Adding Sidechains to Your Structure

Part of the Jmol Training Guide from the MSOE Center for BioMolecular Modeling
Interactive version available at http://cbm.msoe.edu/teachingResources/jmol/jmolTraining/sidechains.html

Introduction

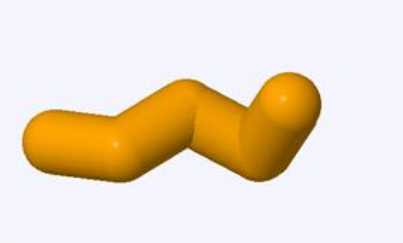
Proteins are long linear sequences of linked amino acids, called polypeptides. These polypeptides fold up into complex 3-dimensional shapes based on the order of their amino acids and the basic chemical properties the amino acids inheritly possess.

Because of this, the specific amino acids in a protein are very important and directly relate to the protein's **structure** (shape) and **function** (job).

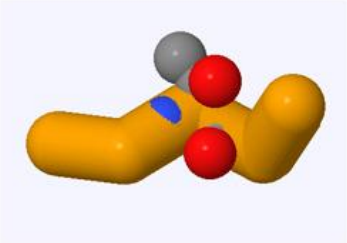
Most protein models designed for **3D Printing** at the MSOE Center for BioMolecular Modeling use **Backbone Format**. In backbone format, only the position of the alpha carbon in each amino acid is shown, representing a bend or kink in the backbone. All of the other atoms within the amino acid are not displayed, including the **Sidechain**, also called the R-Group.

Sometimes you may wish to display an amino acid's sidechain because it is crucially important to telling the story of your protein, such as a sidechain that binds to a substrate or other ligand, even if the rest of your protein structure remains represented in backbone format.

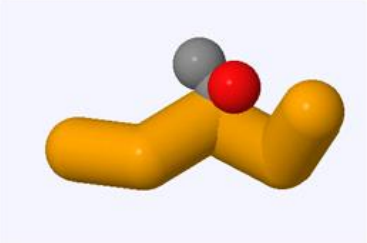
If the interaction only involves sidechain atoms, your model will be less cluttered and more aesthetically pleasing if you do not display the backbone atoms. If these backbone atoms are represented on top of the backbone format, they often poke through the backbone and look like small **bumps**. The amino nitrogen and carbonyl oxygen backbone atoms will protrude from your smooth alpha carbon backbone format. Unless the backbone atoms of the amino acid play a specific role in the story you are telling, you will want to avoid a bumpy backbone.



Section of alpha carbon backbone with no additional atoms shown



Section of alpha carbon backbone with **bumpy backbone atoms** and sidechain shown



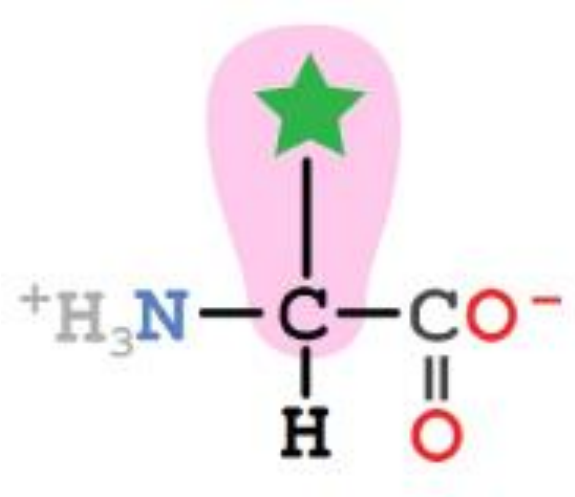
Section of alpha carbon backbone with **clean sidechain** shown

In this section, we will use **Boolean Operators** to select just the atoms in the sidechain and display only these atoms. Please see **The Select Command and Boolean Operators** section of the Jmol Training Guide for a basic introduction to boolean logic in Jmol.

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.

And (Sidechain or Alpha)

To select and display only the atoms of the sidechain of a specific amino acid, and not the "bumpy" backbone atoms, you will use the select command followed by the amino acid name/number and end with the and (sidechain or alpha) command.



This command selects a specific single amino acid, but also limits the selected atoms in that amino acid to the **sidechain** atoms and the **alpha carbon** atom of the backbone, as shown in **magenta** in the figure to the right. It is important to select the alpha carbon atom in addition to the sidechain atoms because this will attach the sidechain atoms to the backbone. Without the alpha carbon being selected, the sidechain would 3D Print as a separate unit from the rest of the protein!

An example of the commands needed to create a "clean" sidechain are shown below.

To add a clean sidechain for Tyrosine 39 in the protein Top 7:

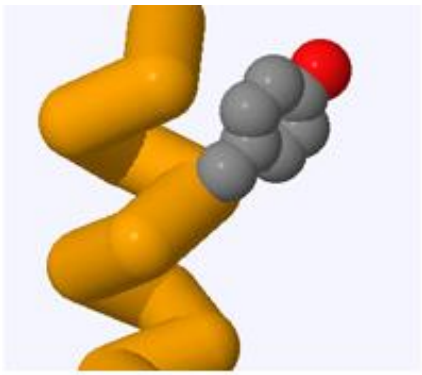
```
select tyr39 and (sidechain or alpha)
spacefill 1.25
wireframe 1.0
```

Note that the alpha carbon backbone format in this display has been colored orange to make the tyrosine sidechain more visible and easily identifiable.

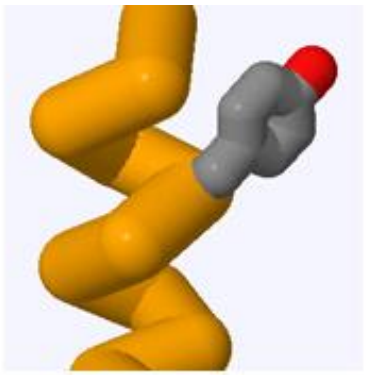
Sidechain Formats

The two commands used to add the "clean sidechain" in the example above (`spacefill 1.25` and `wireframe 1.0`) will generate a "ball and stick" appearance. Even if you don't visually see the wireframe format, if you enter just the spacefill command, the atoms will only be displayed as little spheres that may not be securely connected to one another. Adding the wireframe will ensure that the sidechain builds soundly. You can also enter just the wireframe command and create a "sticks" appearance. We suggest a minimum wireframe size of 1.0 angstroms if you are designing a model for 3D Printing. This will help guarentee that the sidechain builds soundly.

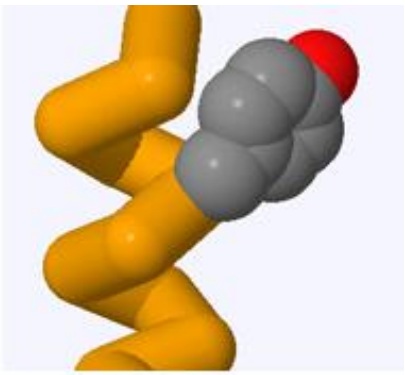
There are also times where a larger spacefill representation of your sidechain atoms would help best tell the story of your molecular structure. Any spacefill above 1.25 angstroms that compliments a wireframe of 1.0 should build soundly.



```
spacefill 1.25
wireframe 1.0
```



```
wireframe 1.0
```



```
spacefill 2.5
wireframe 1.0
```

Displaying Backbone Atoms

Occasionally you'll want to display a backbone atom that is important to your protein's molecular story. In this case, it is acceptable to show the corresponding backbone atom(s). For example, in a potassium channel, the carbonyl oxygen atoms of the amino acid backbones that form the pore in the channel are intigral to the smooth flow of potassium.

To display a backbone atom:

1. Identify the atom number of the particular backbone atom you want to display. You can do this by selecting the entire amino acid and displaying all of the atoms in that amino acid with a spacefill of 1.25.
2. Click on the atom you want to display. Clicking on an atom will show you information about that atom in the **Console**, including the **Atom Number**.
3. Turn the spacefill off on the whole amino acid.
4. Select only the atom number of the backbone atom you want to display and turn the spacefill on. This will now onlyl effect the single atom you have selected.

In the example shown below, the goal is to show and color magenta the carbonyl oxygen atom in the backbone of tyrosine 39.

```
select tyr39
spacefill 1.25
Click on the backbone atom you want to highlight to get the atom number.
spacefill off
select atomno=272
spacefill 1.25
```

Note that the spacefill command uses a larger value than normal so that the atom will protrude from the backbone. You may adjust the spacefill value from 1.25 to 1.6 to determine the size that best displays the backbone atom.