PyMOL – Basics – The GUI

Molecular Visualisation

PyMOL	Intuitive interface	Python compatible
Chimera	Great for larger structures	Advanced visualisations
VMD	Great for trajectory analysis	
QuteMol	Simple stylised visuals	

Pymol Version

Pymol 2.x	Python 3	'Incentive' version (university licence)
Pymol 1.x	Python 2	Open Source version

.pse files will not open between version
.pml and .py scripts contain python will not run between versions

Available for Windows / Mac / Linux

Resources

https://pymolwiki.org/index.php/Main_Page
https://www.uml.edu/docs/PyMOL%20Quick%20Reference%20Guide_tcm18-230352.pdf

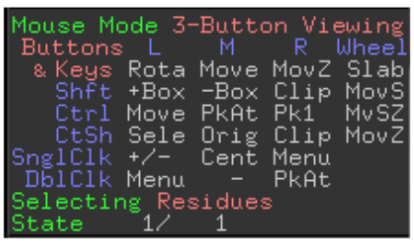
What is a pdb?

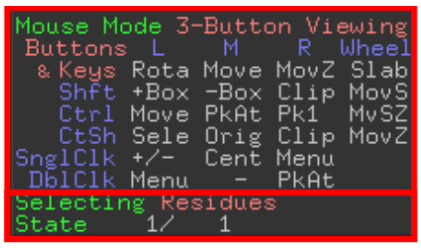
https://www.rcsb.org/
Lets have a look at a PDB file
What is a .cif file? And is this important?

Navigating the GUI

But first we need a structure

```
fetch 2chb
```





Veiw or Edit

Selection type

Mouse Wheel Codes

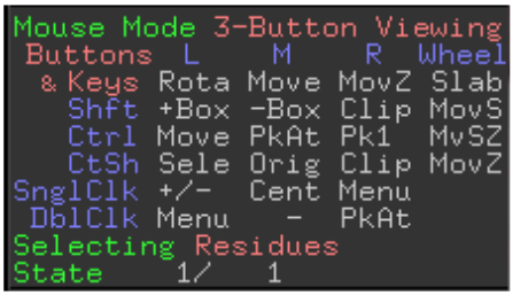
Slab : Adjust the depth of the visible slab (between the clipping planes).
MovS : Move the visible slab.
MvSZ : Move view center relative to the slab.
MovZ : Move the camera along the Z axis (zoom).

Mouse Button Codes for Viewing

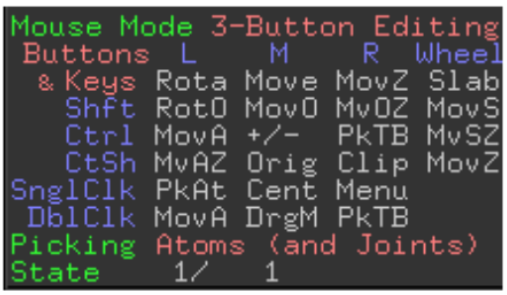
Cent : Center the view on a given atom.
Clip : Move clipping planes using vertical (front) or horizontal (back) motion.
Menu : Activate context-dependent menu.
Move : Translate camera in the XY plane (of the screen).
MovZ : Move the camera along the Z axis (zoom).
Rota : Free camera rotation.
Pk1 : Pick one atom within the molecular graph.
PkAt : Pick atoms within the molecular graph.
Sele : Set the active selection.
Orig : Set the origin (atom) for camera rotation.
+/- : Toggle atom member-ship within the active selection.
+Box : Add atoms to the active selection using a box.
-Box : Remove atoms from selection using a box.

Mouse Button Codes for Editing

DrgM : Activates dragging for a discrete molecule.
Rot_ : Free rotation.
Mov_ : Move in XY plane.
MvZ_ : Move along Z axis.
"_" above is A, D, F, or 0:
A for atom
D for dragged selection
F for fragment
0 for object
PkTB : Pick and (optionally) drag to change bond torsion.



Veiw



Full selection hierarchy

Edit

Only 'atom' selection

Objects and Selection

(de)select all objects
(de)select this object
a named selection
temporary selection

multiple object may be active

only one selection may be avtive

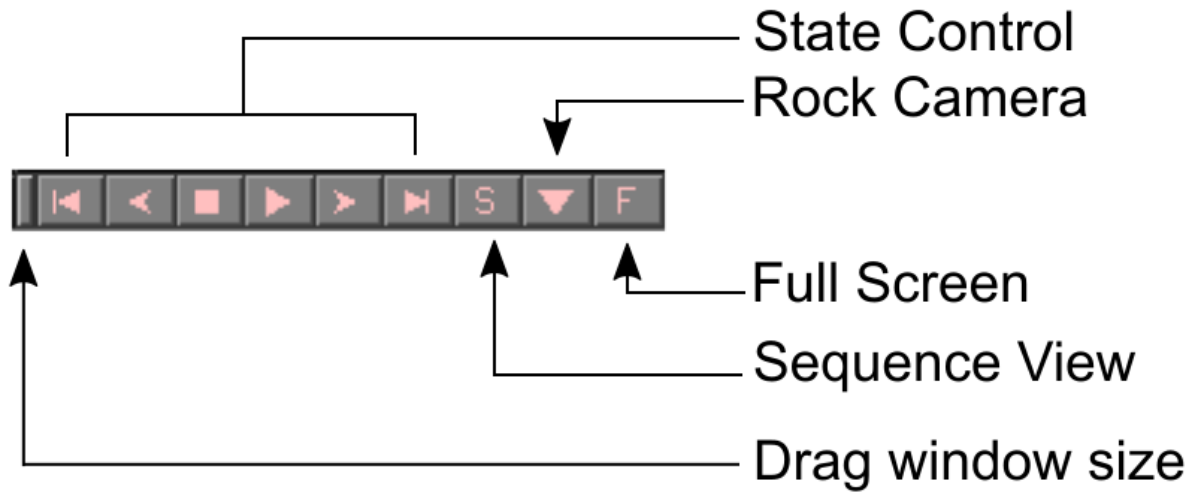
[A] Action

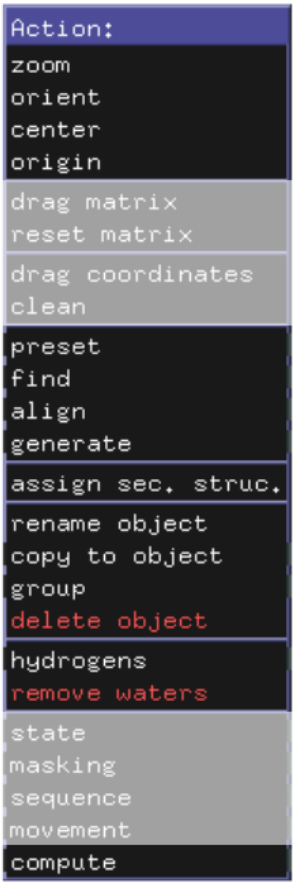
[S] Show

[H] Hide

[L] Label

[C] Colour





Show state control

```
fetch 1j8k
```

```
as sticks
remove hydrogen
```
Find hydrogen bonds
Look at presets

```
split_states 1j8k
delete 1j8k
join_states 1j8k, 1j8k_*
split_states 1j8k
delete 1j8k
```
align all to one

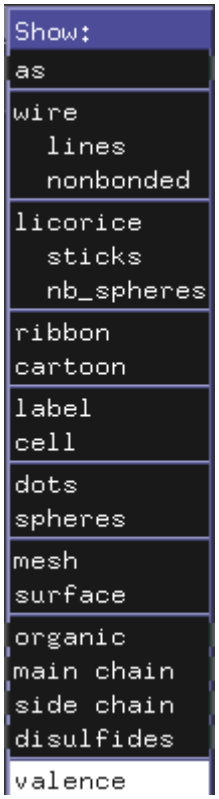
Show alignment

```
fetch 1qoh
```
select chains - take two, extract, align

```
rein
fetch 1qoh, type=pdb1
```

1qoh  > align > to molecule > 2chb

```
align 1qoh, 2chb
cealign 1qoh, 2chb
super 1qoh, 2chb
```



Show – **Add** to the current representation

As – **replace** the current representation

Tip! You can type this also!
as cartoon
show sticks

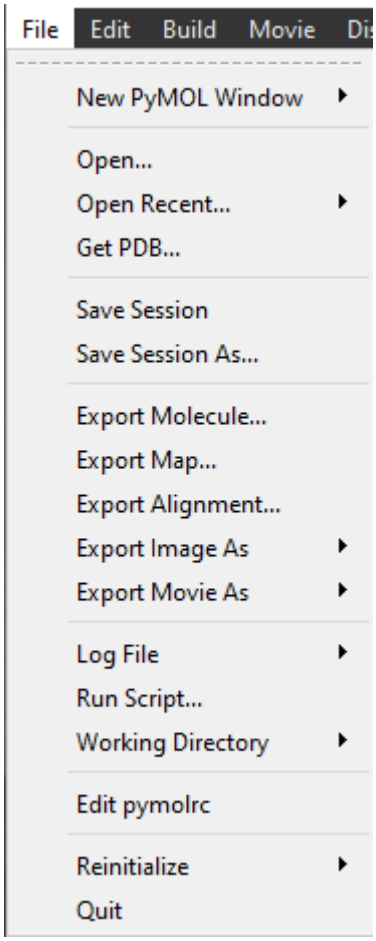
select polymer - selects protein/nucleic acid
select polymer.protein
select organic - selects ligand
select inorganic - selects ions
select solvent - selects water

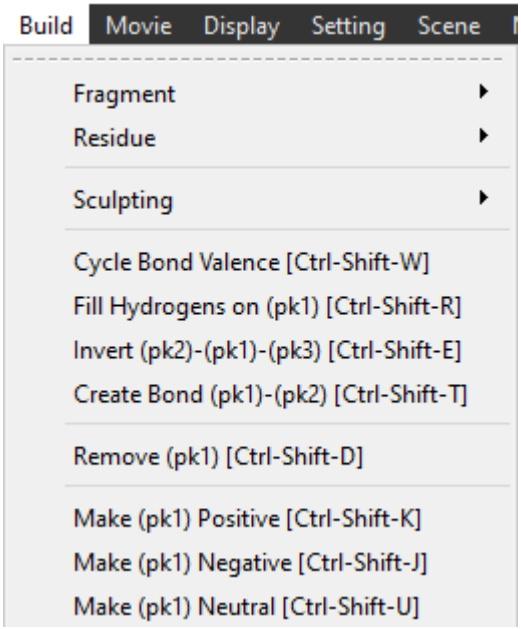
select ! polymer - selects **not** protein/nucleic acid
select ! organic - selects **not** ligand
select ! inorganic - selects **not** ions
select ! solvent - selects **not** water

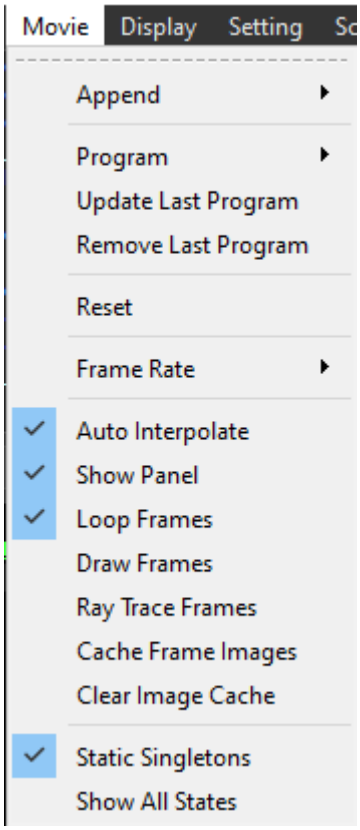

```
By element - first line keeps current C color

By chain - allows chainbows per chain

By ss - colours by secondary structure
      Although limited options, you can try
      color firebrick, ss H
      color forest, ss S
      color density, ss L

command options

util.cbc          cbc = color by chain

util.cnc          cnc = color not carbon

util.chainbows
```

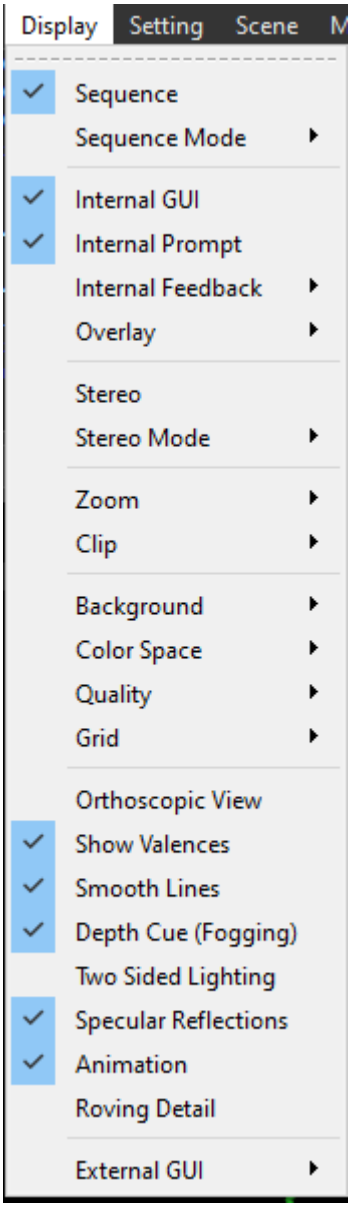
therefore!

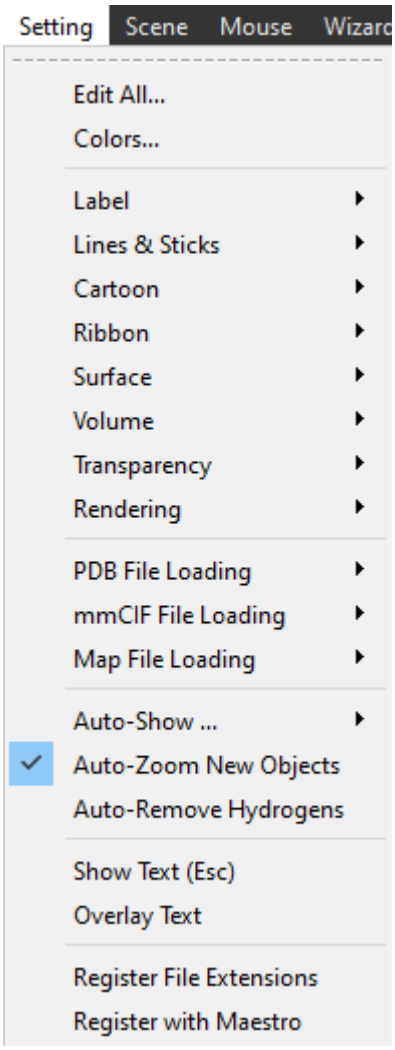
```
rein
fetch 2chb, async=0
remove solvent
remove inorganic
as cartoon
show sticks, organic
util.cbc
color black, organic
util.cnc
bg_color white
orient
```

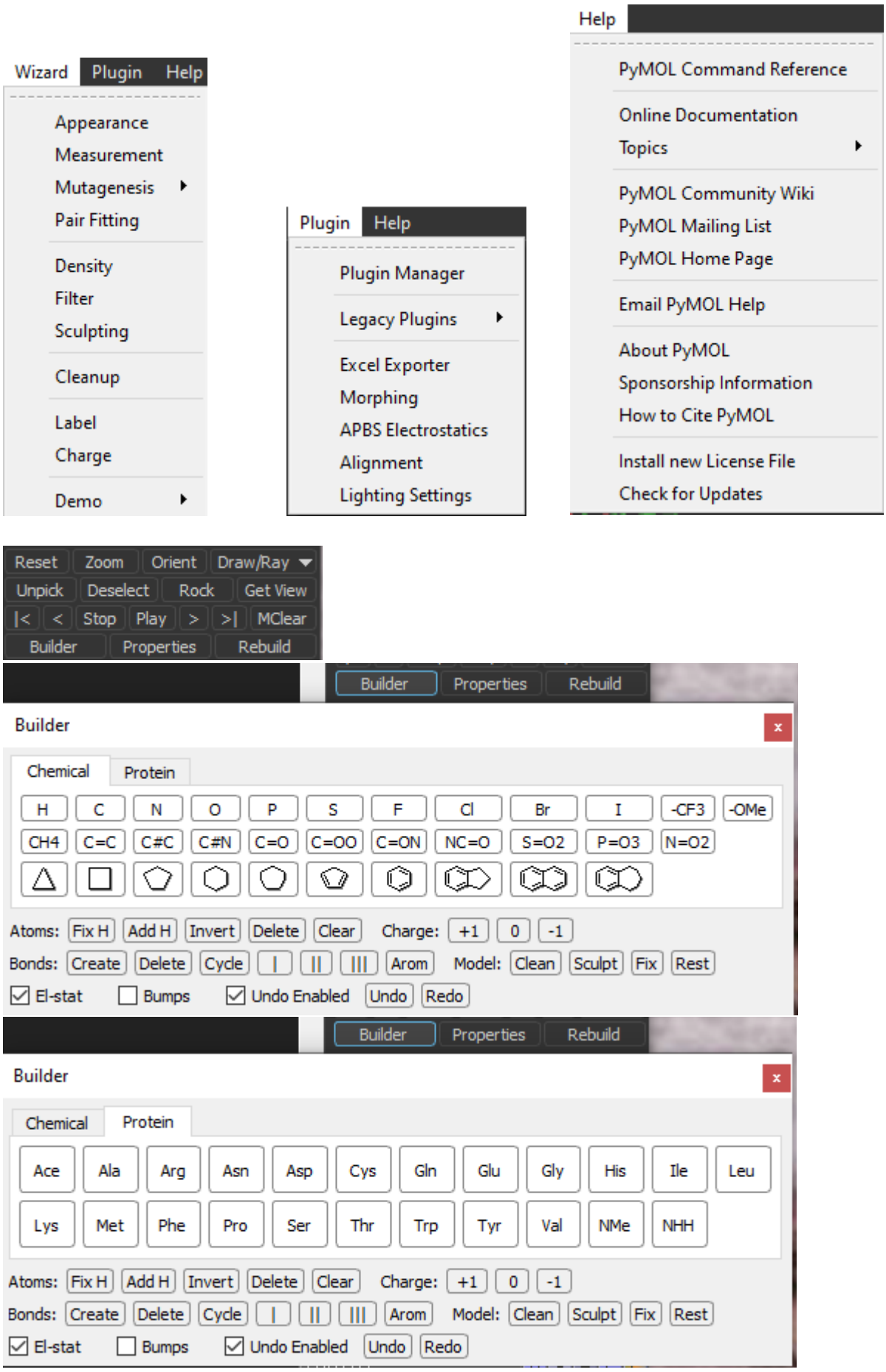

File
Edit
Build
Movie
New PyMOL Window
Open...
Open Recent...
Get PDB...
Save Session
Save Session As...
Export Molecule...
Export Map...
Export Alignment...
Export Image As
Export Movie As
Log File
Run Script...
Working Directory
Edit pymolrc
Reinitialize
Quit


Build
Movie
Display
Setting
Scene
Fragment
Residue
Sculpting
Cycle Bond Valence [Ctrl-Shift-W]
Fill Hydrogens on (pk1) [Ctrl-Shift-R]
Invert (pk2)-(pk1)-(pk3) [Ctrl-Shift-E]
Create Bond (pk1)-(pk2) [Ctrl-Shift-T]
Remove (pk1) [Ctrl-Shift-D]
Make (pk1) Positive [Ctrl-Shift-K]
Make (pk1) Negative [Ctrl-Shift-J]
Make (pk1) Neutral [Ctrl-Shift-U]


Movie
Display
Setting
Append
Program
Update Last Program
Remove Last Program
Reset
Frame Rate
Auto Interpolate
Show Panel
Loop Frames
Draw Frames
Ray Trace Frames
Cache Frame Images
Clear Image Cache
Static Singletons
Show All States


Display
Setting
Scene
Sequence
Sequence Mode
Internal GUI
Internal Prompt
Internal Feedback
Overlay
Stereo
Stereo Mode
Zoom
Clip
Background
Color Space
Quality
Grid
Orthoscopic View
Show Valences
Smooth Lines
Depth Cue (Fogging)
Two Sided Lighting
Specular Reflections
Animation
Roving Detail
External GUI


Setting
Scene
Mouse
Edit All...
Colors...
Label
Lines & Sticks
Cartoon
Ribbon
Surface
Volume
Transparency
Rendering
PDB File Loading
mmCIF File Loading
Map File Loading
Auto-Show ...
Auto-Zoom New Objects
Auto-Remove Hydrogens
Show Text (Esc)
Overlay Text
Register File Extensions
Register with Maestro


Wizard
Plugin
Help
Appearance
Measurement
Mutagenesis
Pair Fitting
Density
Filter
Sculpting
Cleanup
Label
Charge
Demo
Plugin
Help
Plugin Manager
Legacy Plugins
Excel Exporter
Morphing
APBS Electrostatics
Alignment
Lighting Settings
Help
PyMOL Command Reference
Online Documentation
Topics
PyMOL Community Wiki
PyMOL Mailing List
PyMOL Home Page
Email PyMOL Help
About PyMOL
Sponsorship Information
How to Cite PyMOL
Install new License File
Check for Updates
Reset
Zoom
Orient
Draw/Ray
Unpick
Deselect
Rock
Get View
|<
<
Stop
Play
>
>|
MClear
Builder
Properties
Rebuild
Builder
Properties
Rebuild
Builder
Chemical
Protein
H
C
N
O
P
S
F
Cl
Br
I
-CF3
-OMe
CH4
C=C
C#C
C#N
C=O
C=OO
C=ON
NC=O
S=O2
P=O3
N=O2
Atoms:
Fix H
Add H
Invert
Delete
Clear
Charge:
+1
0
-1
Bonds:
Create
Delete
Cycle
|
||
|||
Arom
Model:
Clean
Sculpt
Fix
Rest
El-stat
Bumps
Undo Enabled
Undo
Redo
Builder
Properties
Rebuild
Builder
Chemical
Protein
Ace
Ala
Arg
Asn
Asp
Cys
Gln
Glu
Gly
His
Ile
Leu
Lys
Met
Phe
Pro
Ser
Thr
Trp
Tyr
Val
NMe
NHH
Atoms:
Fix H
Add H
Invert
Delete
Clear
Charge:
+1
0
-1
Bonds:
Create
Delete
Cycle
|
||
|||
Arom
Model:
Clean
Sculpt
Fix
Rest
El-stat
Bumps
Undo Enabled
Undo
Redo