

Bonds and Structural Supports

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

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

Introduction

In addition to covalent bonds between atoms in a molecule, Jmol has the ability to render **Hydrogen Bonds**. These bonds can be shown in a variety of colors and often help highlight the rigidity of secondary structures (specifically, beta pleated sheets) as well as help physically support a model that will be **3D Printed**. Similarly, **Disulfide Bonds** between interacting **Cysteine** amino acids can also be added.

For models that are to be 3D Printed, additional structural supports will most likely also be needed. These **Struts** will not necessarily represent any specific molecular bond or chemical feature, but are simply necessary to produce a solid and stable physical model using 3D printing.

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.

Hydrogen Bonds

Hydrogen bonds (referred to as **hbonds** in Jmol) are essential to the stability of secondary structures in a protein. They form between the backbone oxygen of one amino acid and the backbone nitrogen in a second amino acid.

Adding Hydrogen Bonds

To add hydrogen bonds to secondary structures within your model, you will use the **calculate hbonds** command. We suggest that you typically do not add hydrogen bonds to alpha helices, since they do not add

stability to the model and actually clutter the view of the structure. Adding hydrogen bonds to **beta sheets**, however, provides additional support for the final model and is recommended.

To turn hydrogen bonds on in beta sheets:

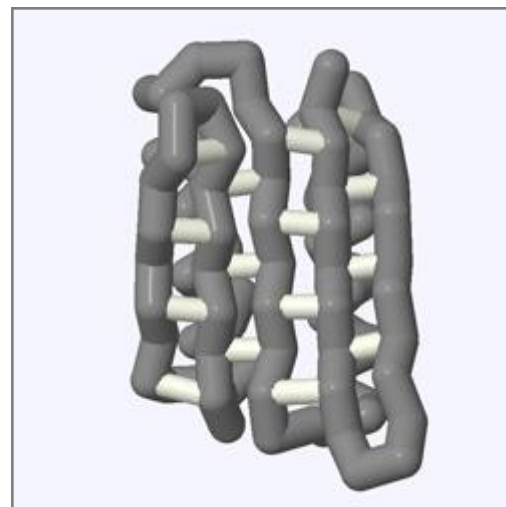
```
select sheet  
calculate hbonds
```

Formatting Hydrogen Bonds

Hydrogen bonds, like wireframe, backbone, and spacefill, can be **thickened** by placing a number after the hbonds command. The standard size we suggest for building a physical model using 3D printing is **1.0 Ångströms**.

The default display for hydrogen bonds is a dashed line. You will need to change this into a solid cylinder for building a physical protein model using 3D printing. You can do this using the **set hbonds solid** command.

By default, hydrogen bonds in Jmol are initially shown to connect the oxygen atom in one amino acid to the nitrogen atom in the second amino acids. However, if you are representing you protein with **backbone format**, these oxygen and nitrogen atoms are now visible and the hydrogen atoms appear to be floating in air. You can move the hydrogen bonds to the alpha carbon using the **set hbonds backbone** command.



Hydrogen bonds can also be colored using the same **color** command and color formats as other areas in a molecular structure. We suggest that you use a subtle color for your hydrogen bonds so they are not visually distracting or overwhelming.

To format your hydrogen bonds:

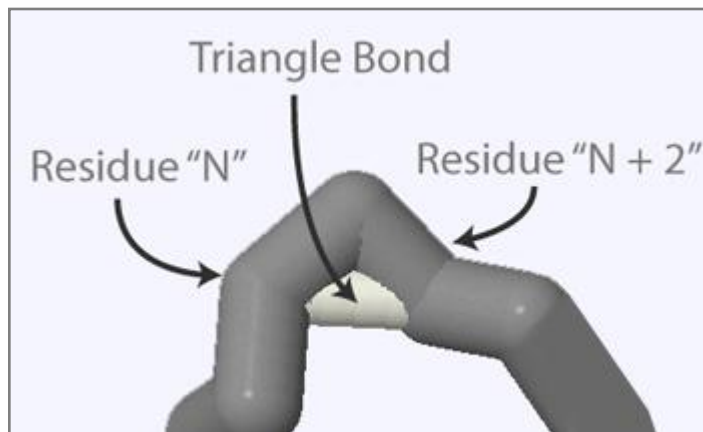
```
hbonds 1.0  
set hbonds solid  
set hbonds backbone  
color hbonds ivory
```

Note that Jmol recognizes both **hbonds** and **hbond** when entering commands. Also note that all of the commands demonstrated above will only affect hydrogen bonds in the currently selected area of the molecular structure.

Editing Hydrogen Bonds

If you use `hbonds off` command, the hydrogen bonds in the currently selected area of the structure will be turned off. To remove just a single hydrogen bond, select only the two amino acids that the hydrogen bond connects and then use the `hbonds off` command.

When Jmol calculates hydrogen bonds, it occasionally inserts a hydrogen bond between two amino acids on the same strand, with a single amino acid between the two. These types of hydrogen bonds create what almost looks like a triangle between two kinks of the alpha carbon backbone and are therefore referred to as **triangle bonds**. For aesthetic reasons, we suggest that triangle bonds be identified and removed from your structure.



If the first amino acid connected by the triangle bond is residue number **N**, then the second amino acid connected by the hydrogen bond is residue number **N + 2**. So to remove a triangle bond, you will need to select two amino acids that have just one amino acid in between them.

To remove a triangle bond that connects amino acid 201 and 203:

```
select 201 or 203  
hbond off
```

Note that before searching for triangle bonds, we suggest you save your model design. You will not want to lose your work if you make a mistake!

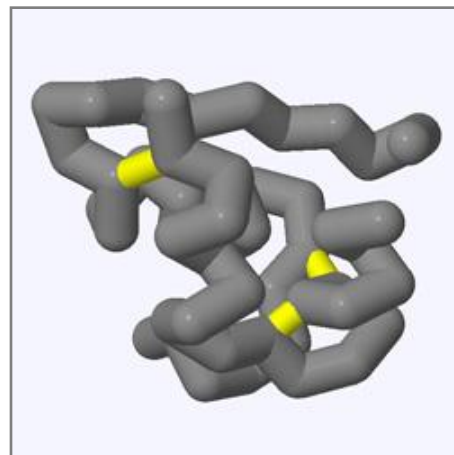
Disulfide Bonds

Some molecules will have **disulfide bonds** (referred to as "ssbonds" in Jmol) that form between two **cysteine amino acids** that lie close to each other in a protein structure.

The basic commands used to add and format a disulfide bond are in essentially the same commands used to add and format hydrogen bonds.

Disulfide bonds form between the two **sulfur atoms** in two **cysteine amino acid sidechains**. Therefore, added disulfide bonds will appear to float if you are only representing your protein with **backbone format**. Similar to hydrogen bonds, you can move the disulfide bonds to the alpha carbon using the **set ssbond backbone** command. If you do choose to display the cysteine amino acid sidechains, you can return the ssbonds to their default position using the **set ssbond sidechain** command.

Note that not every protein structure will have disulfide bonds. Since the Top 7 protein does not have any disulfide bonds, these commands will be demonstrated on a molecule of human insulin from the file 3i3z.pdb.



To add and format disulfide bonds:

```
ssbonds 1.0  
set ssbonds solid  
set ssbonds backbone  
color ssbonds yellow
```

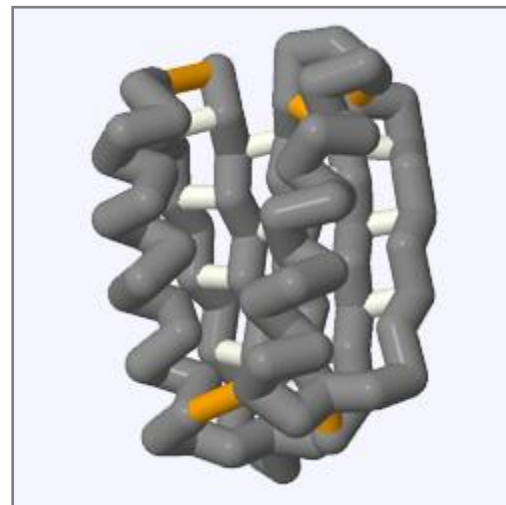
Note that Jmol recognizes both **hbonds** and **hbond** when entering commands. Also note that all of the commands demonstrated above will only affect hydrogen bonds in the currently selected area of the molecular structure.

Struts

Adding and Formatting Struts

When a model is built on a 3D printer, additional support struts are added within the model to provide stability and durability. Struts can be automatically added using the **calculate struts** command.

This command will only add struts to the currently selected area of a molecular structure. If you have already added hydrogen bonds to your beta sheets, you will not need to add struts to the beta sheets and would therefore want to use the **select not sheets** command before adding struts.



Alternatively, you could initially add struts to the entire structure and then remove them from the beta sheets using the `select sheets` command followed by the `connect strut delete` command, which will turn the struts in the selected area off.

The basic commands used to format a strut are also essentially the same commands used to format a hydrogen bond or disulfide bond.

To add struts to everything except the beta sheets:

```
select not sheet
calculate struts
strut 1.0
color strut orange
```

or

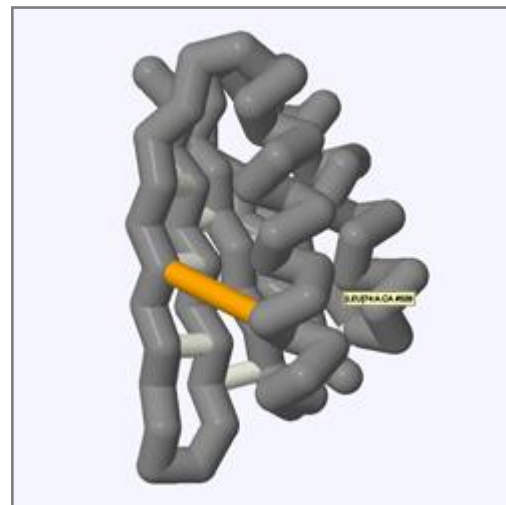
```
select all
calculate struts
select sheets
connect strut delete
strut 1.0
color strut orange
```

Note that Jmol recognizes both `struts` and `strut` when entering commands. Also, the `calculate struts` command will not connect ligands, nucleic acids (DNA and RNA) or ions, and only works on protein chains.

Adding and Removing Individual Struts

Like hydrogen bonds and disulfide bonds, the `strut` commands will only effect areas of the molecular structure that are selected. At times you may want to edit just a single strut (for example, if it goes through a sidechain you have represented). To do this, you will need to select only the two atoms that the strut connects.

Begin by clicking on the two atoms in the **Jmol display window** to identify which two atoms are connected by the strut. Then select only those two atoms using the `select atomno=` command. Then use the `connect strut` command to add the strut. Finally, use the `strut 1.0` command to add a strut or the `connect strut delete` command to remove the bond between the two selected atoms.



Note that you need to have both atoms that a strut connects to selected for these commands to work. You can edit the colors of individual struts using this same technique.

To add and format disulfide bonds:

```
select atomno=120 or atomno=270
connect strut
strut 1.0
color strut orange
```

Adding Struts with the Mouse

The default functionality for left-clicking with the mouse in the **Jmol display window** is to give you feedback about what you clicked such as the atom number, atom type, or residue number. However, you can change this functionality so that left-clicking with the mouse will add struts between two atoms that are clicked on in succession.

To do this, use the **set picking strut** command. You can then click on any two atoms to connect them with a strut. To delete a strut adding with this technique, you will have to click on the two atoms in succession again.

To return left-clicking to its default functionality, use the **set picking ident** command (short for "identification"). You can then click on any atom to get information about it again.

Note that this technique can save you a lot of time when adding struts but is also difficult to master, often resulting in accidental struts that can be difficult to remove. It is highly recommended that you save your work before attempting to add struts using this technique.