

Using Jmol, a quick guide to simple commands

Part 1, Simple Commands:

Zoom alt (or shift) + click and drag vertically (↑)
Display > Zoom > choose preset option

Rotate

click & drag on image

Rotate about X-axis: click & drag horizontally (←→)

Rotate about Y-axis: click & drag vertically (↑)

Rotate about Z-axis: alt (or shift) + click & drag horizontally (←→)

Translate (move along X or Y axis)

shift + double-click and drag

control + right click and drag

Pop-up menu

Right click (control click) image

Change view

View > choose preset option

Pop-up menu > View > choose preset option

Spin on/off

Pop-up menu > Spin > On (Off)

Change size of atom

Display > atom > choose preset option

Pop-up menu > style > Atom > choose preset option

Change bond size

Display > Bonds > choose preset option

Pop-up menu > Style > Bonds > choose preset option

Measure distance between any two atoms

Double click first atom (+) > double click second atom

To change units: Pop-up menu > Measurement > choose preset option

Measure bond angle

Double click first atom (+) > click second atom > double click third atom

Measure dihedral angle (angle between two bonds)

Double click 1st atom (+) > click 2nd atom > click 3rd atom > double click 4th atom

Reset to front view and center

Away from molecule: shift + double-click

Part 2, Complex commands: Pop-up menu >

Select

All

Elements > Choose from list

Protein >

By residue name > Choose from list

All

Backbone

Side chains

Polar residues

Nonpolar residues

Basic Residues

Acidic Residues

Uncharged Residues

Nucleic

By residue name > Choose from list

All

Backbone

Bases

DNA

RNA

AT pair

AU pairs

GC pairs

Hetero

By HETATM > Choose from list

All PDB "HETATM"

All solvent

All water

Ligand (hetero and not solvent)

Nonaqueous HETATM (HETATM and not water)

Nonaqueous solvent (solvent and not water)

Carbohydrate

None of above

Style

Scheme

CPK Spacefill

Ball and Stick

Sticks

Wireframe

Cartoon

Trace

Atoms

Labels

Bonds

Hydrogen Bonds

Disulfide Bonds

Structures

Off

Backbone

Cartoon

Cartoon Rockets

Ribbons

Rockets

Strands

Trace

Axes

Color

Atoms

Bonds

Hydrogen Bonds

Disulfide Bonds

Structure

Backbone

Cartoon

Ribbons

Rockets

Strands

Trace

Surface

Labels

Vectors

Axes

Boundbox

Background

Surfaces

Dot Surface
van der Waals surfaces
Solvent-Accessible Surface (VDW + 1.4Å)
Solvent Surface (1.4 Å probe)
Molecular Surface
Make Opaque
Make Translucent
Off

Animation >

Measurement >

Set Picking >

Console >

Show >

Part 3, Other:

Hide water:

First select the water: Select > Hetero > All Water
Display the water in Spacefill: Style > Scheme > CPK Spacefill
Turn the atoms off: Style > Atoms > Off

Color each chain differently:

Select > All (or Protein > All)
Style > Scheme > Cartoon
Color > Structure > Cartoon > By Scheme > Chain

Change the color of a cartoon:

First select the particular part of a structure in cartoon that you wish to change.
Then change the color of the cartoon:
Color > Structure > Cartoon > By Scheme > element cpk
Other choice may also be made for the last two steps (...By Scheme > element cpk).

Placing figures into a Word document:

Have desired figure in Jmol.
Zoom in or out for desired perspective. The contents and only the contents of the Jmol window will become the figure.
Make background white if desired.
Pop-up menu > Color > Background > White
Edit > Copy Image
Go to Word document and paste.