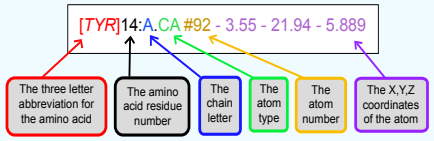
MSOE Center For BioMolecular Modeling - Jmol Quick Reference Sheet

Center for BioMolecular Modeling

Mouse Movements

Clicking on an atom provides information in the console window. This information is explained in detail below.



Rotate on the X-Y axes:

Zoom in and out: Shift

Translate the Molecule: Ctrl Alt

Rotate on the Z axis: Shift

Display Formats

wireframe *(displays stick bonds)*
wireframe <value> *(displays stick bonds with specific thickness)*
example: `wireframe 1.0`

spacefill *(displays atoms as spheres with atom radii equal to their Van der Waals radius)*
example: `spacefill`
spacefill <value> *(displays atoms as spheres with specific radius)*
example: `spacefill 1.25`

backbone *(displays alpha carbon backbone)*
backbone <value> *(displays backbone with specific thickness)*
example: `backbone 1.5`

Exporting Images and Saving

To export a Jpeg file, click File>Export>Export Image from the top left of the display window.

An exported Jpeg file (.jpg) contains the information for both an image of your model as it appears in the display window at the time of exporting, as well as a record of your current state or progress.

To load your past progress using the saved information in an exported Jpeg file, drag the saved Jpeg file into the Jmol Display Window. This will automatically load your saved state or progress.

*Note: The Jpeg file must be located in the same folder as the PDB file that it uses in order to load correctly.

Color Formats

Method 1: select <selection type>
color <color name>
example:
```
select hydrophobic
color yellow
```

Method 2: color <selection type>
color <code[R,G,B]>
example:
```
select helix
color [15,255,110]
```

Default color mode: `color CPK`
Color secondary structures: `color structure`

For a full list of the predefined colors available in Jmol, visit: http://jmol.sourceforge.net/jscolors/

Selection and Restriction

select <selection type> *(selects part of the file)*
example: `select helix`

restrict <selection type> *(removes the display of everything except what was restricted)*
example: `restrict water`

List of Common Selection Types:

backbone	sidechain	hydrophobic
hydrophilic	charged	hetero
water	nucleic	protein
helix	sheet	

`*<letter>` *(for selecting by chain letter)*
`<number>` *(for selecting by residue number)*
`<number>-<number>` *(for selecting by residue range)*
`atomno=<number>` *(for selecting by atom number)*
`atomno>=<number> and atomno<=<number>` *(for selecting by atom range)*
`<atom type>` *(for selecting by atom type)*

Standard Sizes for SMART Team Models

backbone 1.5	hbond 1.0
wireframe 1.0	strut 1.0
spacefill 1.25	ssbond 1.0

Bonds and Struts

Hydrogen Bonds:

`calculate hbonds` *(adds hydrogen bonds to all selected areas)*
`hbonds off` *(removes all hydrogen bonds in a selected area)*
`hbonds <number>` *(displays hydrogen bonds with specific thickness)*
`color hbonds <color>` *(colors hydrogen bonds)*
`set hbonds solid` *(displays hydrogen bonds as solid lines)*
`set hbonds backbone` *(connects hydrogen bonds to the alpha carbon)*
`set hbonds sidechain` *(connects hydrogen bonds to the nitrogen and oxygen atoms)*

To add or remove a single hbond, select only the two **amino acids** that that the hbond connects and use the `hbonds 1.0` or `hbonds off` command

example:
```
select 716 or 1341
hbonds 1.0
```
example:
```
select 14 or 342
hbonds off
```

Disulfide Bonds:

`ssbonds on` *(adds disulfide bonds to all selected areas)*
`ssbonds off` *(removes disulfide bonds)*
`ssbonds <number>` *(displays with specific thickness)*
`color ssbonds <color>` *(colors disulfide bonds)*
`set ssbonds backbone` *(connects disulfide bonds to the alpha carbon)*
`set ssbonds sidechain` *(connects disulfide bonds to the nitrogen and oxygen atoms)*

To add or remove a single ssbond, select only the two **amino acids** that that the ssbond connects and use the `ssbonds 1.0` or `ssbonds off` command

example:
```
select 716 or 1341
ssbonds 1.0
```
example:
```
select 14 or 342
ssbonds off
```

Struts:

`calculate struts` *(adds structural supports called struts to all selected protein areas)*
`struts off` *(removes struts)*
`struts <number>` *(displays with specific thickness)*
`color struts <color>` *(colors struts)*

To add or remove a single strut, select only the two atoms that that the strut connects and use the `strut` or `strut off` command

example:
```
select atomno=716 or atomno=1341
connect strut
strut 1.0
```
example:
```
select atomno=14 or atomno=342
connect strut delete
```

Adding a "Clean" Sidechain:

To select and display only the atoms of the sidechain of a specific amino acid, you want to use the `select` command followed by the amino acid name/number and end with the `and (sidechain or alpha)` text.

```
select cys30 and (sidechain or alpha)
spacefill 1.25
wireframe 1.0
```

To remove an incorrectly displayed sidechain:

```
select cys30
spacefill off
wireframe off
```

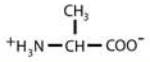
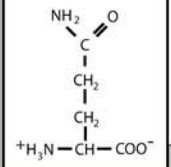
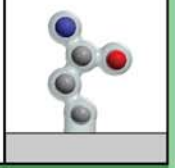
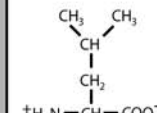
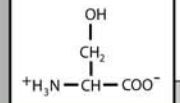
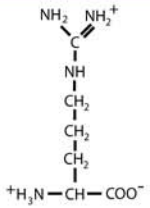
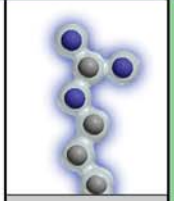
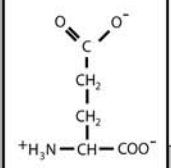
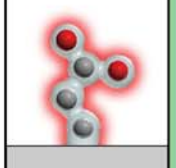
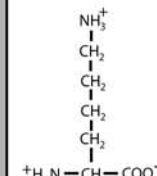
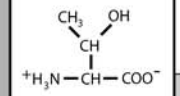
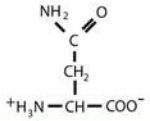
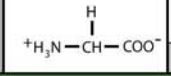
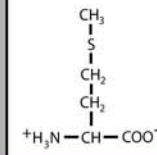
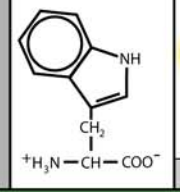
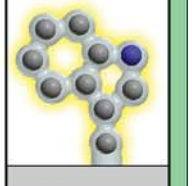
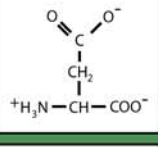
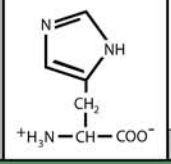
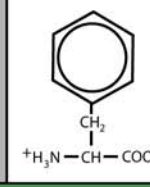
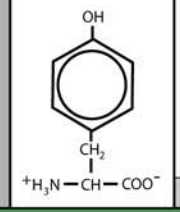
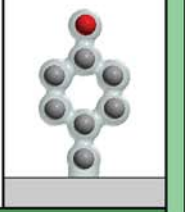
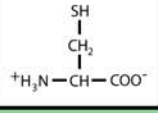
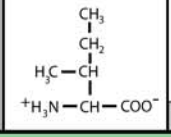
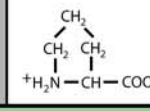
Additional Resources:

General Protein Structure:
http://cbm.msoe.edu/stupro/so/ProteinStructure.html
Official Jmol Command Database:
http://jmol.sourceforge.net
CBM Jmol Training Guide E-book
http://cbm.msoe.edu/teachRes/jmol/trainingguide/
RSCB Protein Data Bank
http://www.pdb.org
Jmol Wiki Page
http://wiki.jmol.org/index.php/

version 1.0

Amino Acid Sidechain List

Dual Color Scheme:
1. Color of amino acid name and sidechain shading indicate: hydrophobic amino acids (yellow); hydrophilic non-charged amino acids (white); positive charged amino acids (blue); negative charged amino acids (red); cysteine (green).
2. Atom type indicates carbon (gray), oxygen (red), nitrogen (blue) and sulfur (yellow).

Name	Amino Acid	Sidechain	Name	Amino Acid	Sidechain	Name	Amino Acid	Sidechain	Name	Amino Acid	Sidechain
Alanine Ala A			Glutamine Gln Q			Leucine Leu L			Serine Ser S		
Arginine Arg R			Glutamic Acid Glu E			Lysine Lys K			Threonine Thr T		
Asparagine Asn N			Glycine Gly G			Methionine Met M			Tryptophan Trp W		
Aspartic Acid Asp D			Histidine His H			Phenylalanine Phe F			Tyrosine Tyr Y		
Cysteine Cys C			Isoleucine Ile I			Proline Pro P			Valine Val V