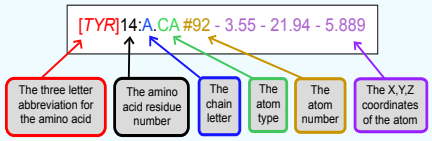
MSOE Center For BioMolecular Modeling - Jmol Quick Reference Sheet

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)*

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`

Saving and Reloading Your Work

write pngj filename.png *(exports a "PNJ + Jmol" document, which contains an image of your design, the script needed to reload your work, and a copy of the PDB file you are using.)*

example: `write pngj myDesign1.png`

history *(displays a history of all the commands you entered in the console, which can be copied and pasted into a word document for future review/use.)*

example: `history`

Color Formats

Method 1: select <selection type>
color <color name>

example:
```
select hydrophobic
color yellow
```

Default color mode: `color cpk`

Color secondary structures: `color structure`

Color each chain uniquely: `color chain`

Color a specific color: `color [R,G,B]`

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
polar	charged	hetero
water	nucleic	protein
helix	sheet	

`:<letter>` *(use a colon 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 plaster 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, use the same technique as described above for hydrogen bonds.

Struts:

`calculate struts` *(adds structural supports called struts to all selected protein areas)*
`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 `connect strut` or `connect strut delete` command

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

`set picking struts` *(allows you to add struts manually by clicking with the mouse on the two atoms you would like to connect. Be careful, this can be a bit tricky!)*

`set picking ident` *(turns off "set picking struts" and returns you to the normal/default mouse clicking)*

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 it and use `spacefill off` followed by `wireframe off`.

Additional Resources:

CBM Jmol Resources:
http://cbm.msoe.edu/teachingResources/
Official Jmol Command Database:
http://jmol.sourceforge.net
RSCB Protein Data Bank
http://www.pdb.org
Jmol Wiki Page
http://wiki.jmol.org/index.php/

3-D Molecular Designs
...where molecules become real™

Amino Acid Side Chain Chart©

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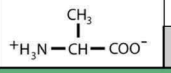
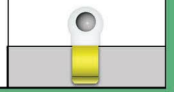
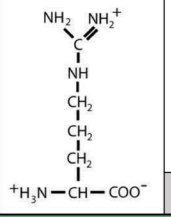
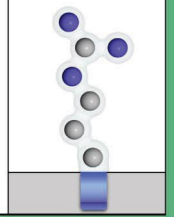
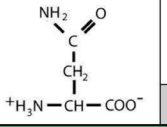
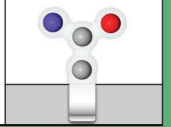
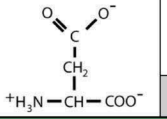
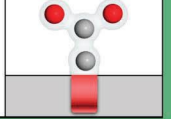
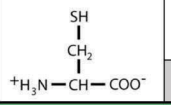
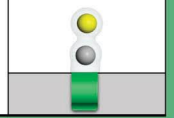
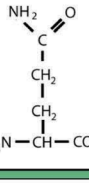
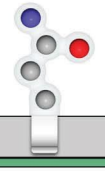
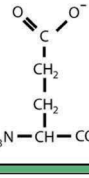
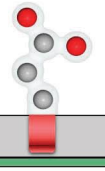
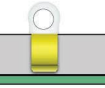
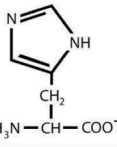
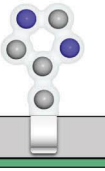
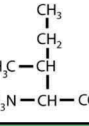
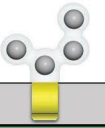
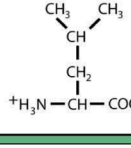
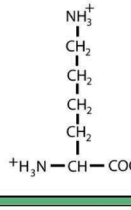
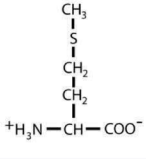
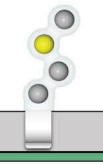
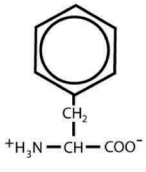
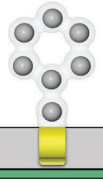
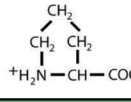
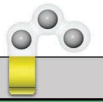
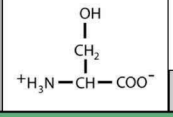
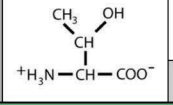
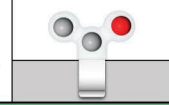
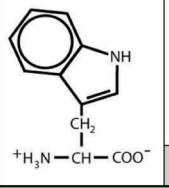
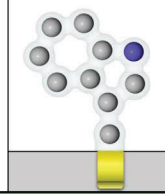
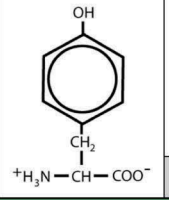
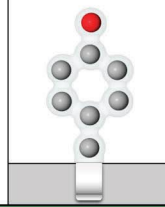
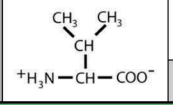
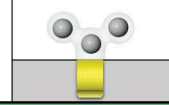
Name	Amino Acid	Side Chain
Alanine Ala A		
Arginine Arg R		
Asparagine Asn N		
Aspartic Acid Asp D		
Cysteine Cys C		

Name	Amino Acid	Side Chain
Glutamine Gln Q		
Glutamic Acid Glu E		
Glycine Gly G		
Histidine His H		
Isoleucine Ile I		

Name	Amino Acid	Side Chain
Leucine Leu L		
Lysine Lys K		
Methionine Met M		
Phenylalanine Phe F		
Proline Pro P		

Name	Amino Acid	Side Chain
Serine Ser S		
Threonine Thr T		
Tryptophan Trp W		
Tyrosine Tyr Y		
Valine Val V		

Atom Color Key

Carbon · Oxygen · Nitrogen · Sulfur · Hydrogen

Amino Acid Property Key

Amino acid clip color and name color indicate property

Negative Charge · Positive Charge · Hydrophilic · Cysteine · Hydrophobic