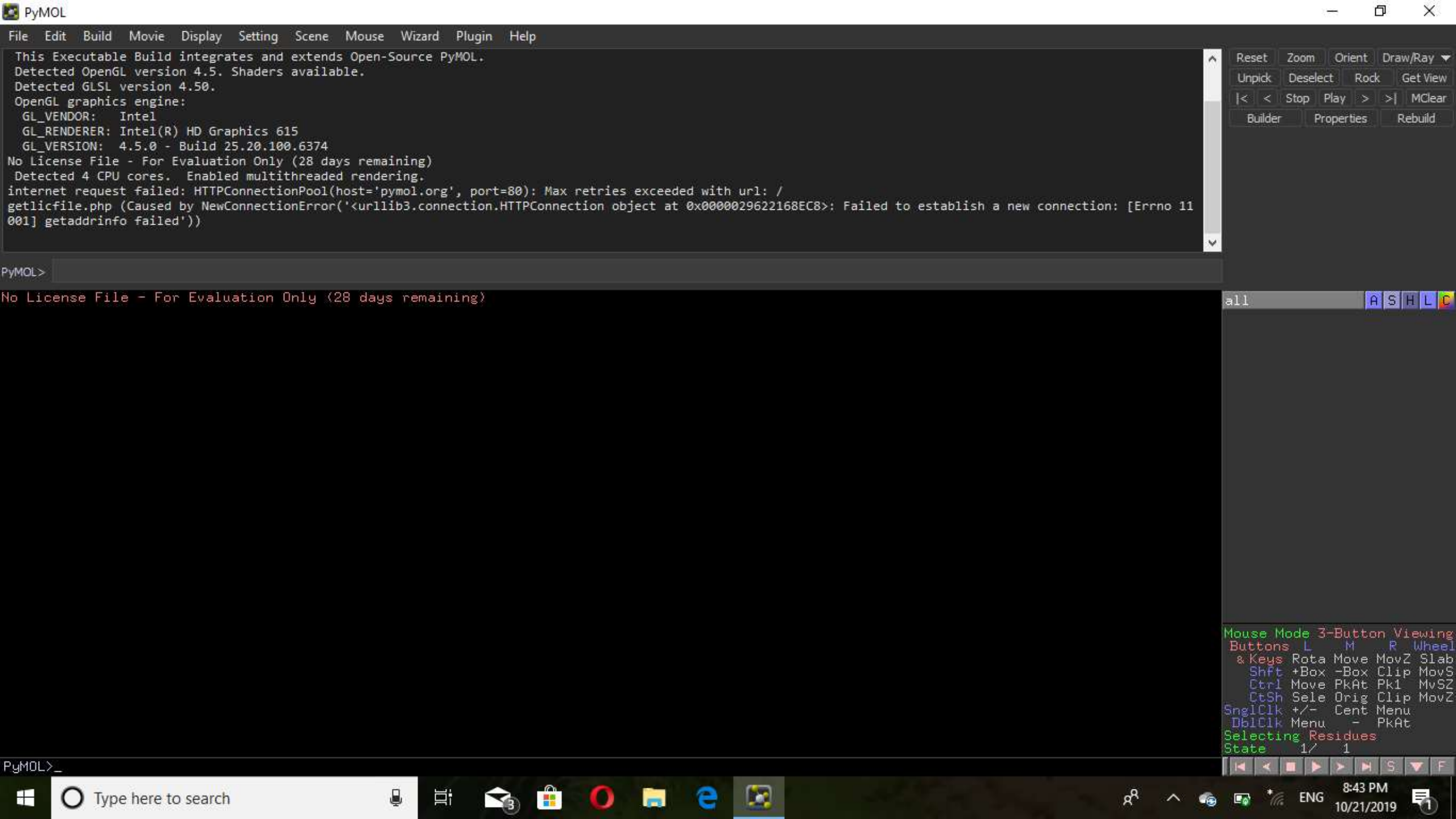
PYMOL SOFTWARE

Introduction to PyMOL

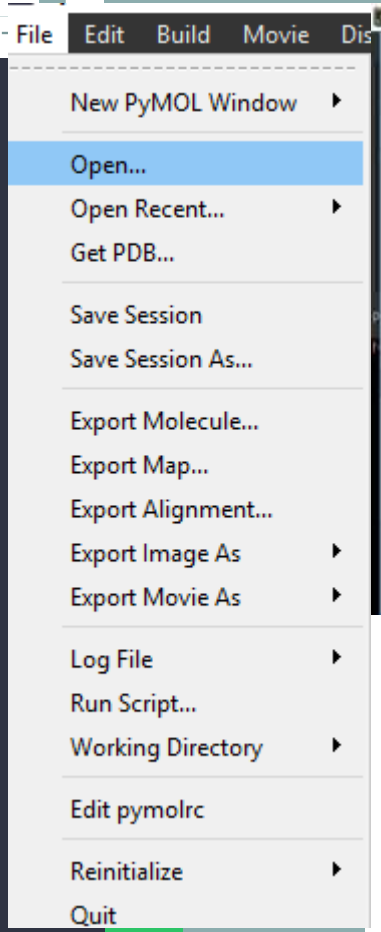
- PyMOL is an open source molecular visualization program which provides high quality of rendering, speed and versatility especially crystallography. PyMOL was created by Warren Lyford DeLano. It license is free but not in all forms. Py in PyMOL refers to the Pytho language which enables automation with simple command scripts Schrödinger took over PyMOL in 2010.
- PyMOL is written in C, C++ and Python. It provides the capabilitie of traditional molecular graphic packages having a plus of integrat python interpreter. This software is used popularly among structu biologists and crystallographers

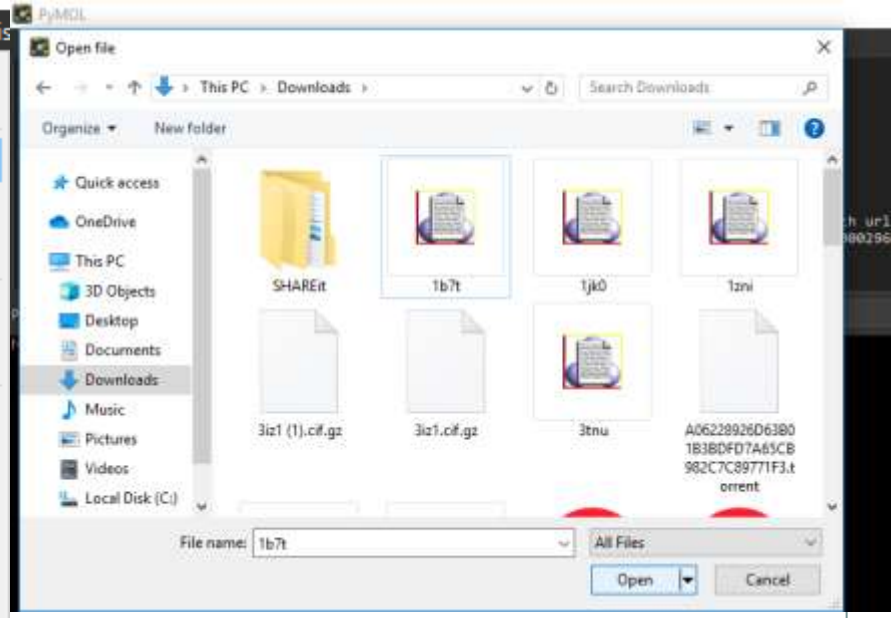

PyMOL
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help
This Executable Build integrates and extends Open-Source PyMOL.
Detected OpenGL version 4.5. Shaders available.
Detected GLSL version 4.50.
OpenGL graphics engine:
GL_VENDOR: Intel
GL_RENDERER: Intel(R) HD Graphics 615
GL_VERSION: 4.5.0 - Build 25.20.100.6374
No License File - For Evaluation Only (28 days remaining)
Detected 4 CPU cores. Enabled multithreaded rendering.
internet request failed: HTTPConnectionPool(host='pymol.org', port=80): Max retries exceeded with url: /
getlicfile.php (Caused by NewConnectionError('<urllib3.connection.HTTPConnection object at 0x0000029622168EC8>: Failed to establish a new connection: [Errno 11
001] getaddrinfo failed'))
Reset Zoom Orient Draw/Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear
Builder Properties Rebuild
PyMOL>
No License File - For Evaluation Only (28 days remaining)
all A S H L C
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1
PyMOL>_
Type here to search
ENG
8:43 PM
10/21/2019

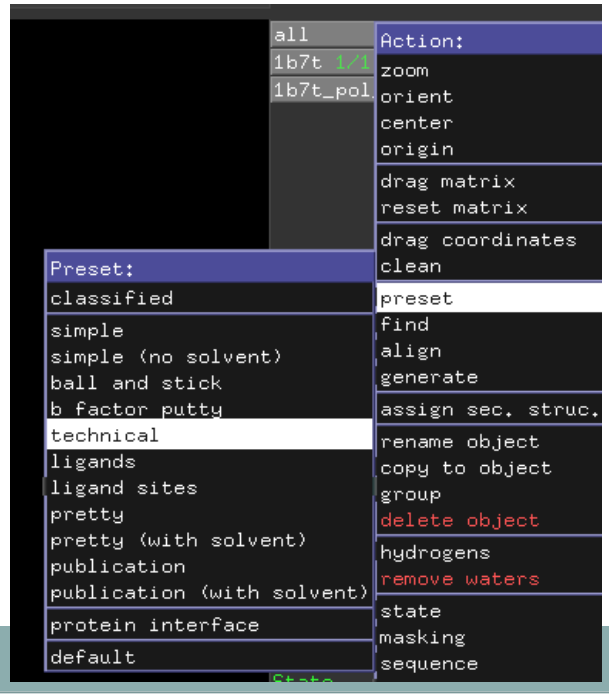
Features
Visualization Presets

PDB file can be opened by going to file.

PyMOL comes with an array of preset visualizations for example technical view or simple view. Command: A > Action > Preset > Simple or Technical.



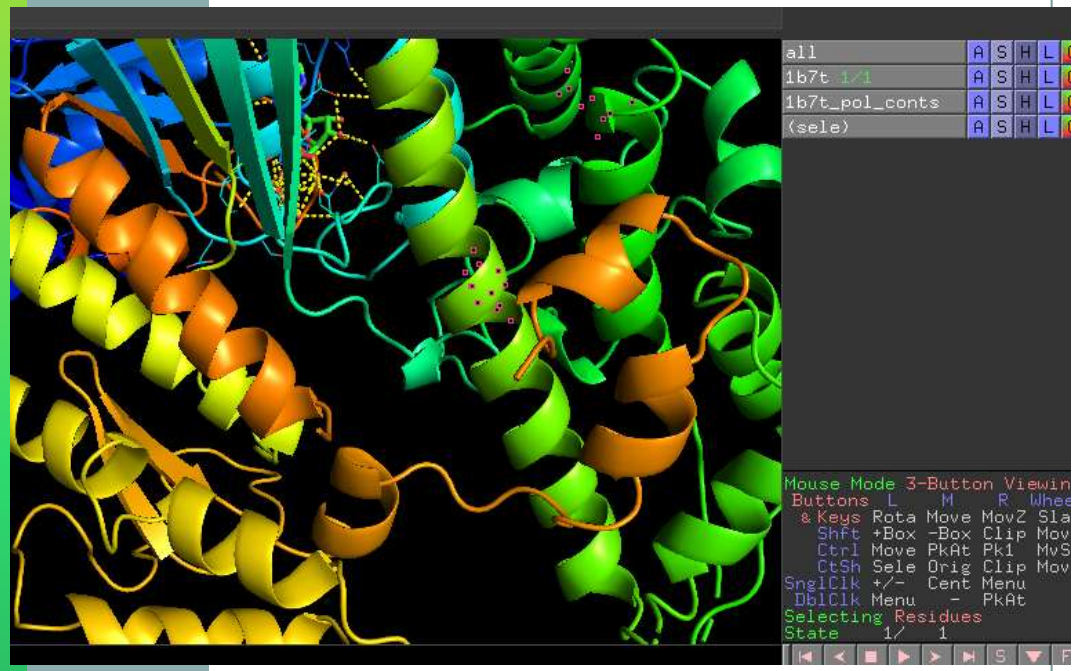


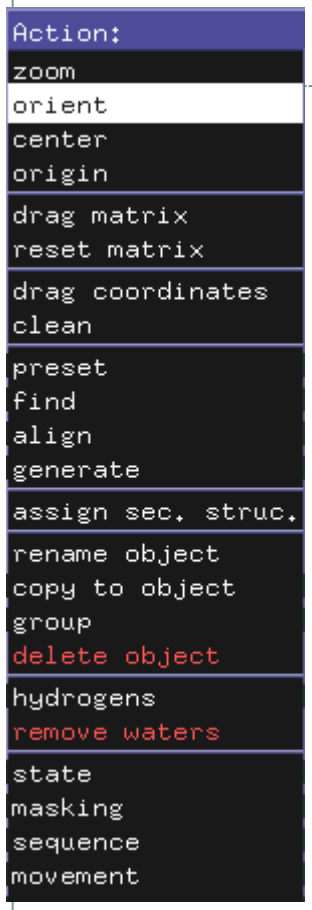


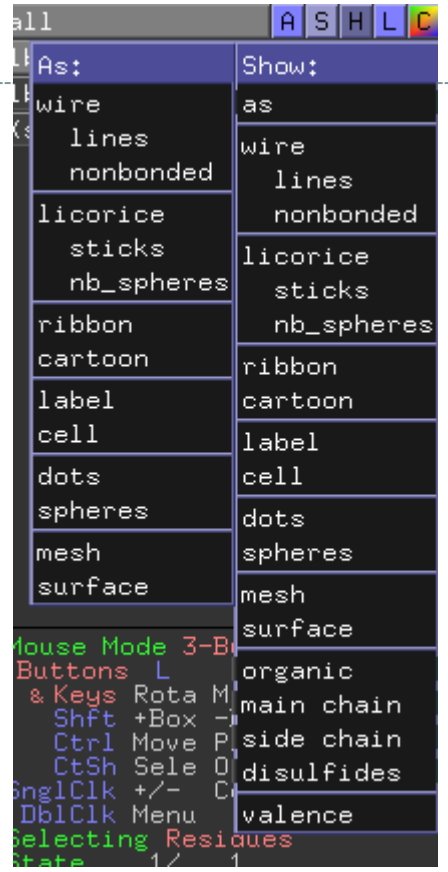
Representations and Selections

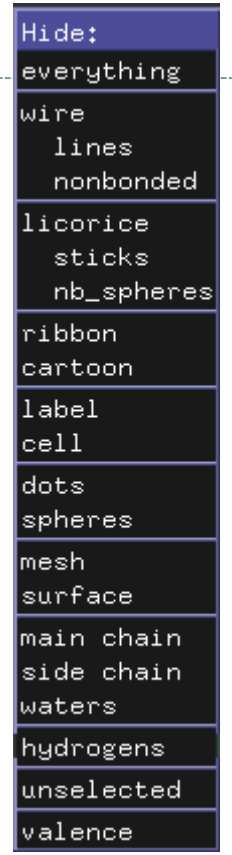
Representations in PyMOL is controlled through S (Show), H (Hide), L (Label), C (Color) popup menus. Cartoon representation of PyMOL is quite near to that of MolScript.

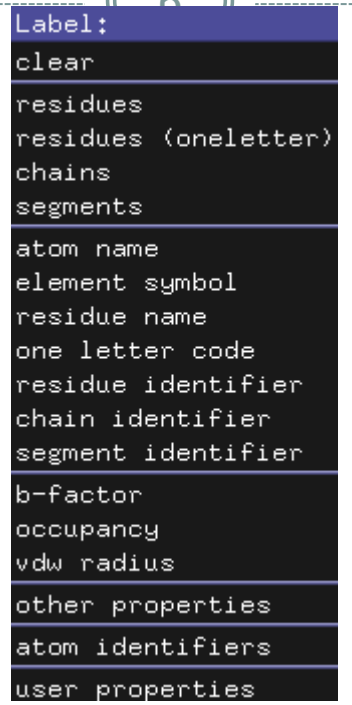
Selections in PyMOL are just set of atoms that you define and do not have any properties of their own other than a name. Selection names appear in viewer window in parenthesis as in (sele) to distinguish them from objects.

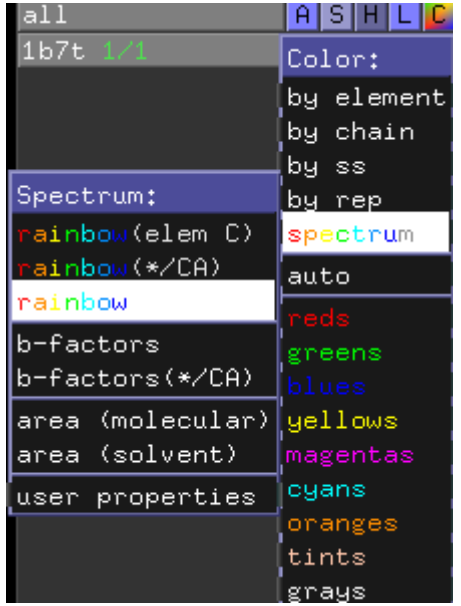


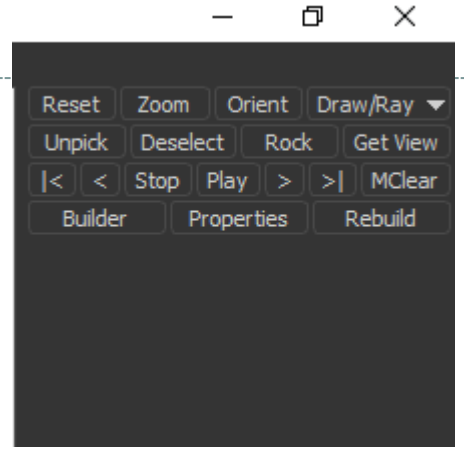

Action:
zoom
orient
center
origin
drag matrix
reset matrix
drag coordinates
clean
preset
find
align
generate
assign sec. struc.
rename object
copy to object
group
delete object
hydrogens
remove waters
state
masking
sequence
movement


all
A S H L C
As:
wire
lines
nonbonded
licorice
sticks
nb_spheres
ribbon
cartoon
label
cell
dots
spheres
mesh
surface
Show:
as
wire
lines
nonbonded
licorice
sticks
nb_spheres
ribbon
cartoon
label
cell
dots
spheres
mesh
surface
organic
main chain
side chain
disulfides
valence
Mouse Mode 3-B
Buttons L
& Keys Rota M
Shft +Box -
Ctrl Move P
CtSh Sele O
SnglClk +/- C
DblClk Menu
Selecting Resi ues
State 1/ 1


Hide:
everything
wire
lines
nonbonded
licorice
sticks
nb_spheres
ribbon
cartoon
label
cell
dots
spheres
mesh
surface
main chain
side chain
waters
hydrogens
unselected
valence


Label:
clear
residues
residues (oneletter)
chains
segments
atom name
element symbol
residue name
one letter code
residue identifier
chain identifier
segment identifier
b-factor
occupancy
vdw radius
other properties
atom identifiers
user properties


all
A S H L C
1b7t 1/1
Spectrum:
rainbow(elem C)
rainbow(*/CA)
rainbow
b-factors
b-factors(*/CA)
area (molecular)
area (solvent)
user properties
Color:
by element
by chain
by ss
by rep
spectrum
auto
reds
greens
blues
yellows
magentas
cyans
oranges
tints
grays

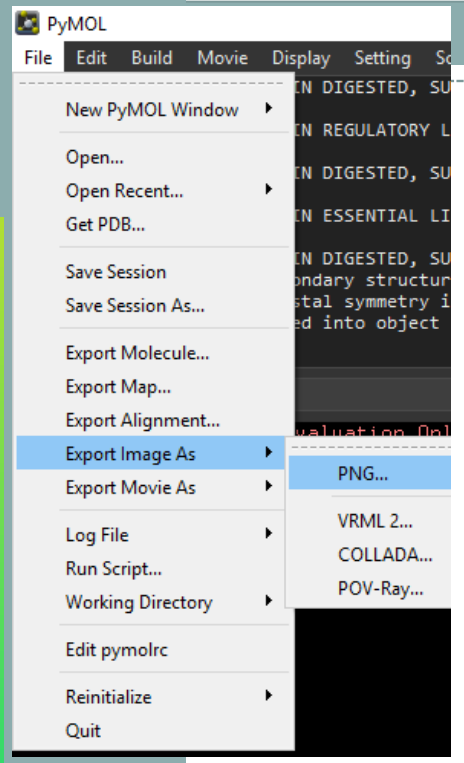

Reset
Zoom
Orient
Draw/Ray
Unpick
Deselect
Rock
Get View
|<
<
Stop
Play
>
>|
MClear
Builder
Properties
Rebuild

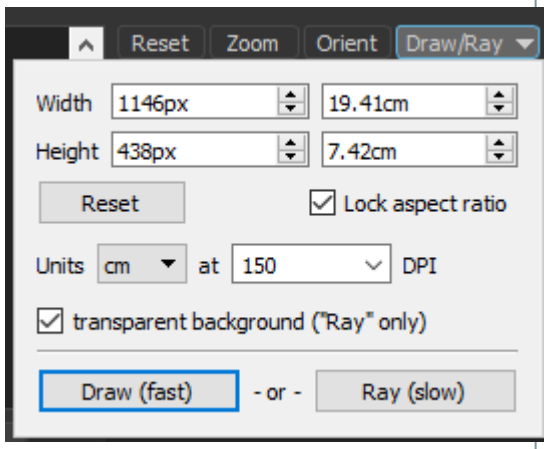

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Atoms
State 1/ 1
S F

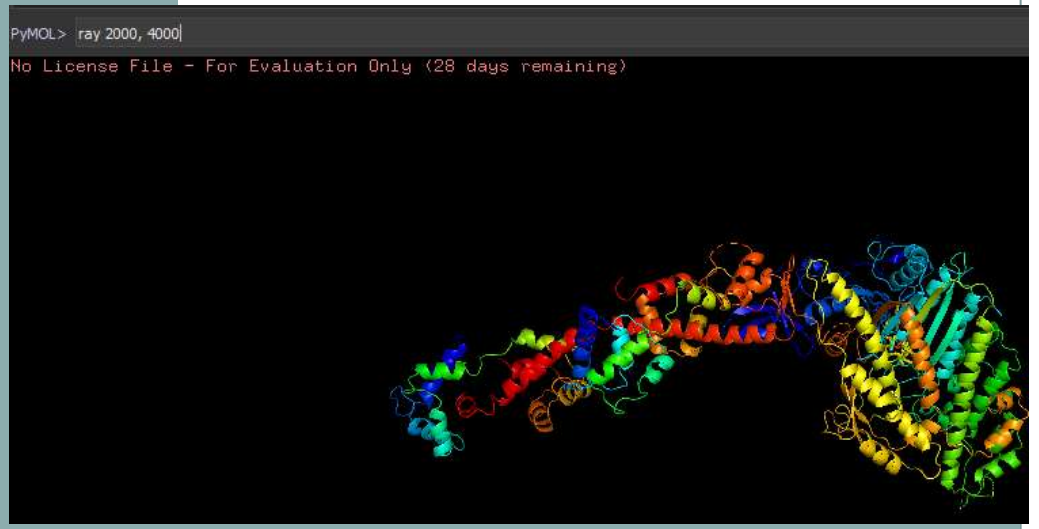
Image Saving

PyMOL provides the privilege to save image in high definition in PNG format. The resolution or Dots Per Inch (DPI) are usually very high. It provides transparency of background. It can also save ray traced image which draws scenes with superior detail.

Command: Type “ray W, H” at PyMOL command. File > Save/Export Image As > PNG. W and H can be calculated by multiplying height and width times the DPI.





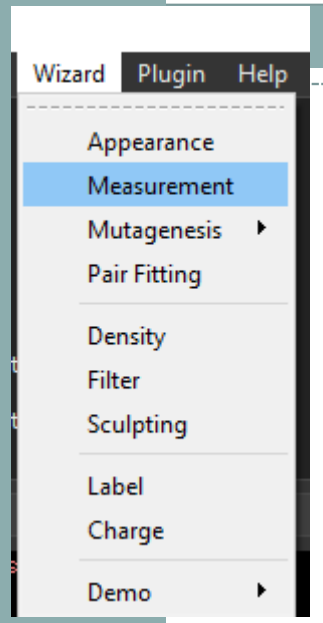


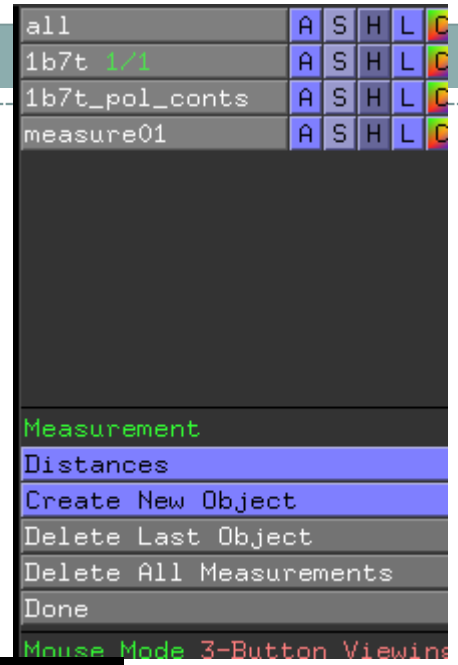
Measurements

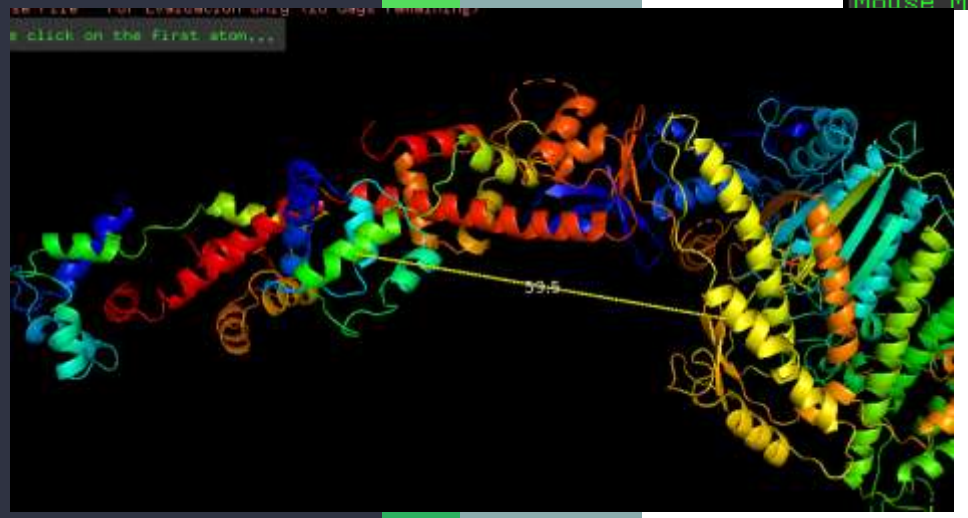
PyMOL can take measurements of the distances, angles, dihedrals, neighbors (polar/ heavy) of the macromolecules being analyzed. PyMOL Wizard is used for this purpose. Wizard can be used to create dashed lines between atoms.

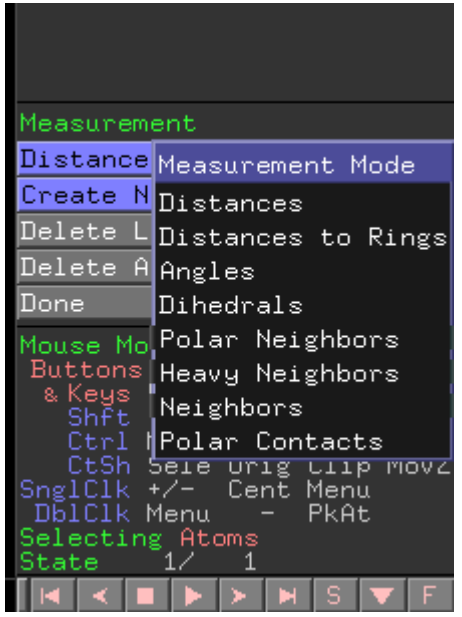
Commands: S > Show > As > Lines.

Wizard > Measurement (Click on any atom) > Measurement Mode: Distances/ Angles/ Dihedrals etc.







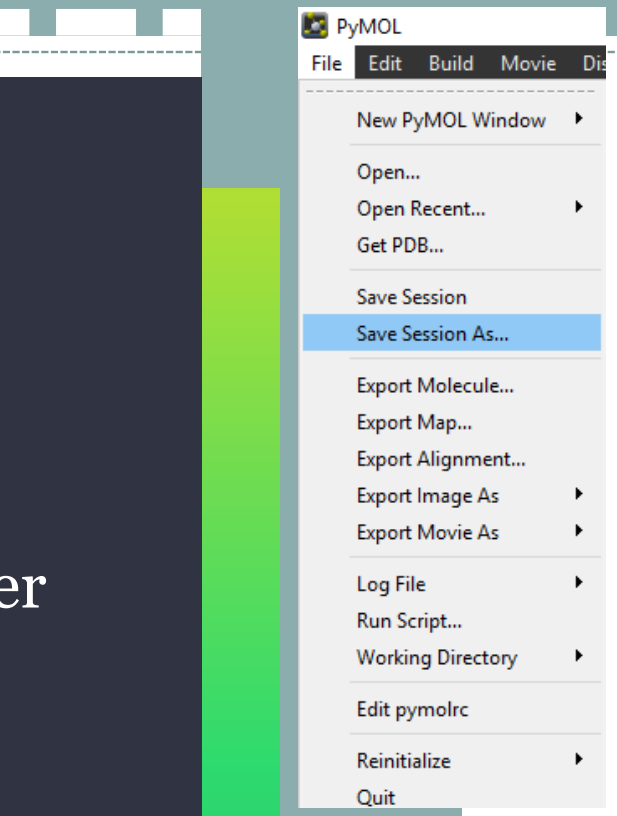


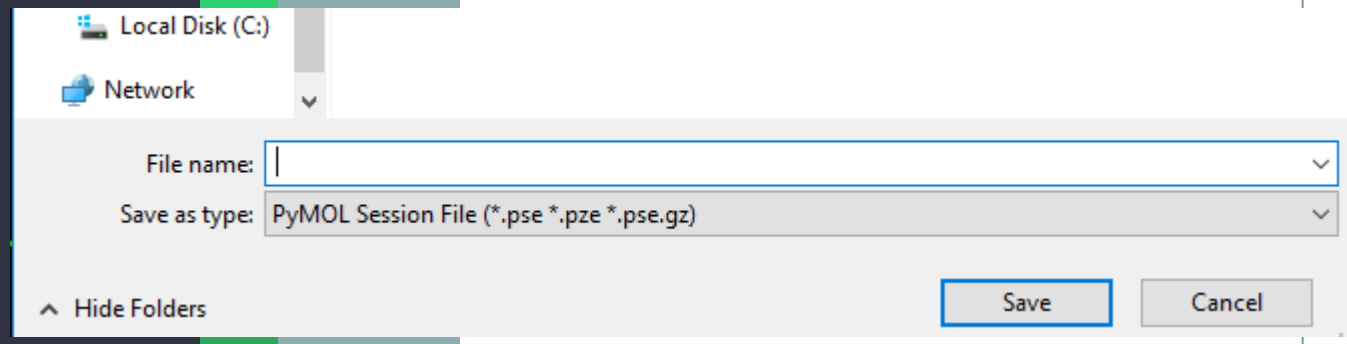
PyMOL Sessions

Sessions store all your objects, selections, views, scenes, representations, etc. to work on later or sharing it with others.

Commands: File > Save Session As >. pse

The file can be opened by double clicking .pse file

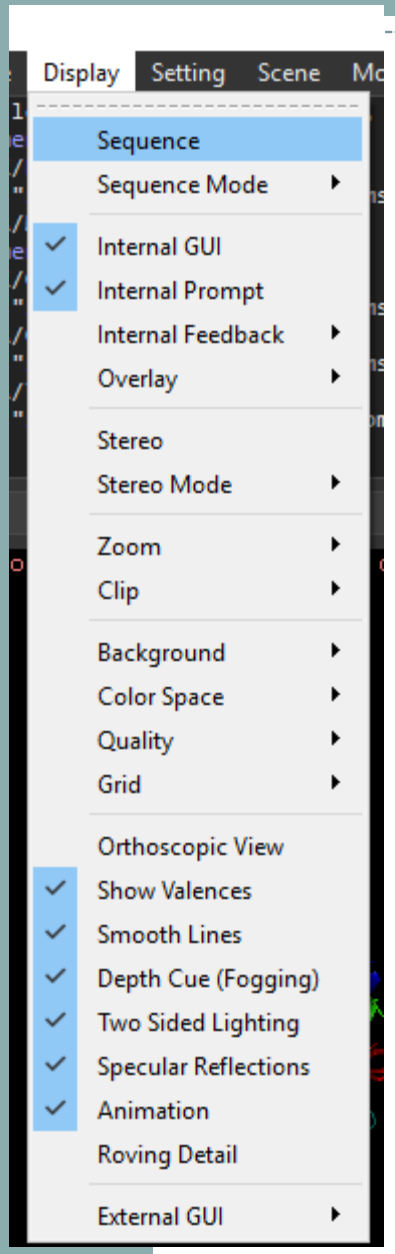




Sequence viewer

Amino acid sequences of protein can be viewed in familiar one letter codes. Residues can also be viewed in form of purple dots.

Command: Display > Sequence (from upper control window)



PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

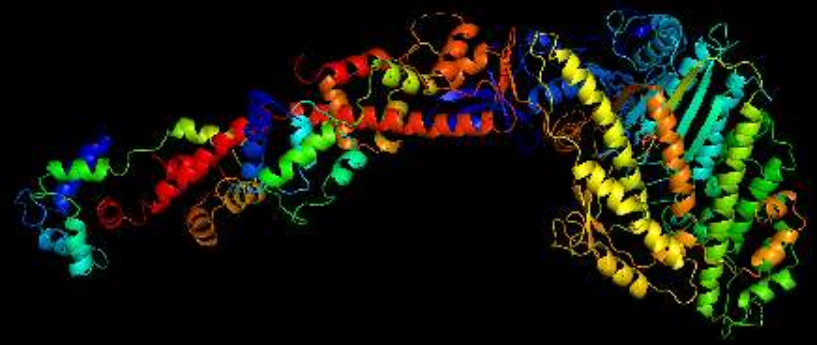
```
PyMOL>wizard measurement
 You clicked /1b7t//Z/PRO`70/CA
 Selector: selection "sele" defined with 1 atoms.
 You clicked /1b7t//A/MET`518/CA
PyMOL>wizard measurement
 You clicked /1b7t//Z/GLU`66/CA
 Selector: selection "sele" defined with 1 atoms.
 You clicked /1b7t//A/GLU`344/CA
 Selector: selection "sele" defined with 9 atoms.
 You clicked /1b7t//A/TYR`431/CA
 Selector: selection "sele" defined with 21 atoms.
 Setting: seq_view set to on.
```

PyMOL>

Reset Zoom Orient Draw/Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear
Builder Properties Rebuild

```
/1b7t//A/5     11   16        27  31   36   41   46   51   56   61   66   71   76   81   86   91   96   101  106  111  116  121  126  131  136
        FSDPDFQNLAMI---...---AFDGKKNCWFDERGFASAEIQSSKGDEITVKIVADSSTRTVKKIDDIQSMNPPKFEKLEDMANMTYLNEASVLYNLRSRYTSGLIYTYSGLFCIAVNPYRRLPIYTDSVIAK
```

No License File - For Evaluation Only (28 days remaining)



all A S H L C
1b7t 1/1 A S H L C
1b7t_pol_conts A S H L C
(sele) A S H L C

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
&Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1

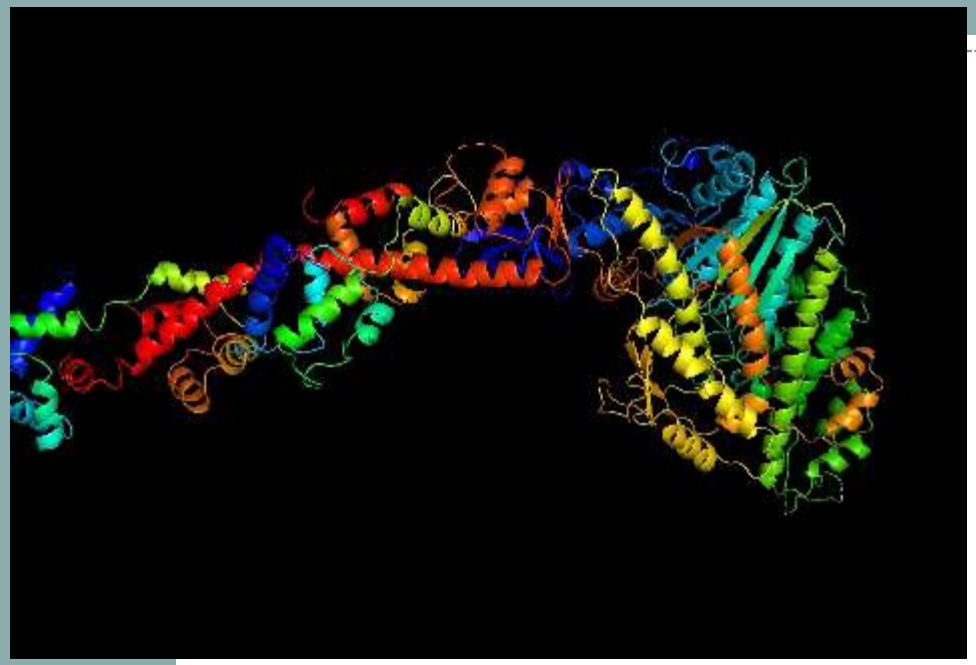
PyMOL>_

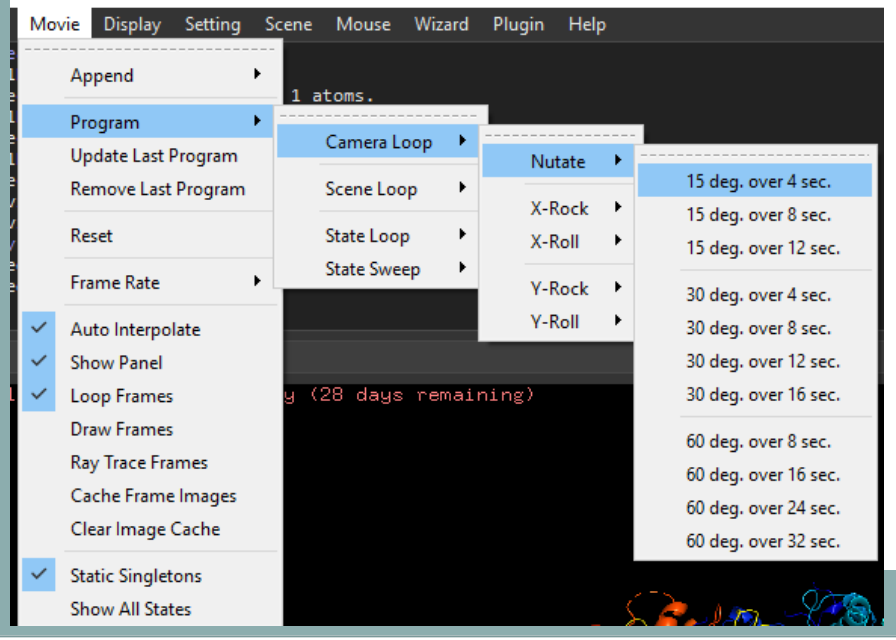
Scenes, Shows and Movies

A scene in PyMOL is simply a memory snapshot which saves current colors, visualizations, representations and camera position. Command: A > Actions > Orient. Scene > Append.

A show is an interactive movie as you advance or reverse through your predefined scenes.

Movies can be made with commands as: Movie > Append (for no. of seconds), to program: Movie > Program > Camera Loop/ Scene Loop/ State Loop/ State Sweep.

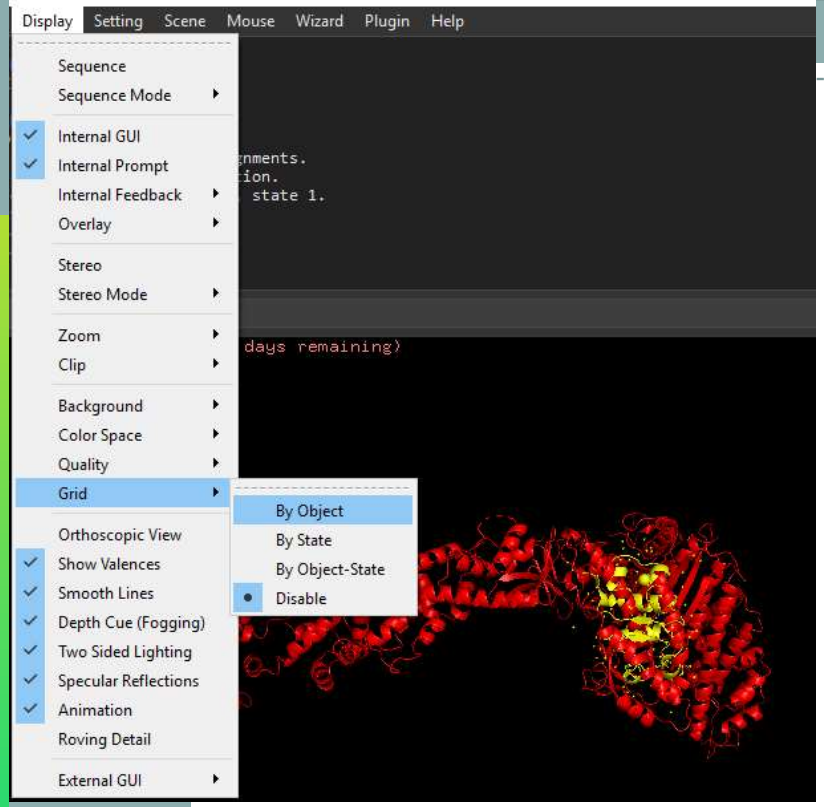


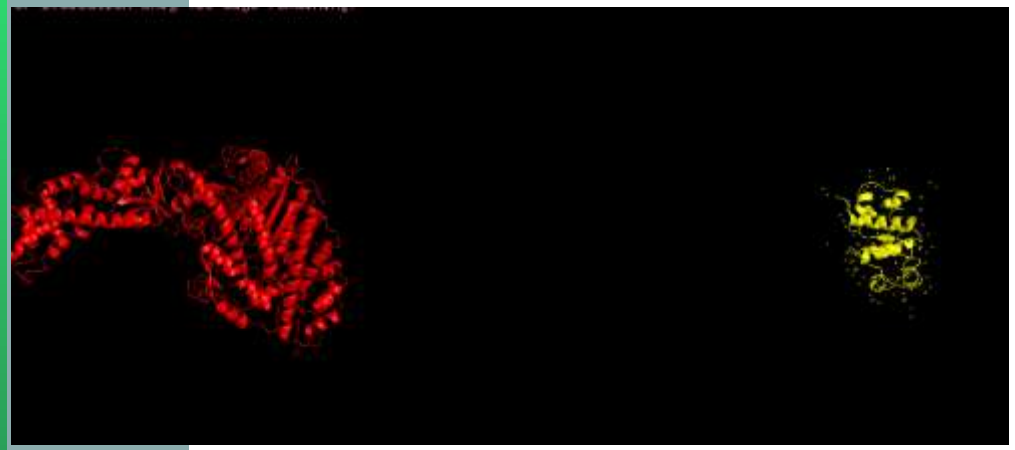


Working with Multiple Objects and Selection

PyMOL can be used to simultaneously visualize dozens of structures or more. It has a feature called as a grid mode which subdivides the Display Area into equal sized rectangles on screen each having a structure.

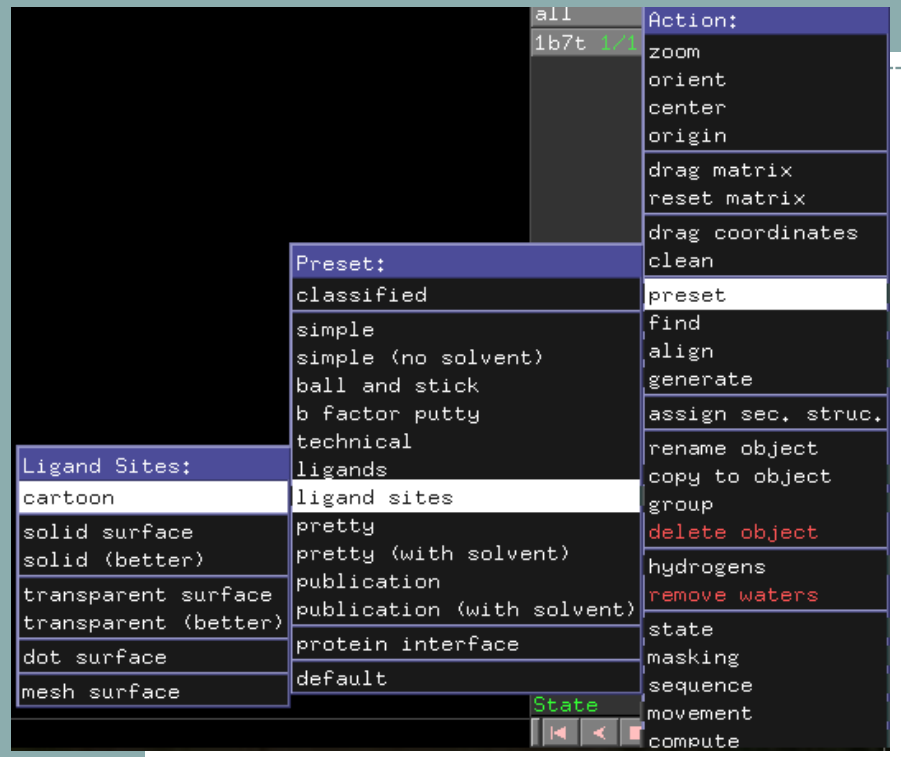
Command: Display > Grid > By Object

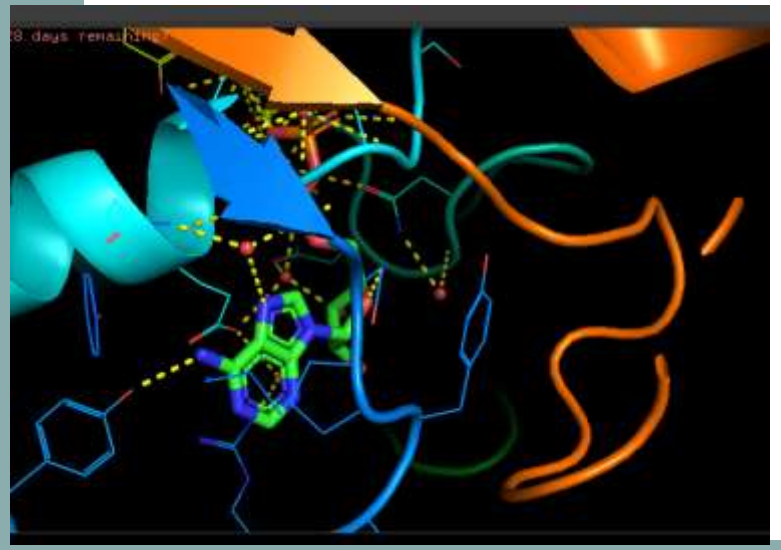




Ligand sites

PyMOL can also show the ligand sites as well as any selected residual in the structure of molecule.

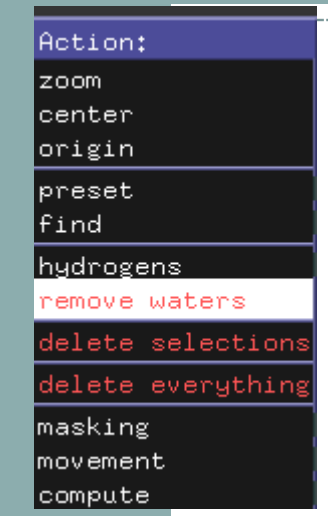


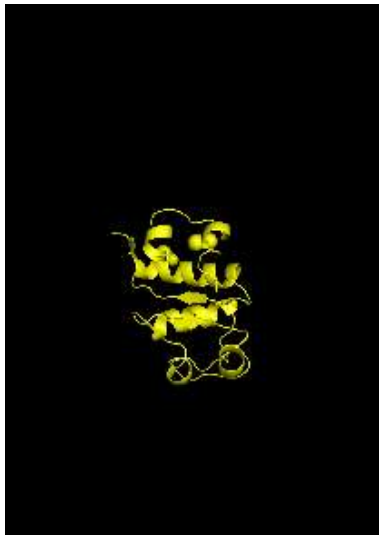


Editing molecular objects

PyMOL allows to create or replace bonds, atoms, residues and commonly used chemical groups. After modification the structure can be cleaned using MMFF (Merk Molecular Force Field).

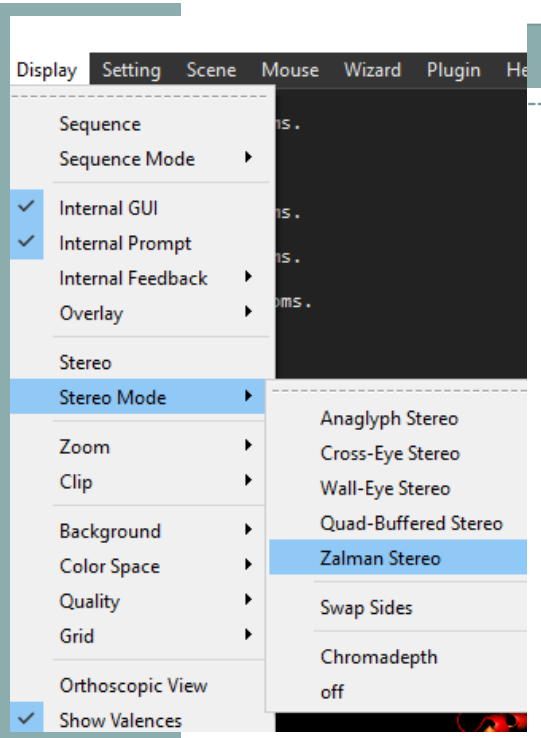
Command: A > Actions > Remove Waters/ Remove Hydrogens/ Remove Atoms.

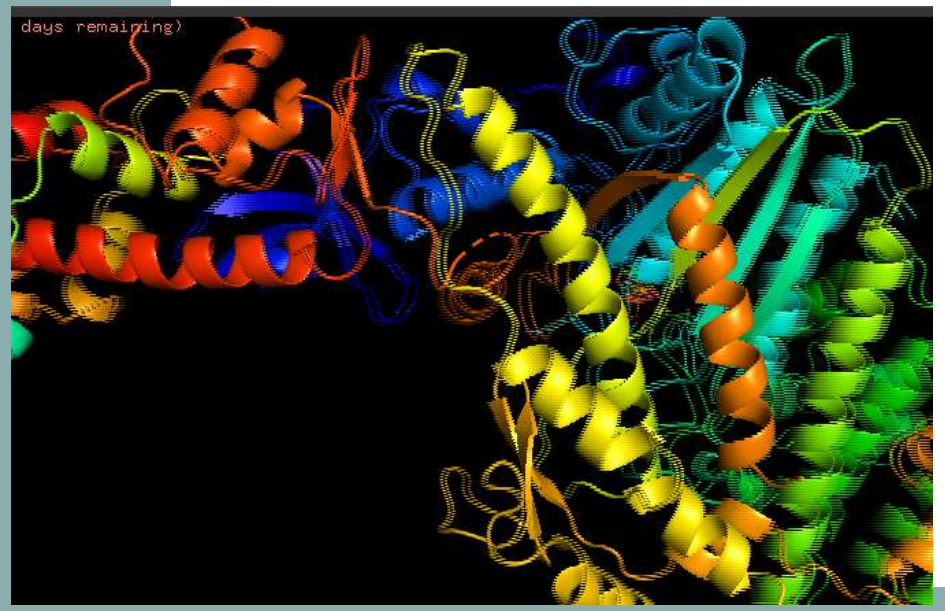




Stereo Modes

Different stereo graphic options are supported by PyMOL, for example, Crosseye stereo, Walleye Stereo, Hardware Stereo, etc.





Advantages

- **Cross–Platform**. A single code base supports both Unix, Macintosh, and Windows, using OpenGL and Python and a small set of Open–source external dependencies.
- **Command–Line and GUI Control** Real world applications require both.
- **Molecular Splits/Joins**. Structures can be sliced, diced, and reassembled on the fly and written out to standard files (i.e. PDB).
- **Scripting**. The best way to control PyMOL is through reusable scripts, which can be written in the command language or in Python.
- **Rendering**. A built–in ray tracer gives you shadows and depth on any scene. You also render externally.
- **Output**. PNG files output from PyMOL can be directly imported into PowerPoint
- Electron Density Maps can also be made using PyMOL
- **Conformational Editing**. Click and drag interface allows you to edit conformations naturally. Sculpting allows the molecule to adapt to your changes

disadvantages

- **User Interface**. Development has been focused on capabilities, not on easy–of–use for new users.
- **Documentation**. Only recently has any documentation become available.
- **Object–Orientation**. There is a single monolithic, functional API.
- **Electrostatics**. PyMOL is not yet a replacement for Delphi/Grasp.
- **No Mechanics Engine** Although PyMOL sports potent molecular editing features, you can't yet perform any "clean–up".
- PyMOL lacks a general undo command so sessions must be saved periodically (every 5 minutes for extended tasks).


THANK YOU