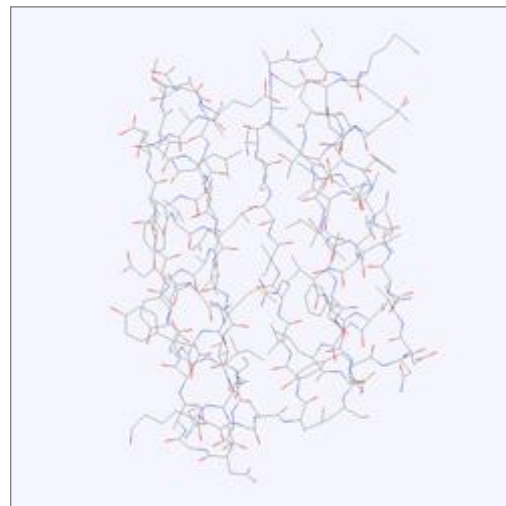
`wireframe on`

To turn wireframe off:

`wireframe off`

To turn all other formats off and turn **only** wireframe on:

`wireframe only`



## Backbone Format

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 backbone on:

`backbone on`

To turn backbone off:

`backbone off`

To turn all other formats off and turn **only** backbone on:

`backbone only`



## Spacefill Format

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 spacefill on:

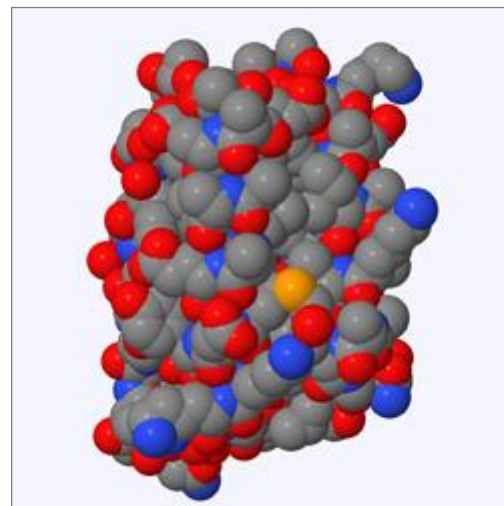
```
spacefill on
```

To turn spacefill off:

```
spacefill off
```

To turn all other formats off and turn only spacefill on:

```
spacefill only
```



## Cartoon Format

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 gently pleated structure. The direction of the protein chain can also be identified by arrows at the ends of beta strands.

To turn cartoon on:

```
cartoon on
```

To turn cartoon off:

```
cartoon off
```

To turn all other formats off and turn only cartoon on:

```
cartoon only
```



## Strands Format

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 strands on:

```
strands on
```

To turn strands off:

```
strands off
```

To turn all other formats off and turn only strands on:

```
strands only
```



## Advanced Display Formats

### Adding Thickness to Display Formats

Many of the display formats can be further altered by changing the **thickness**. To do this, simply add a number after any display format when typing the command into the console.

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 x 10<sup>-10</sup> meters). So if you enter backbone 1.0, you will be showing a Display Format with a one Ångström diameter backbone. Omitting the decimal reverts to a Rasmol scale, in which 1 Ångström = 250 Rasmol units.

**Note** that the standard scale for designing models for 3D printing is **backbone 1.5**. The suggested size used for e-posters and computer visualizations is **backbone 0.9**.

To display wireframe format with a **0.25 angstrom** thickness:

```
wireframe 0.25
```

To display backbone format with a **1.0 angstrom** thickness:

```
backbone 1.0
```

To display spacefill format with a 2.5 angstrom atom diameter:

```
spacefill 2.5
```

To display cartoon format with a 1.5 angstrom thickness:

```
cartoon 1.5
```

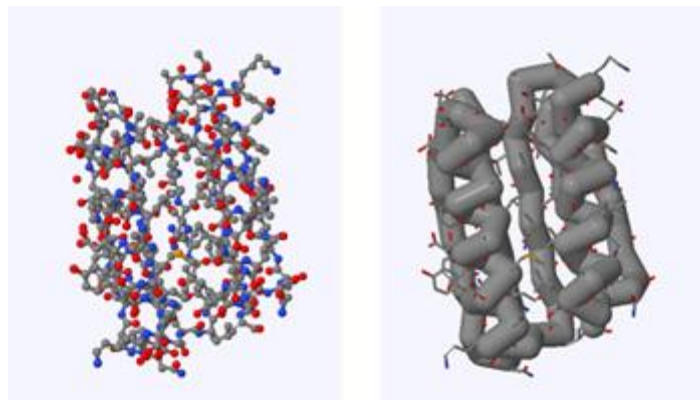
To display strands format with a 0.5 angstrom thickness:

```
strands 0.5
```

## Multiple Display Formats at the Same Time

More than one display format can be turned on at the same time, allowing you to create more complicated molecular representations. Two examples are given below, but they in no way represent all of the possibilities - so experiment on your own as well!

**Note** that when we show two Jmol commands on two separate lines, it implies that you will submit the first command by hitting "enter" or "execute" before entering the second command.



To create a "ball and stick" effect, combine a 0.25 angstrom wireframe with a 0.5 angstrom spacefill

```
wireframe 0.25
```

```
spacefill 0.5
```

To create a highly visible backbone with more subtle sidechains, combine a 0.1 angstrom wireframe with a 1.5 angstrom backbone

```
wireframe 0.2
```

```
backbone 1.5
```

## Pros and Cons of Various Display Formats

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 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** that cartoon and strand formats are generally 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 yet sturdy model for 3-D printing.

## Different Display Colors

Just like the various display formats, the colors for your molecular visualization can be customized. Jmol has a number of 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 the commands needed to apply the color and a Jmol button that will let you see the command demonstrated.

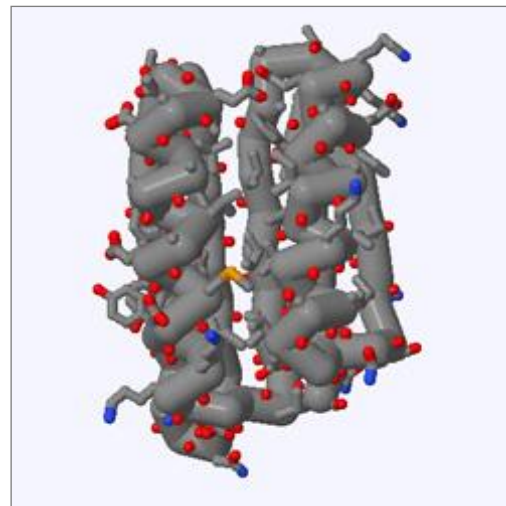
**Note** that for the following color format sections, the Top 7 protein will be shown with a backbone of 1.5 and a wireframe of 0.5.

## CPK

This is one of the default display colors used in Jmol and was developed by Corey and Pauling and later improved by Koltin. In the CPK color scheme, 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. (Many chemistry texts use CPK coloring, except that carbon is black instead of gray.)

To color CPK:

```
color cpk
```



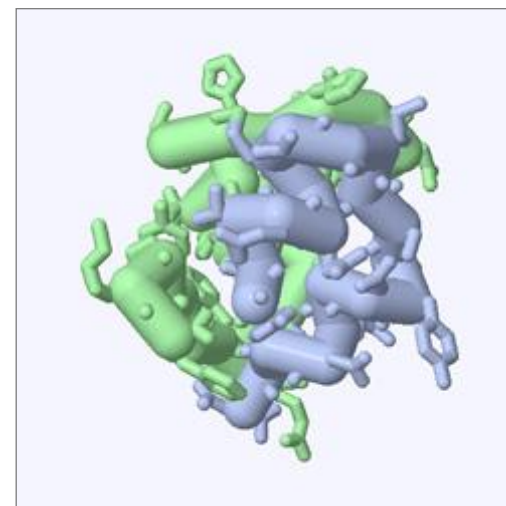
## Chain

If a PDB file has multiple chains (also known as polypeptides), this color option will color each chain a different color. This is often a great way to initially explore a new structure and get a feel for its overall shape.

**Note** that the Top 7 protein has only one 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.

To color by chain:

```
color chain
```



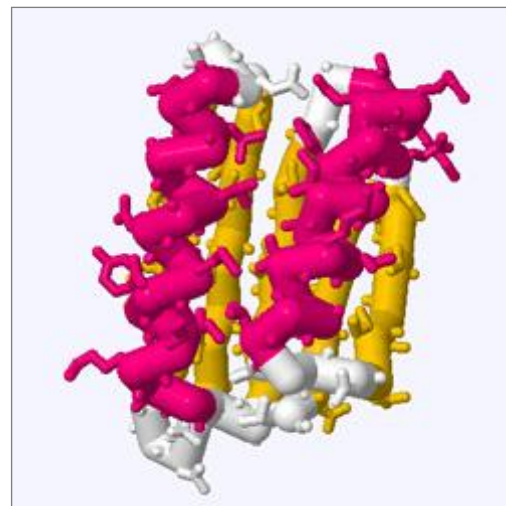


## Structure

This option will color the model based on protein secondary structures. **Magenta** is used to highlight helices, **yellow** to indicate beta sheets, and **white** for loop regions.

To color by secondary structures:

`color structure`

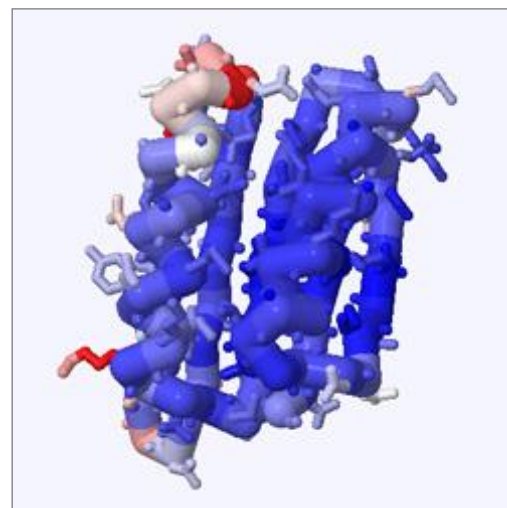


## Temperature

Proteins are flexible, dynamic structures. The arrangement of the atoms within the protein, as captured in a structure file, is much like a still photo. If a particular atom is moving, the electron density is blurred. The B-value or **temperature** factor is a measure of the sharpness or blurriness of the electron density around each atom, and hence, the certainty of the location of that atom in the protein. Low B-values indicate stable atoms and are colored **dark blue**. High B-values indicate moving atoms and are colored **red**. Typically, lower B-values are found in the core of the protein, while higher B-values may be found on the surface of the protein.

To color by temperature:

`color temperature`



## Custom Colors

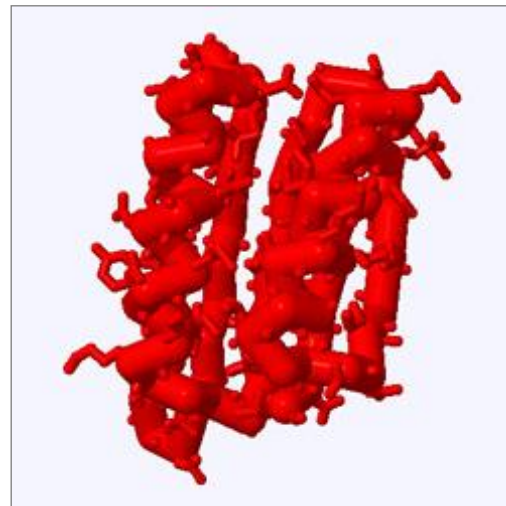
This option allows you to color your molecule any custom solid color. Jmol recognizes a wide range of color by name (such as "red", "blue", and "green"), or you can use RGB color codes entered between brackets and separated by commas [R,G,B] to specify a more specific color. For a complete list of color names, visit the **Source Forge Jmol Color List** (<http://jmol.sourceforge.net/jscolors/>).

To color by color name:

```
color red
```

To color by RGB Value:

```
color [245, 107, 82]
```



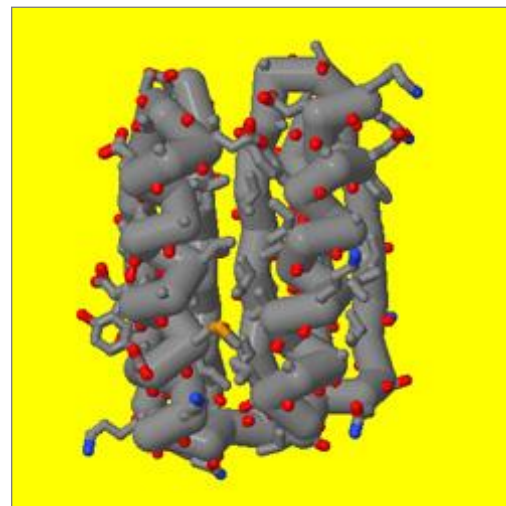
## Coloring the Background of the Display Window

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.

**Note** that 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.

To color the background:

```
color background yellow
```



## Source Forge Jmol Color List

Jmol uses a large range of color schemes and offers a near limitless number of options for coloring your molecular structure. For a complete list of color names and values, visit the **Source Forge Jmol Color List** (<http://jmol.sourceforge.net/jscolors/>).