Getting Started

Accessing Jmol

Access the CBM's "Jmol user Design Environment" at:
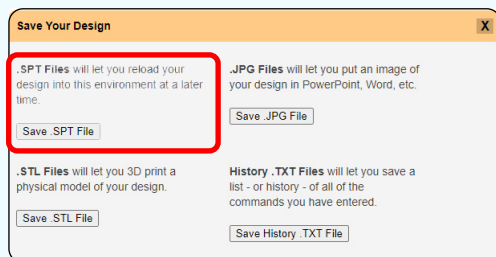**cbm.msoe.edu/modelingResources/jmolUser DesignEnvironment/**

Loading Structures

To load SMILES Sequences or Public PDB Files, click the "Open a New Molecular Structure" tab, enter the SMILES sequence or PDB ID, and click "Load"

Open a New Molecular Structure   X

SMILES sequence   COC=CC   Load
Public .PDB file (by ID)   1a3n   Load
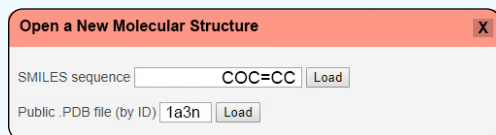
Saving and Reloading

To save your work, click the "Save Your Design" tab and select the file format you wish to export. We recommend using Script (.spt) files for standard saving.

Save Your Design   X

.SPT Files will let you reload your design into this environment at a later time.
Save .SPT File

.JPG Files will let you put an image of your design in PowerPoint, Word, etc.
Save .JPG File

.STL Files will let you 3D print a physical model of your design.
Save .STL File

History .TXT Files will let you save a list - or history - of all of the commands you have entered.
Save History .TXT File

To reload your work, simply drag and drop your script (.spt) file into the Jmol Display Window.
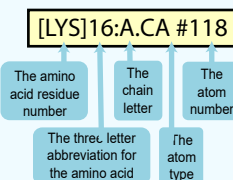
Rotate on the X-Y axes:

Translate the Molecule: Ctrl Alt

Zoom in and out: Shift

[LYS]16:A.CA #118

The amino acid residue number
The chain letter
The atom number
The three letter abbreviation for the amino acid
The atom type

center visible - *centers the view on currently visible atoms*

Simplifying Your Protein

Display Formats

wireframe - *displays bonds as sticks*
spacefill - *displays atoms as spheres*
backbone - *displays alpha carbon backbone*

examples: `wireframe`
`spacefill 200%`
`backbone 1.25`
`wireframe off`

Colors

color chains - *colors each protein chain uniquely*
color structure - *colors by secondary structures*
color cpk - *colors by atom element*
color <color name> - *colors by color names*
color [R, G, B] - *colors by RGB color values*
color group - *colors the backbone as a rainbow gradient*

examples: `color cpk`
`color orange`
`color [212, 138, 50]`

Select

select backbone - *selects all backbone atoms*
select sidechain - *selects all sidechain atoms*
select helix - *selects all alpha helix atoms*
select sheet - *selects all beta sheet atoms*
select :<chain ID> - *selects atoms in specific chain*
select <residue number/range> - *selects by residue #*
select @<atom number> - *selects by atom #*
select <element> - *selects by periodic table element*
select <amino acid abbreviation> - *selects by amino acid type*

examples: `select backbone`
`select :A`
`select 15-25`
`select @1382`
`select carbon`
`select his`

set selectionhalos on/off - *shows currently select atoms*

Booleans

and - *selects atoms in both of two selection groups*
or - *selects atoms in one or the other of two selection groups*

Adding the Details

Adding Sidechains

select <amino acid> and sidechain - *displays a specifc amino acid sidechain without a "bumpy backbone" (backbone atoms)*

examples: `select his29 and sidechain`
`spacefill 1.25`

Adding Bonds and Struts

Hydrogen Bonds - *a series of commands that will add hydrogen bonds to whatever area of your structure is currently selected:*

`calculate hbonds`
`set hbonds solid`
`set hbonds backbone`
`color hbonds white`
`hbonds 0.75`

Disulfide Bonds - *a series of commands that will add disulfide bonds to whatever area of your structure is currently selected:*

`set ssbonds backbone`
`color ssbonds yellow`
`ssbonds 0.75`

Calculate Struts - *adds support struts to any area of the protein backbone that is currently selected.*

`calculate struts`
`color strut gray`
`strut 0.75`

Editing Individual Struts - *to add or delete an individual support strut by selecting only the two atoms that the strut will connect.*

`select @34 or @713`
`connect strut`

`select @812 or @1103`
`connect strut delete`

Recommended Sizes

*If you plan to 3D print a physical model of your Jmol design, we recommend the following sizes. These can be **doubled** if you are using a plastic (FDM) 3D printer and are having trouble getting a successful print.*

Backbones: `backbone 1.25`

Sidechains: `spacefill 1.25`

Bonds: `strut 0.75`   `hbond 0.75`   `ssbond 0.75`

Amino Acid Side Chain Chart ©

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

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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 — Hydrophilic — Hydrophobic
Positive Charge — Cysteine

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