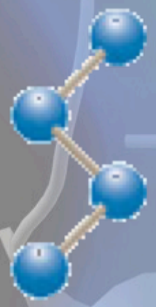
Advanced Visualization with Pmv



TSRI

Instructors:

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Stefano Forli, Ph.D. (TSRI)

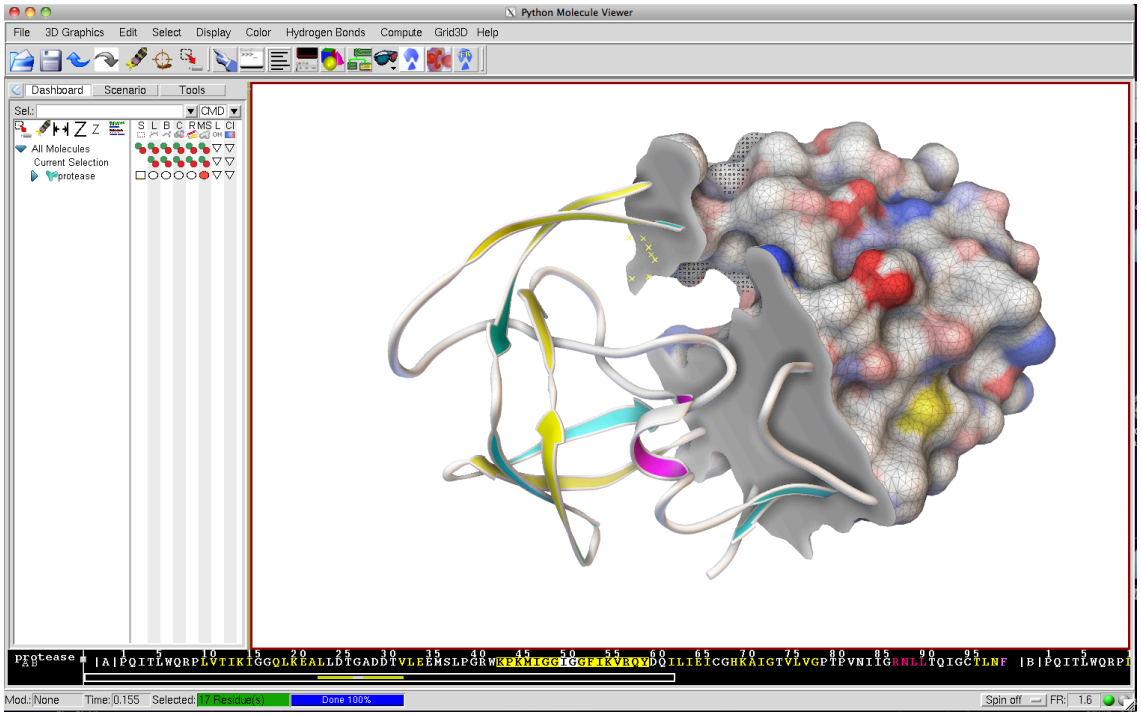
Handouts in ~/Desktop/TutorialData/PDFs and at http://www.scripps.edu/~sanner/collab/PmvTut.pdf

Overview

- Introduction to Pmv
- The Dashboard Panel
- Advanced Rendering
- Vision Programming

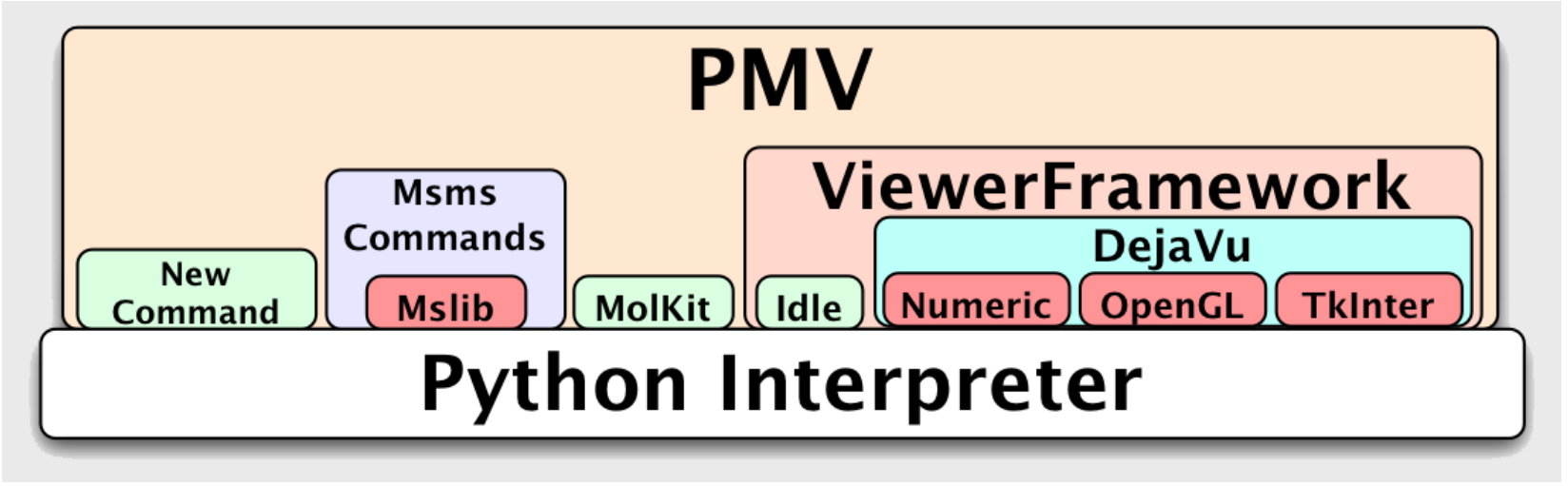
Not Yet Another Molecular Viewer

- Component based architecture



Pmv is underlying:

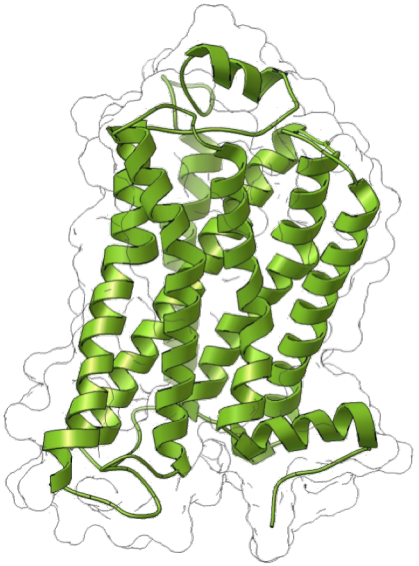
- ADT
- Raccoon
- PyARTK
- ePmv
- Continuity GUI

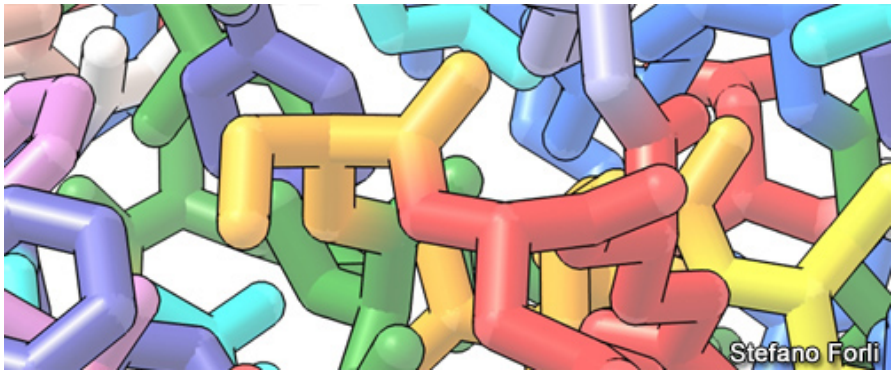


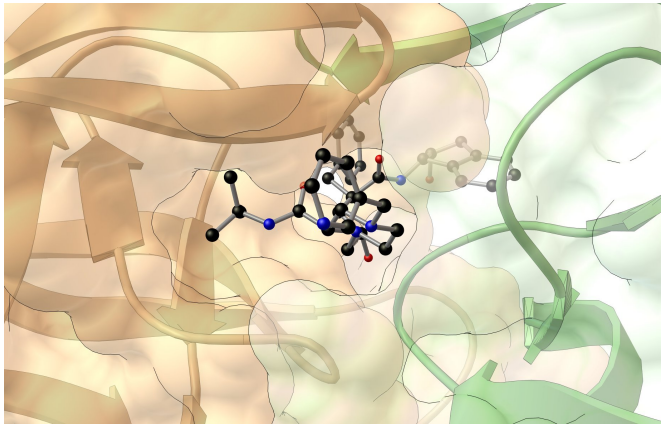
Unique Design Features

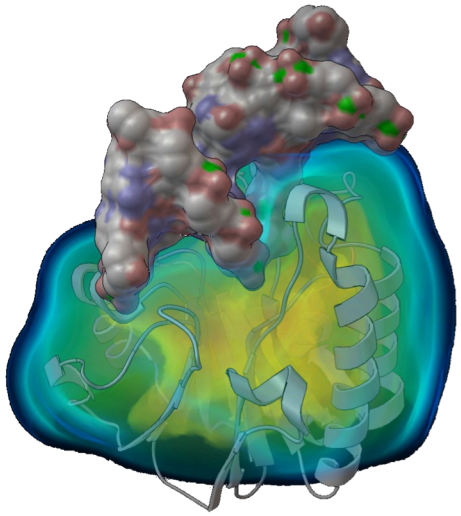
- Written in Python (i.e. Fully scriptable)
- Automatic command log generation
- Customizable commands (loaded dynamically)
- Programmable through visual programming
- Dynamically extensible data structures
- Advanced rendering capabilities
- Amination capabilities

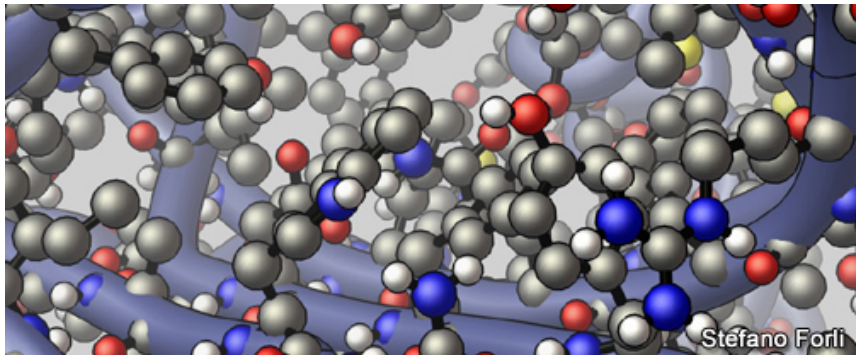
Powerful 3D graphics

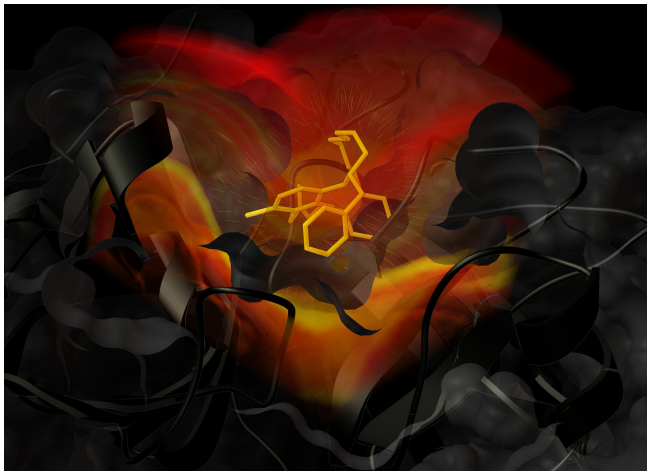


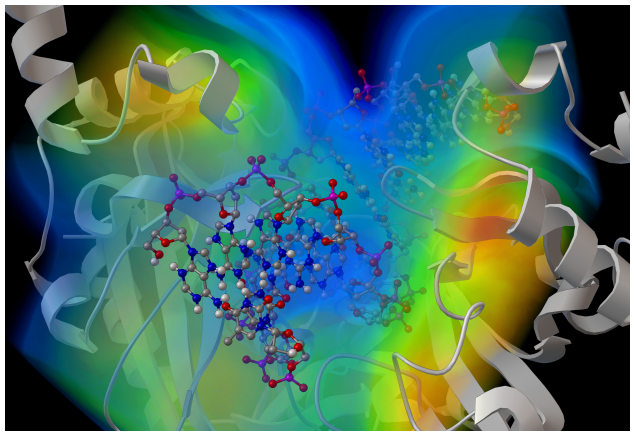


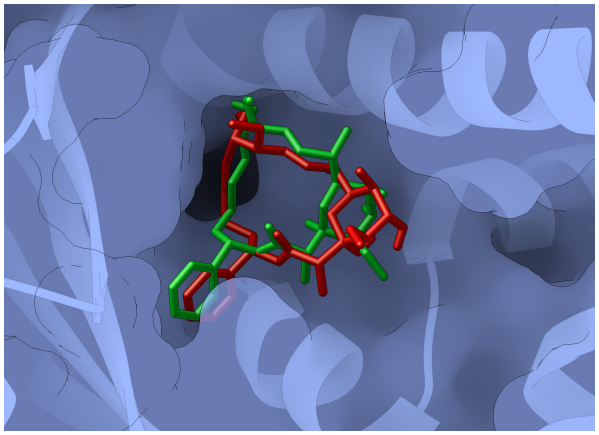


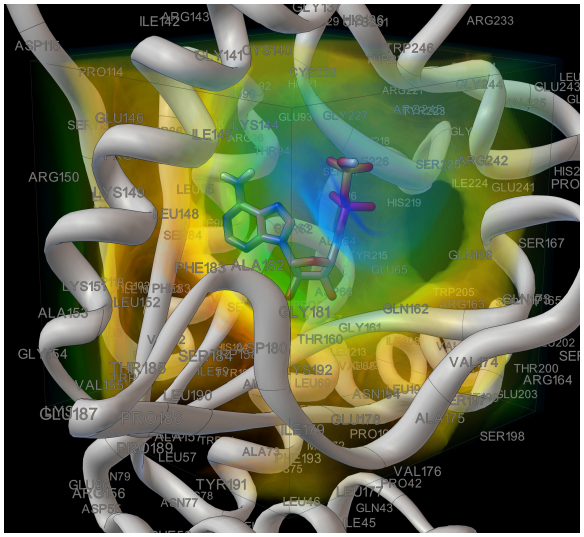






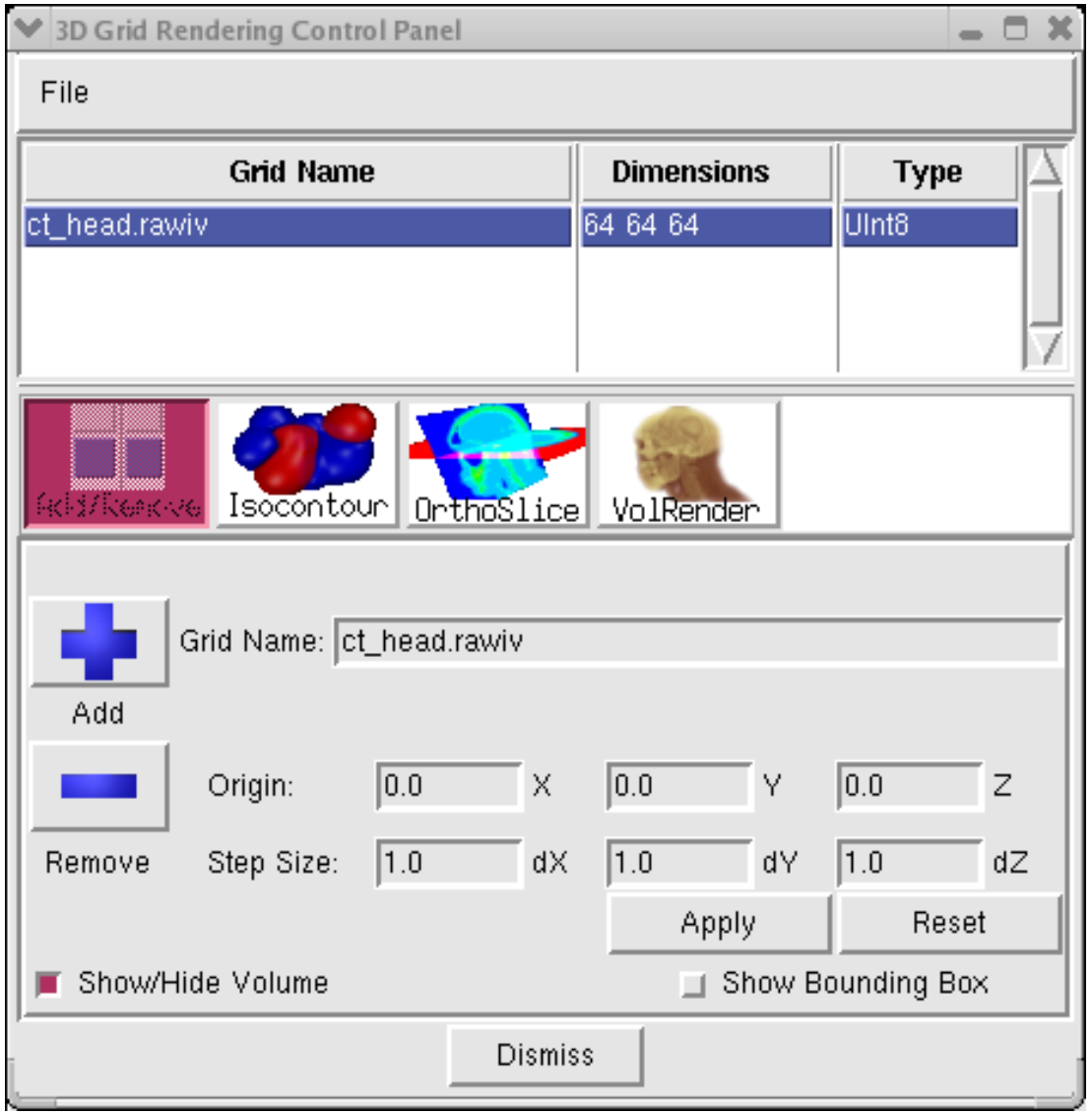


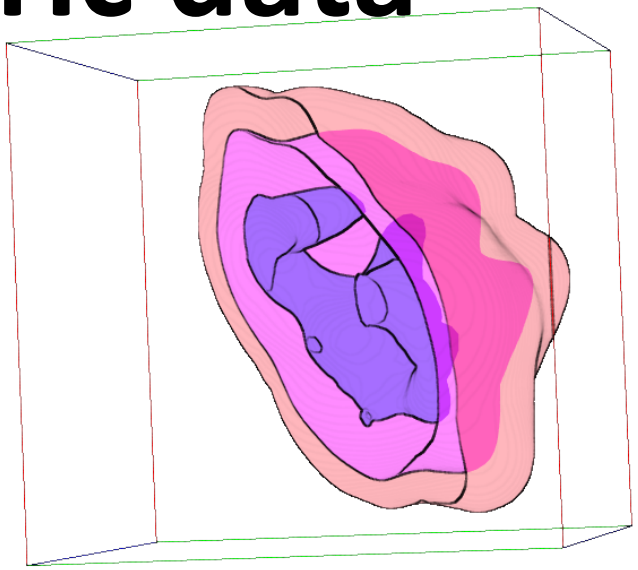


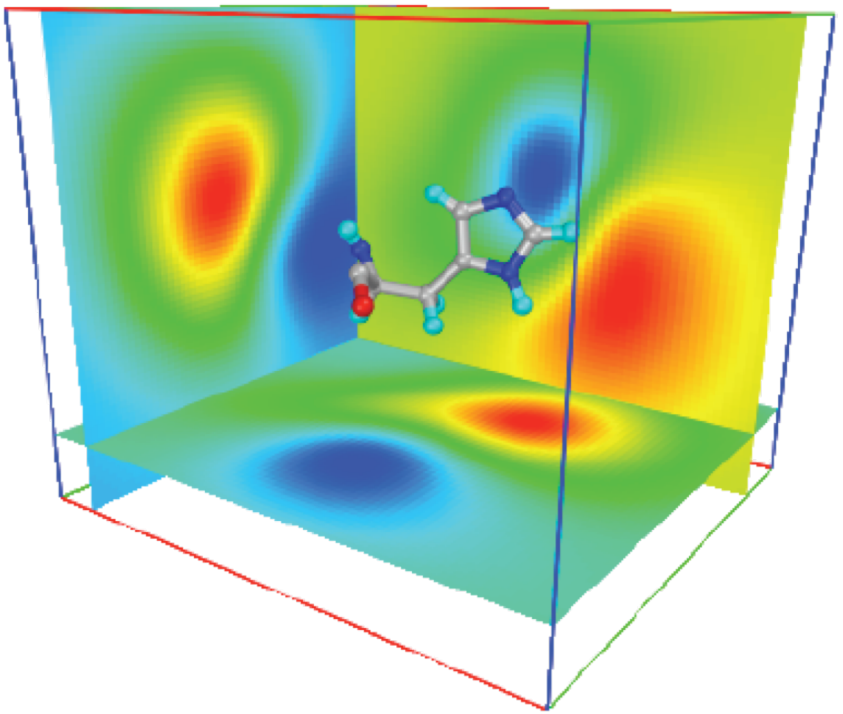


Rendering: Volumetric data

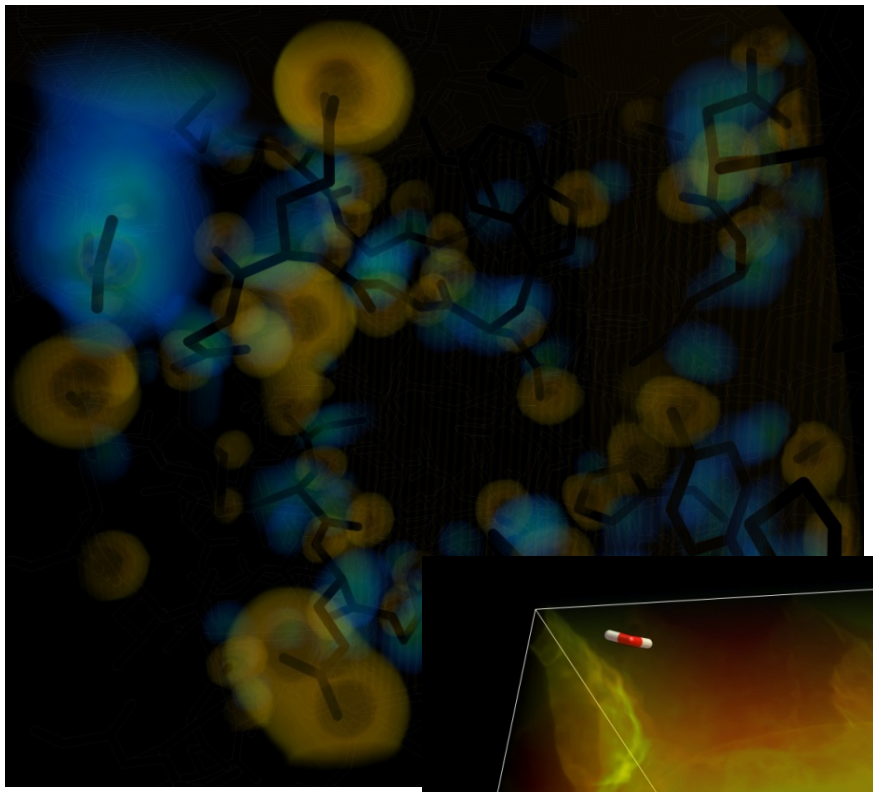
- The Pmv interface to Volume

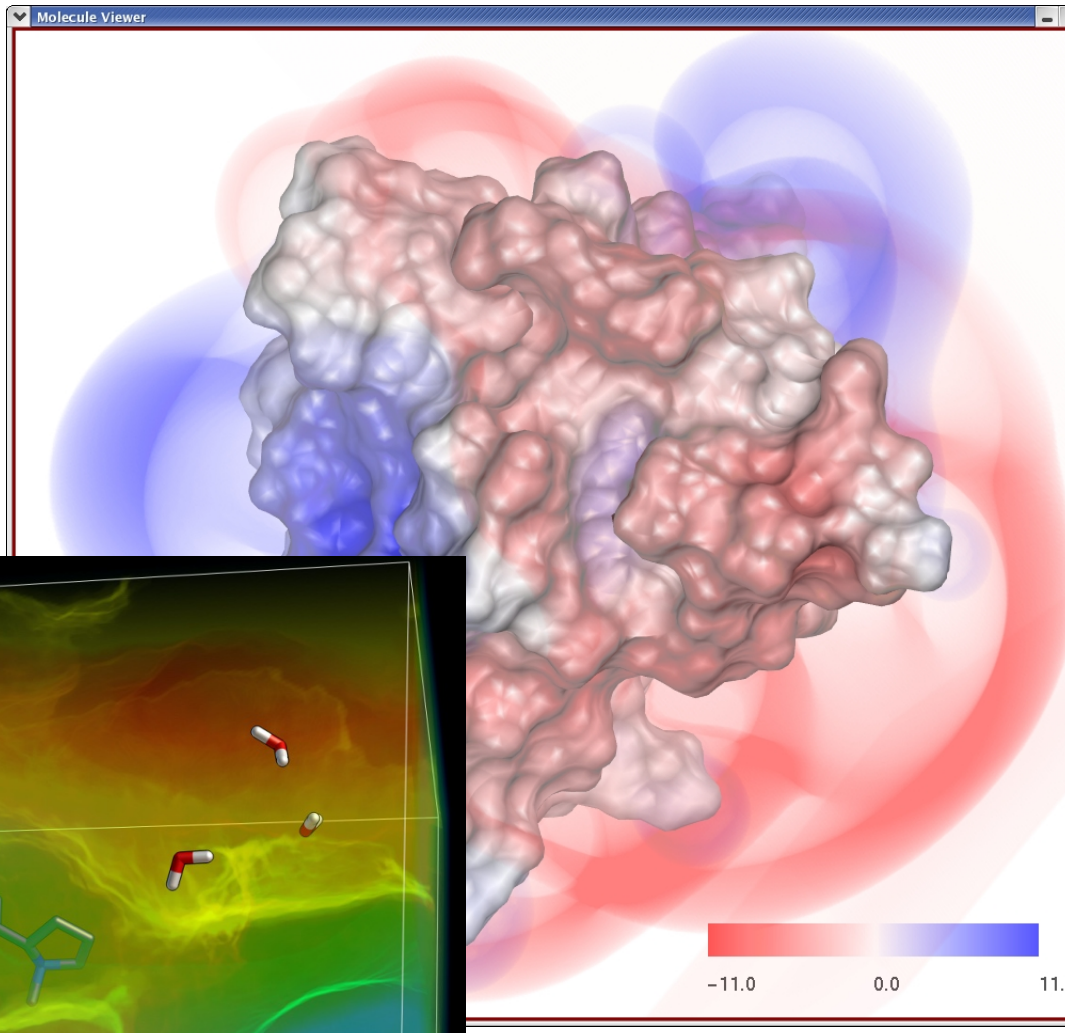


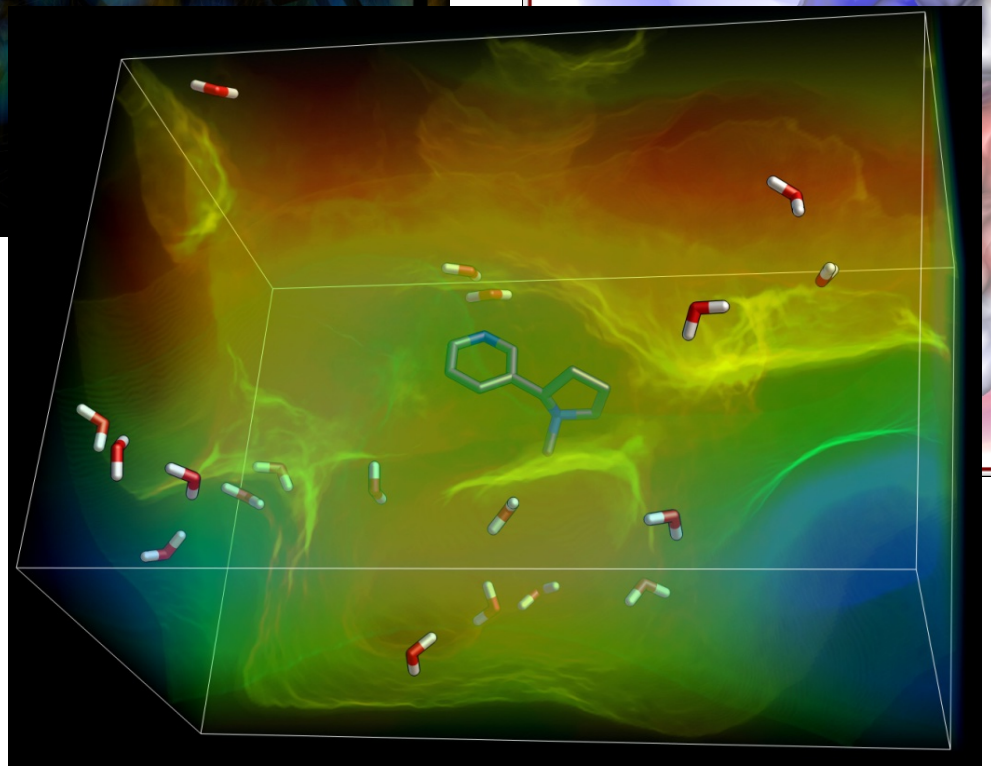




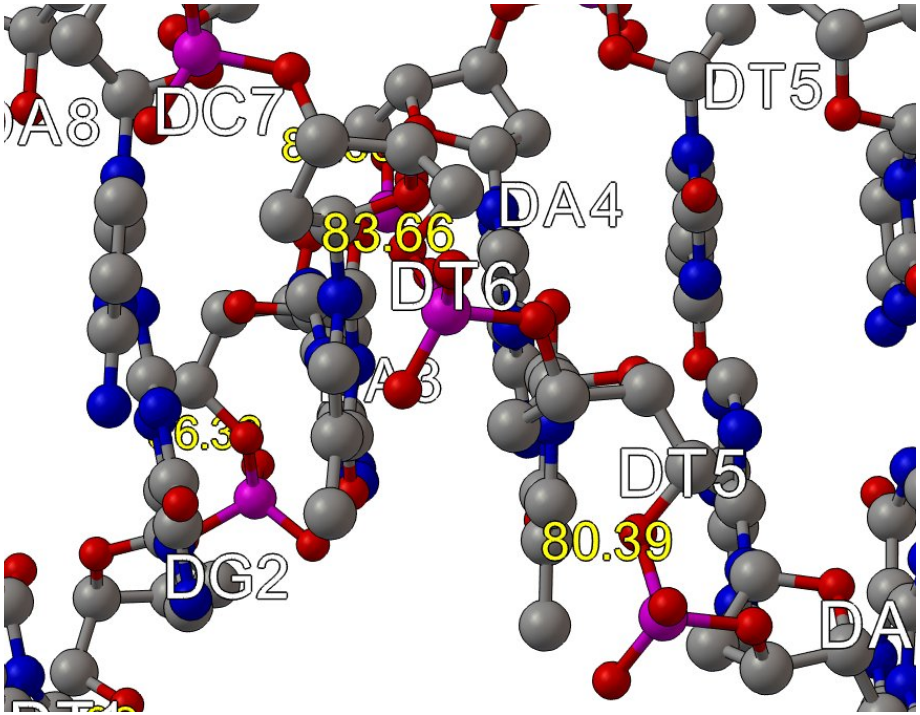
Rendering Volumetric data

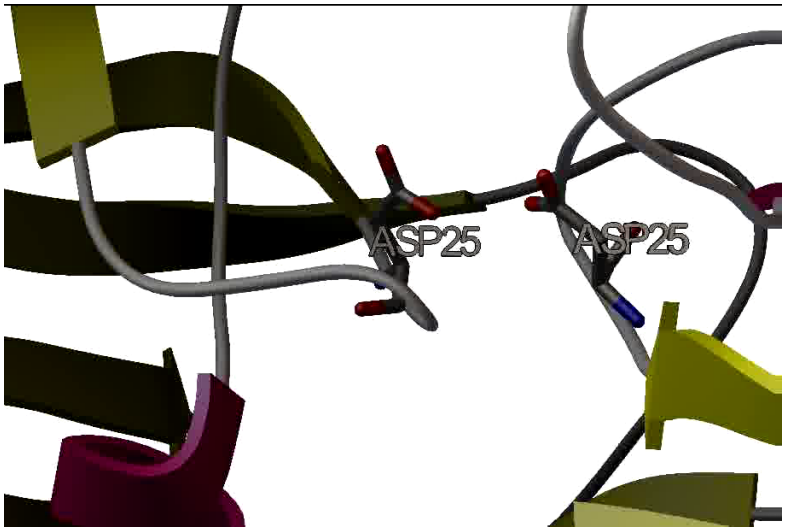


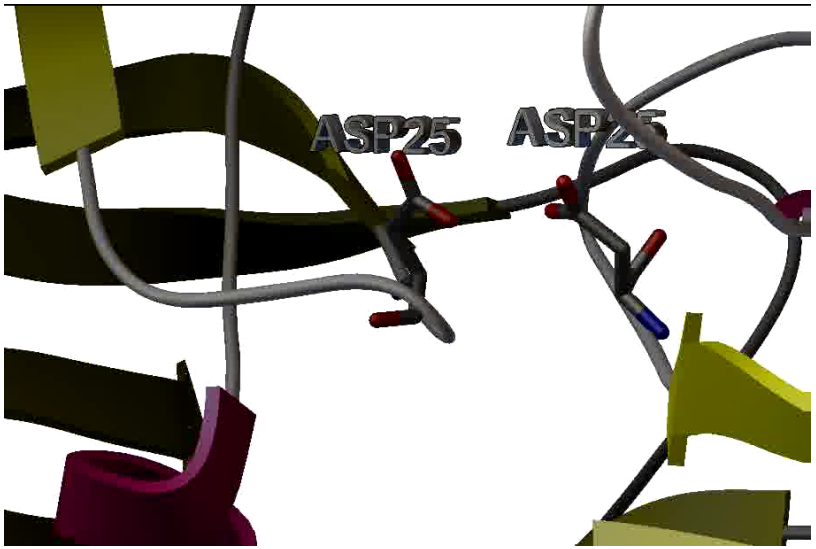




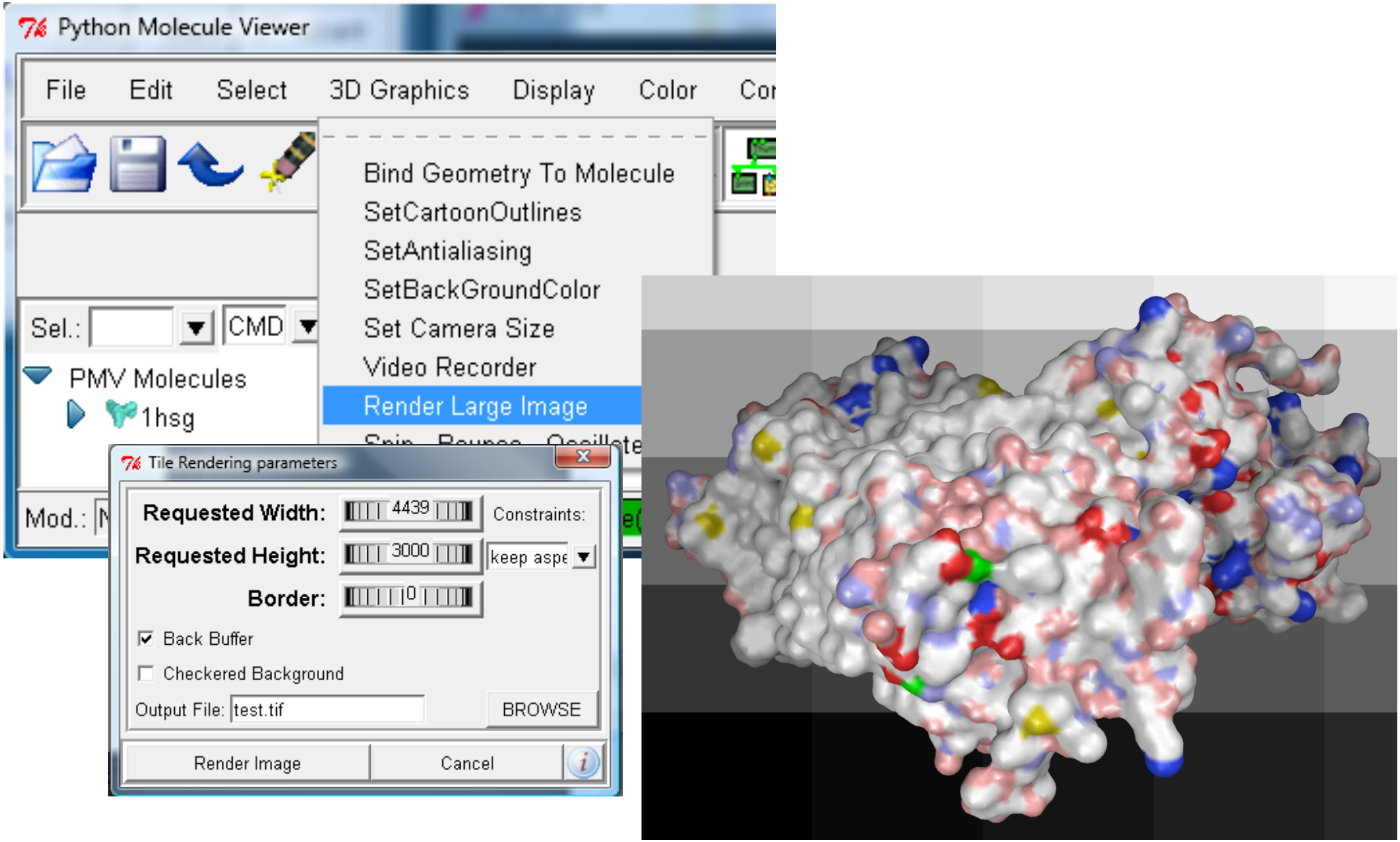
Rendering: 3D Labels



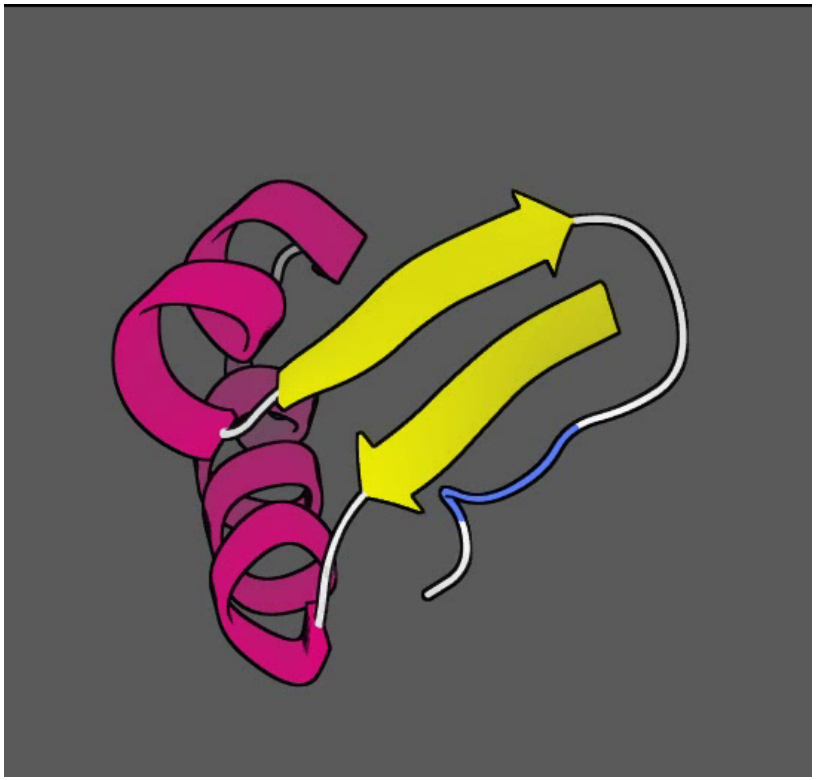


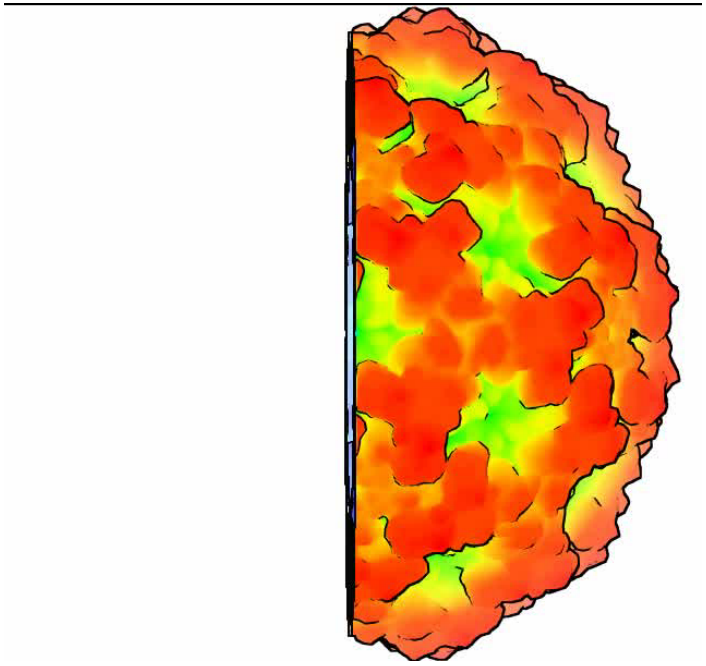


Rendering Modes: Large Images

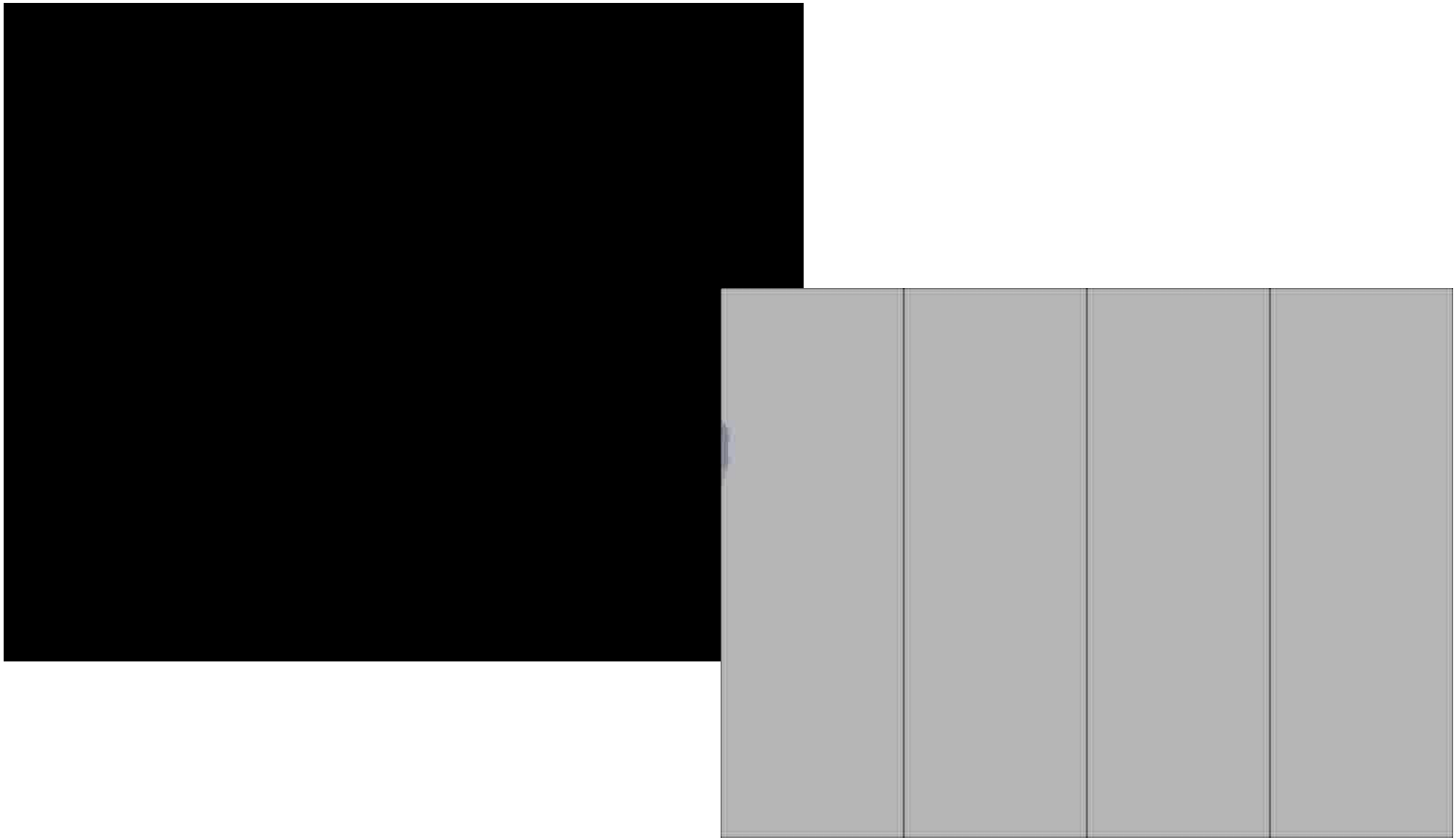


Rendering Modes: NPR

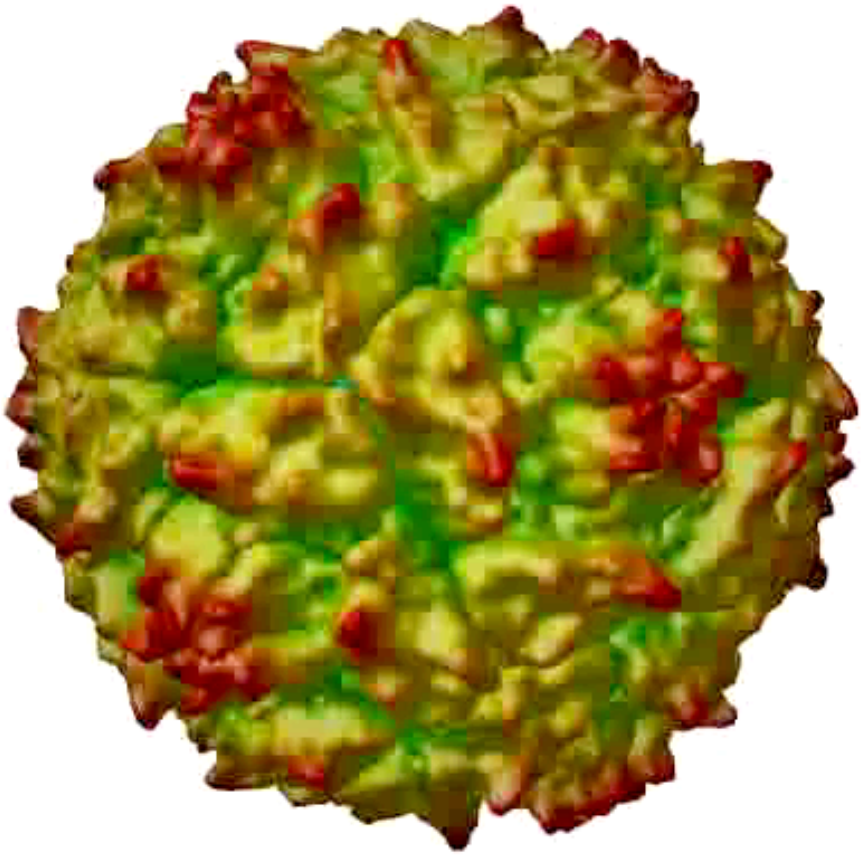




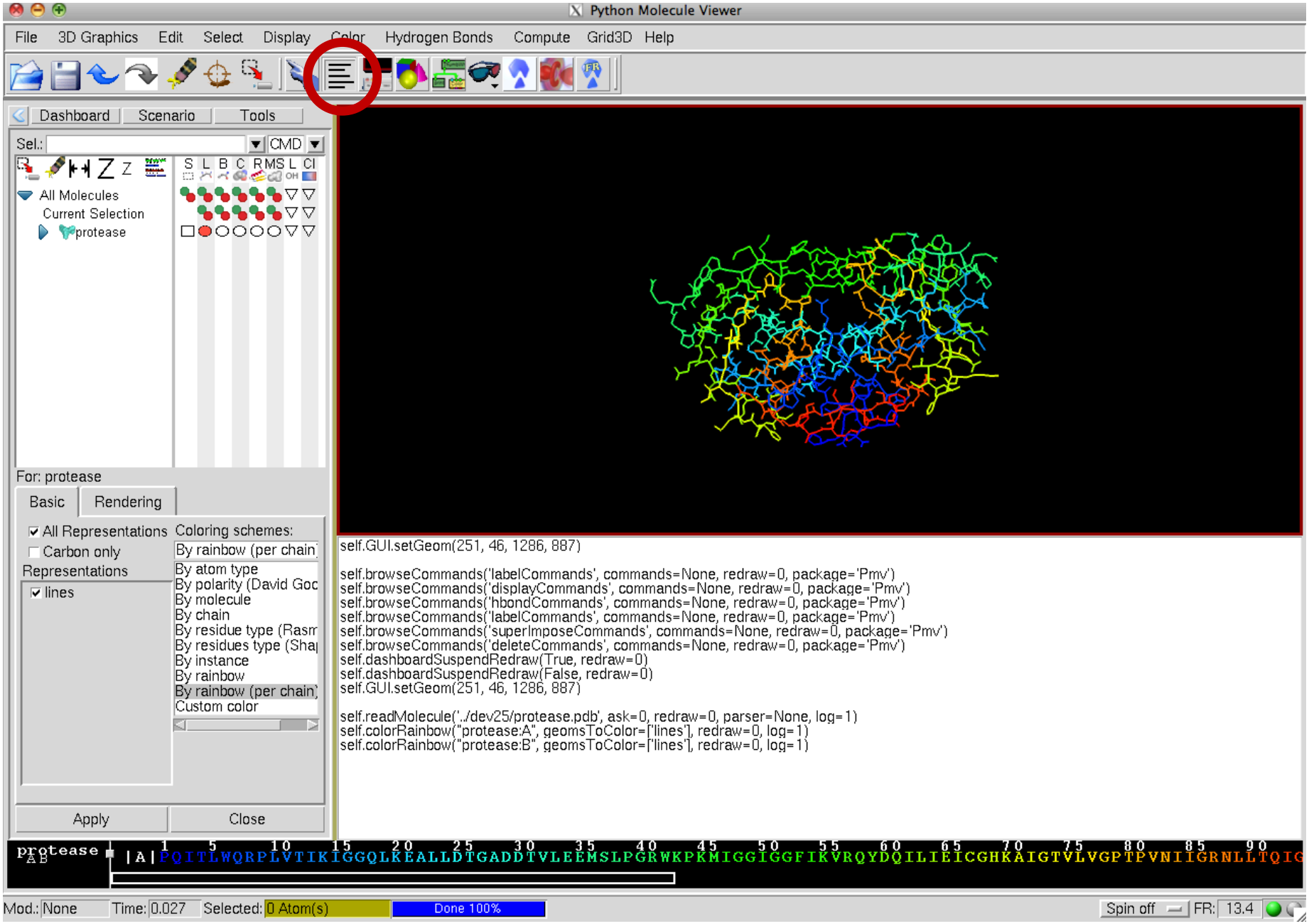
OpenGL Scissors



Support for point symmetry

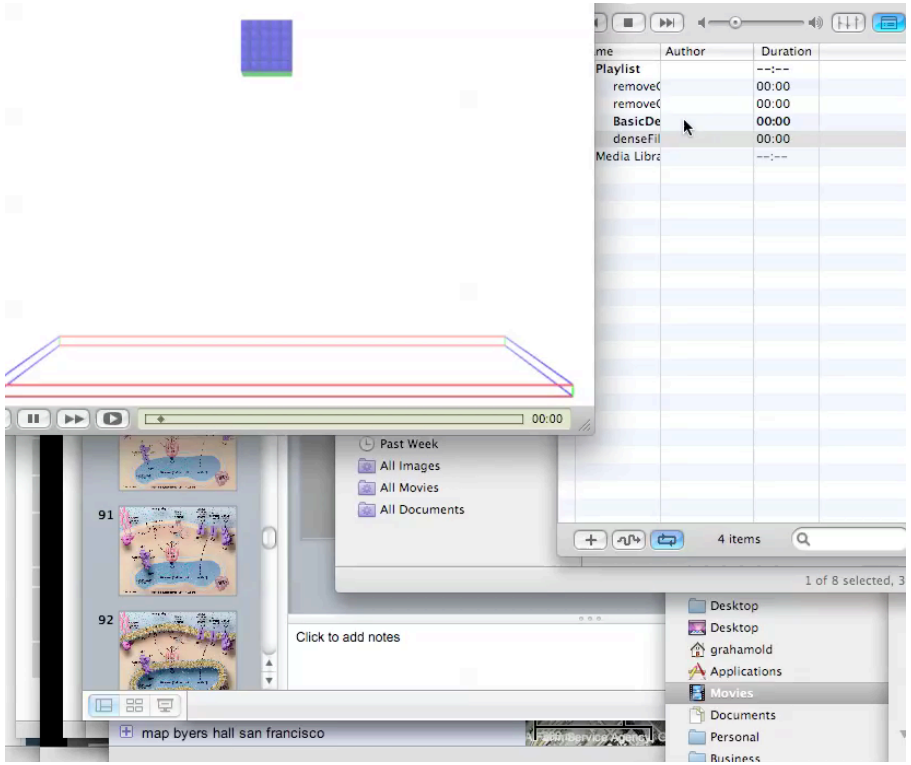


Vision: scripting Pmv



Animations

- Scripted in Python
- Frame grabbing
- Using Vision
- Using Scenario



Antigen-antibody encounter reactions:
simple laws explain complex dynamics

Advanced animation
Brownian dynamics (1000 steps of 1 nano second each)

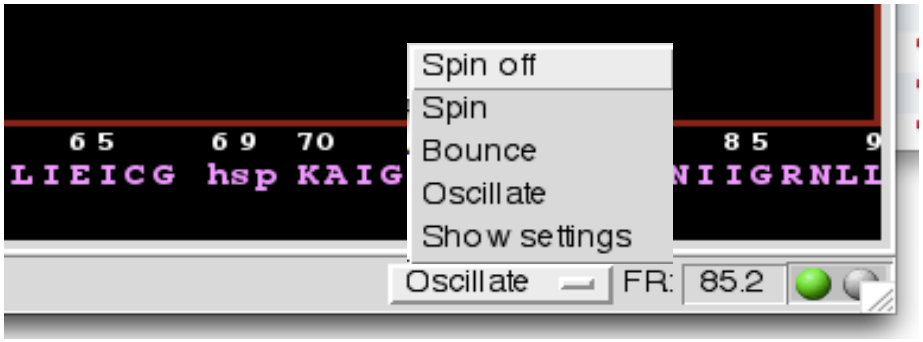
L. Bongini, D. Fanelli, F. Piazza,
P. De Los Rios, S. Sandin, M. Sanner, U. Skoglund

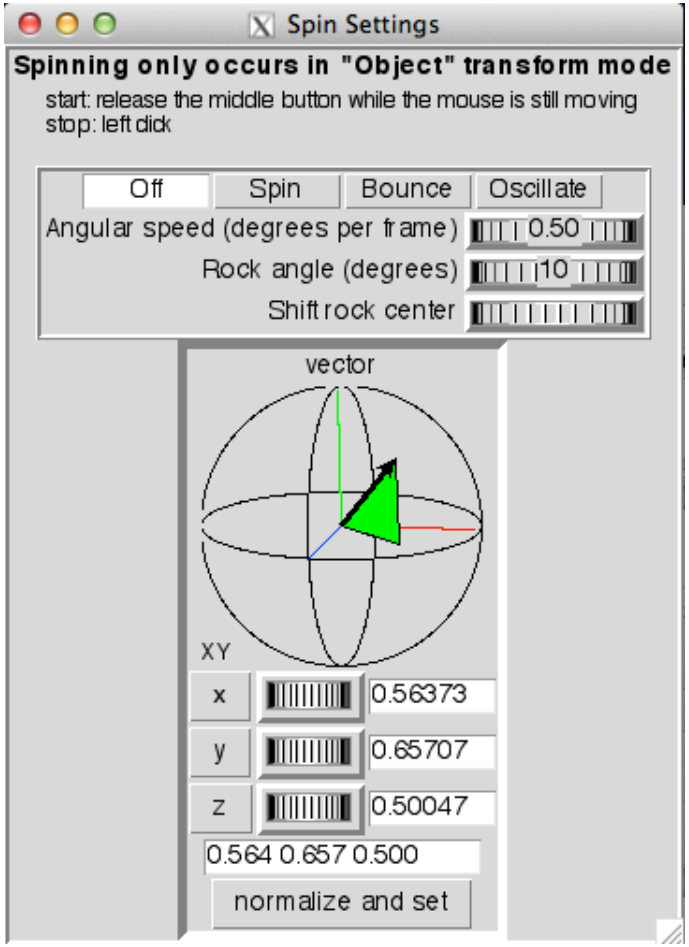
May 2005

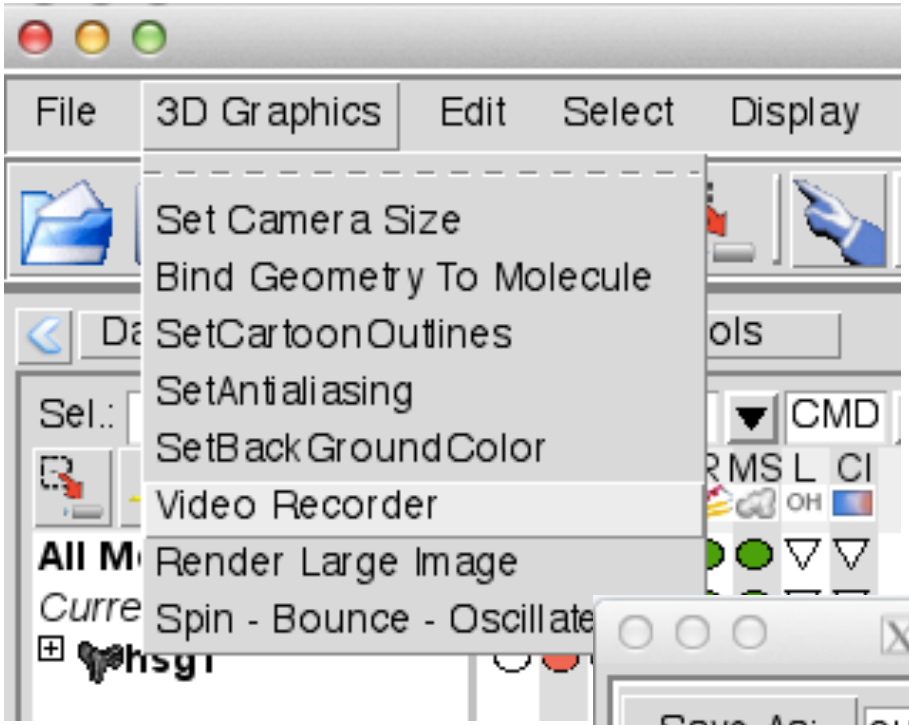
375 lines of Python code

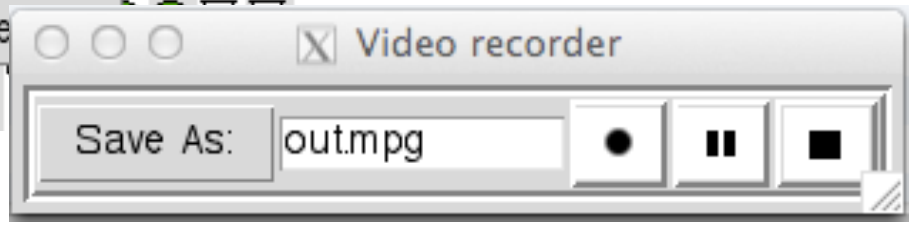
Interactive Frame grabbing

Pmv: simple animations

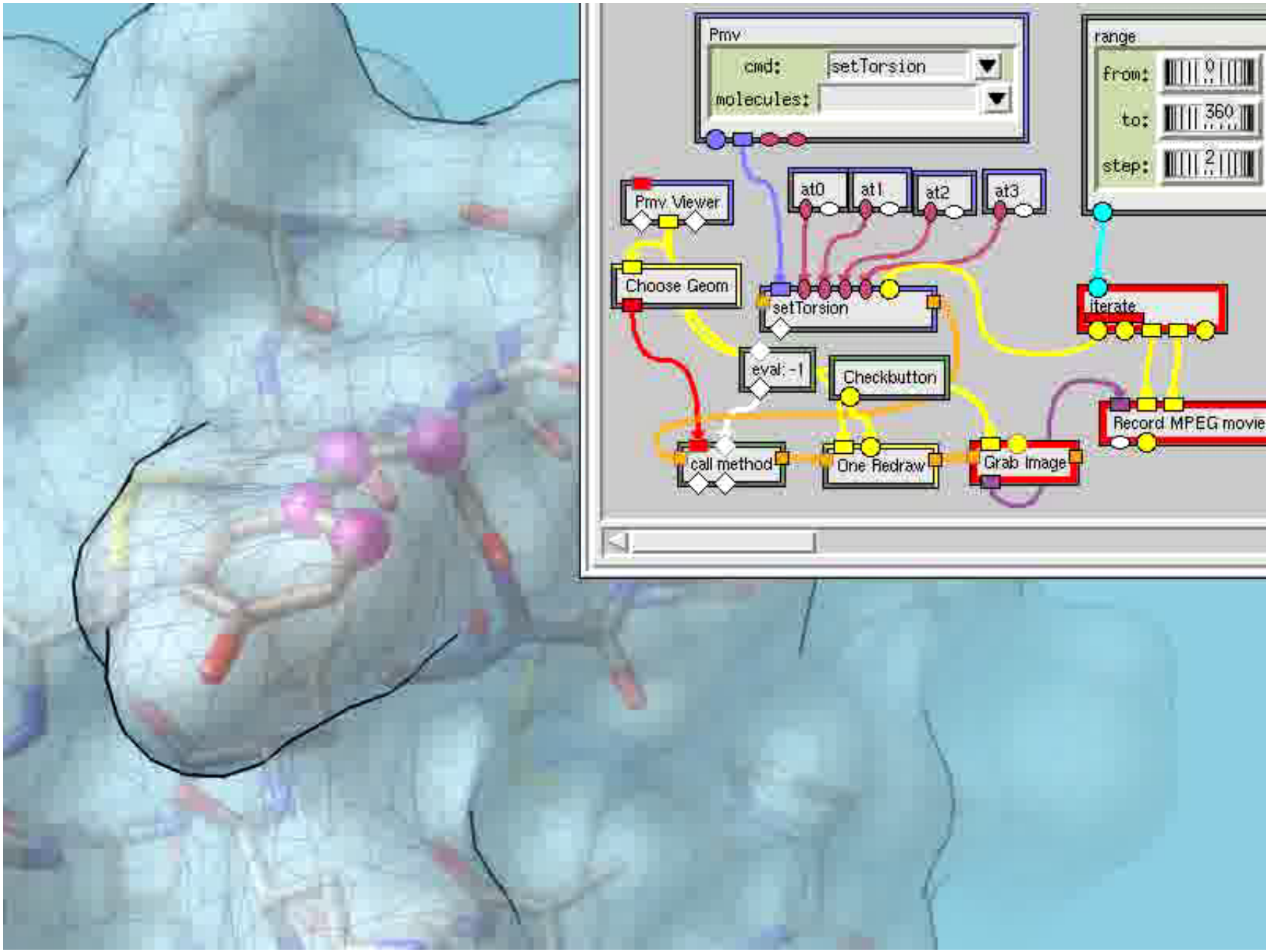




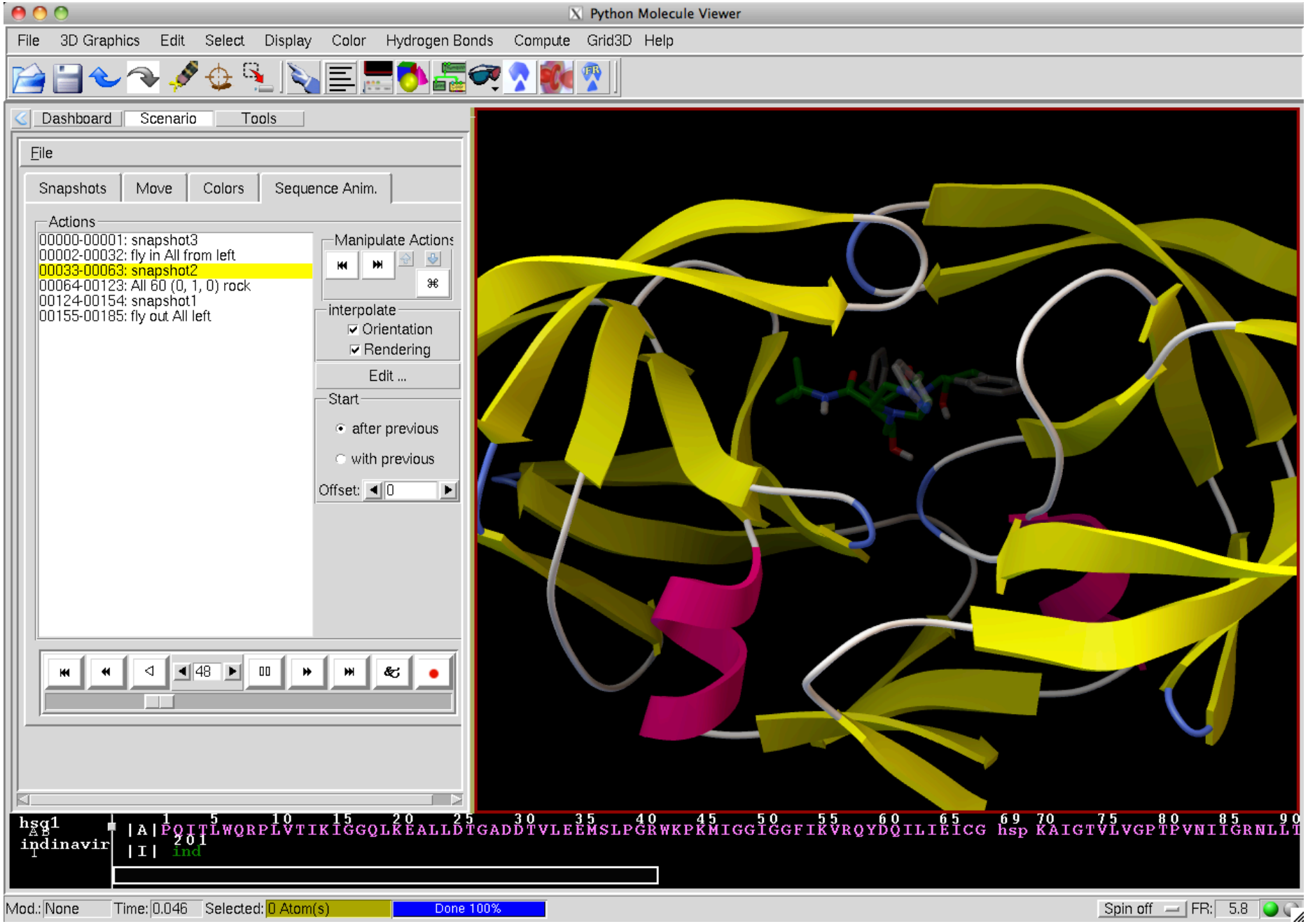


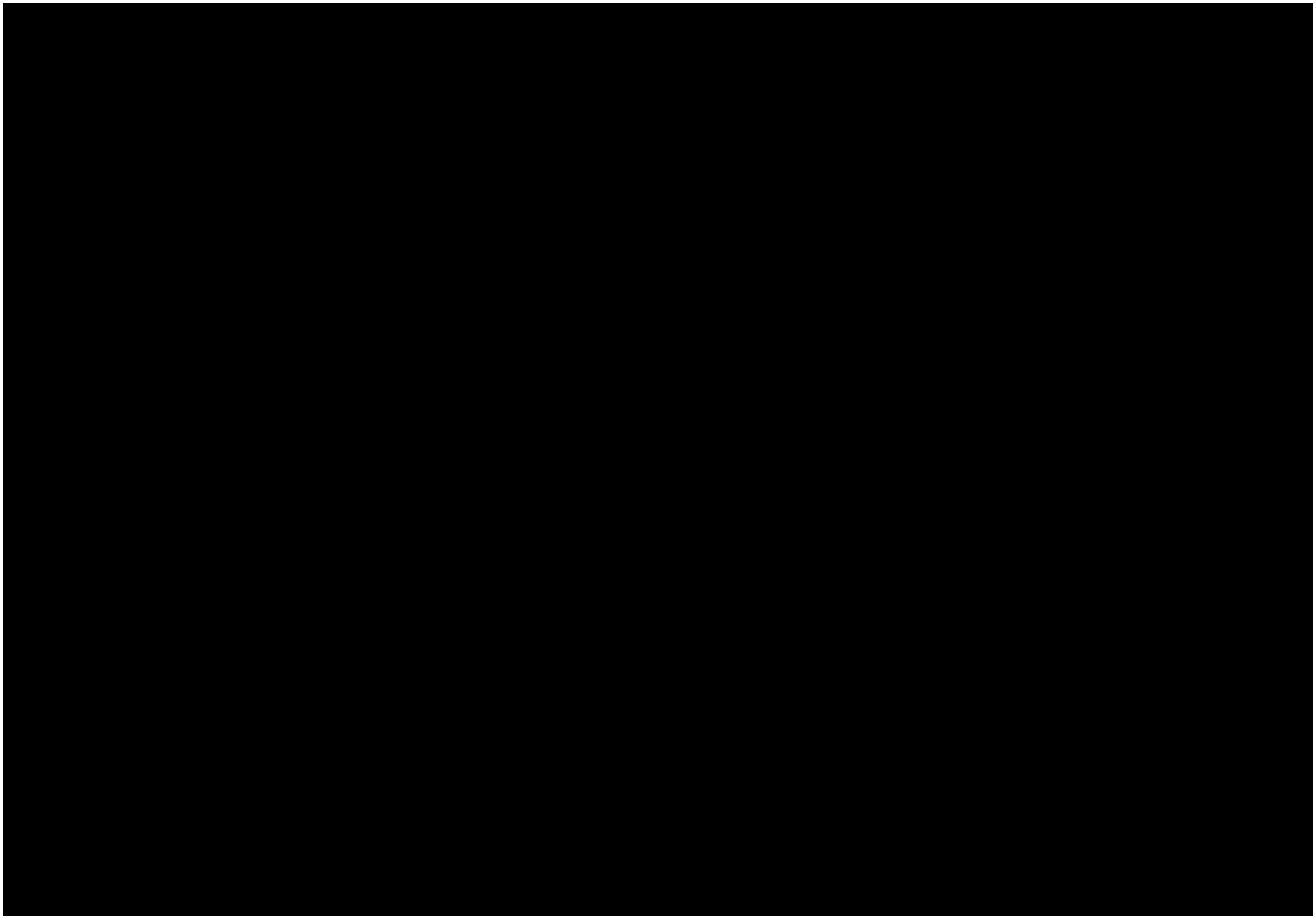


Animation: Vision



Amination: Scenario

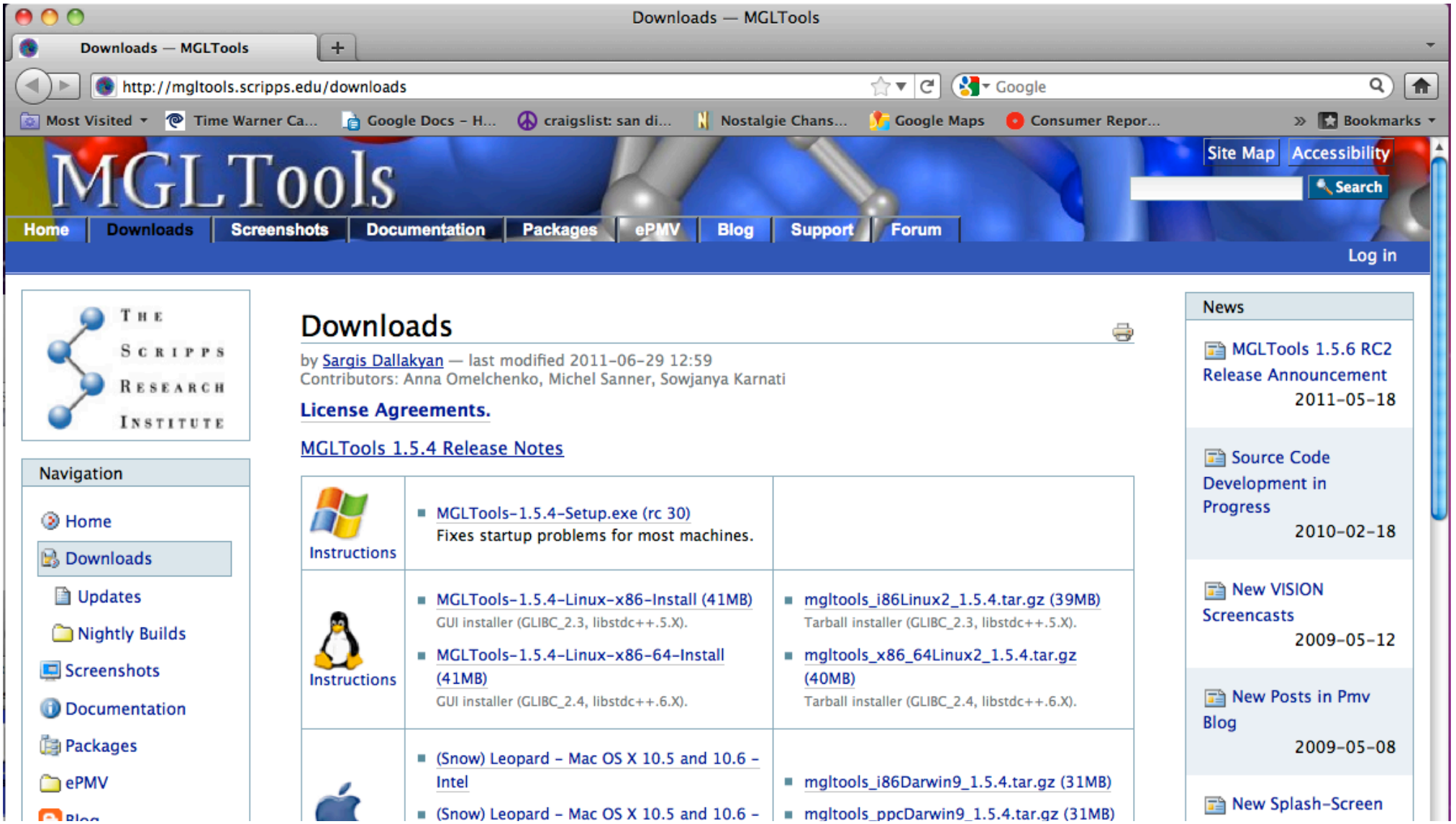




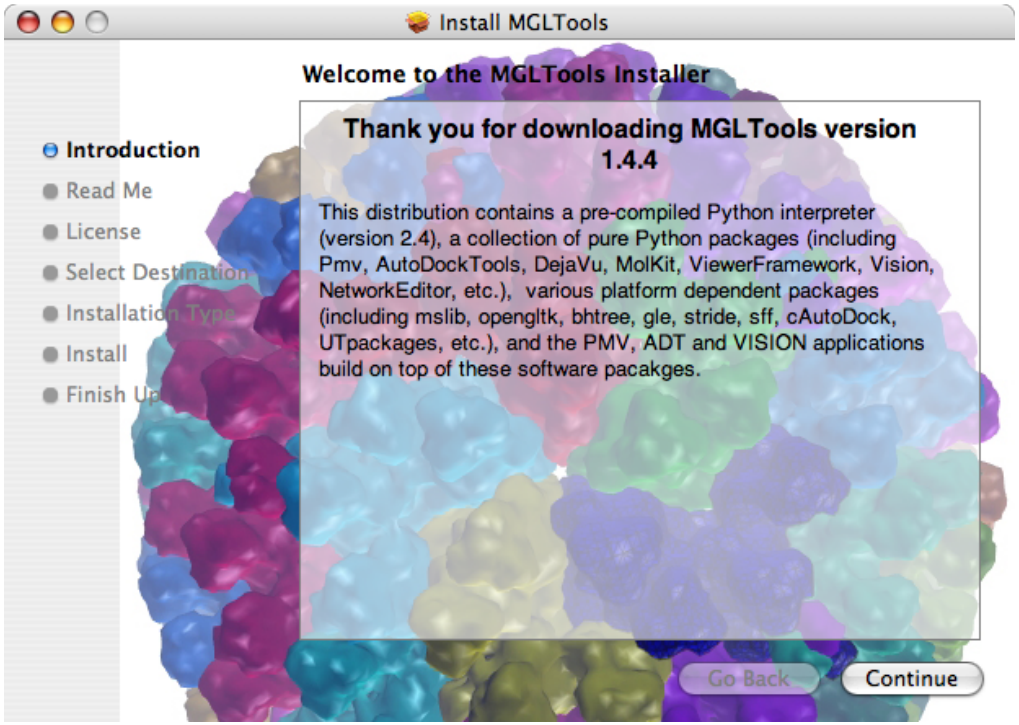
Installing Pmv

http://mgltools.scripps.edu/downloads

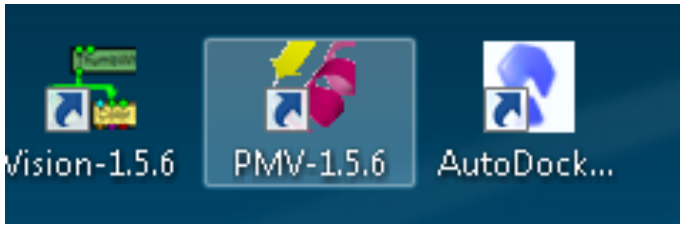
http://www.scripps.edu/~sanner/collab/TutorialData.zip



Installing Pmv



Starting Pmv

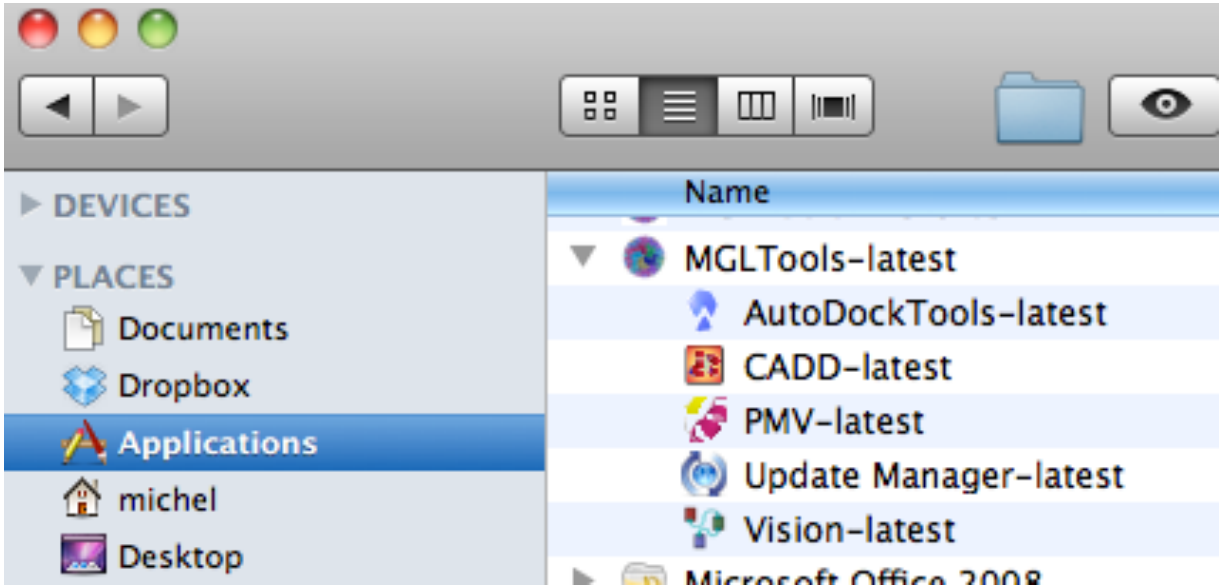


The installer placed 3 icons on the desktop. To start Vision double click on the Vision Icon.

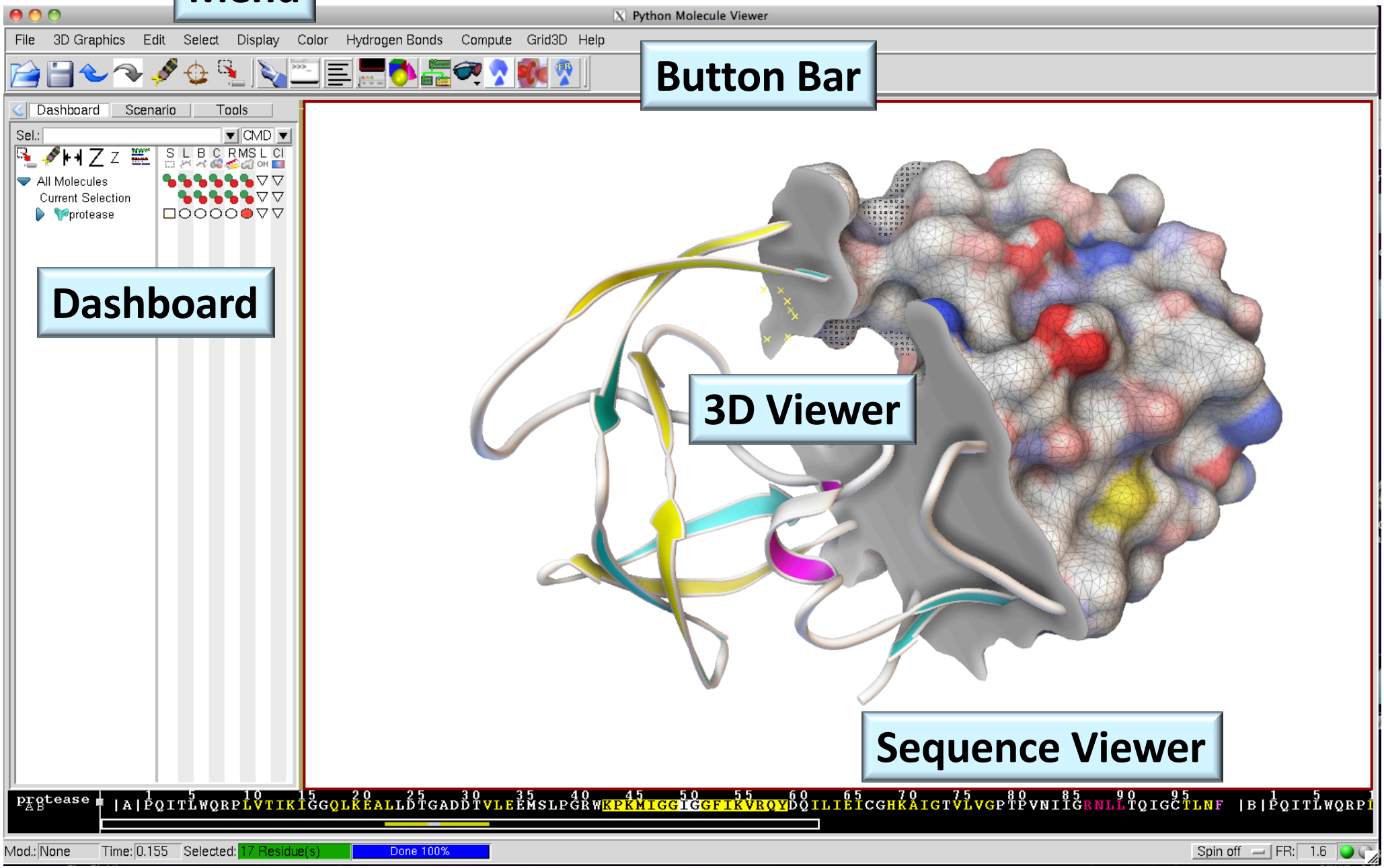
The installer created the pmv shell script

$MGLROOT/bin/pmv.

Where MGLROOT is the folder you chose to install the software



Starting Pmv

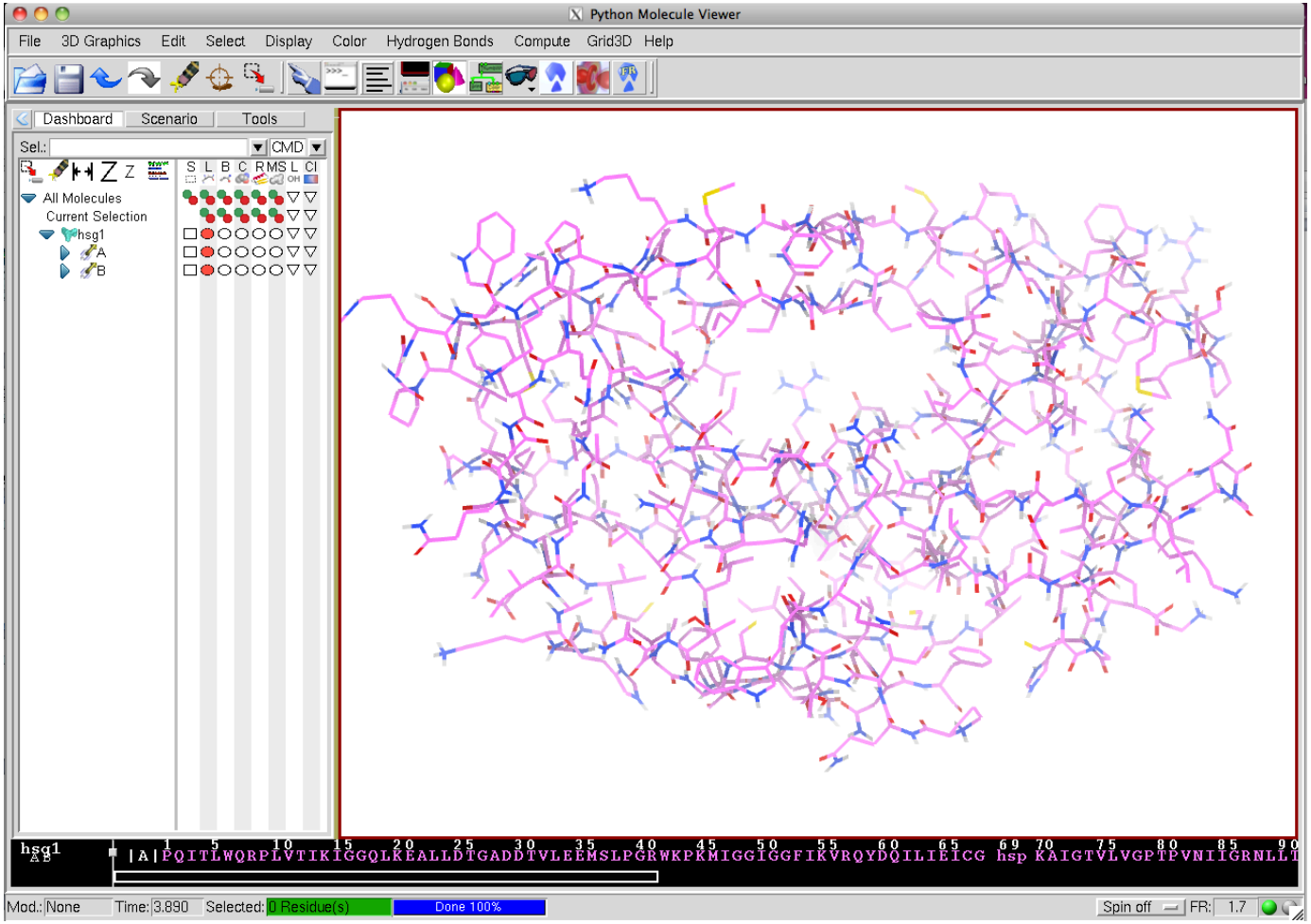


Exercise: start Pmv

Task: loading molecules into PMV

1 – start Pmv

2 – load the molecule hsg1.pdbqs is located in Desktop/TutorialData
using the menu entry File -> Read Molecule



Exercise: Loading molecules

Task: alternatives for loading molecules into PMV

1 – right click on “All Molecules” in dashboard
2 – File -> Read Molecule
3 – File -> Recent Files
4 – File -> Import -> Fetch From Web
5 – using command line: pmv mymol.pdb

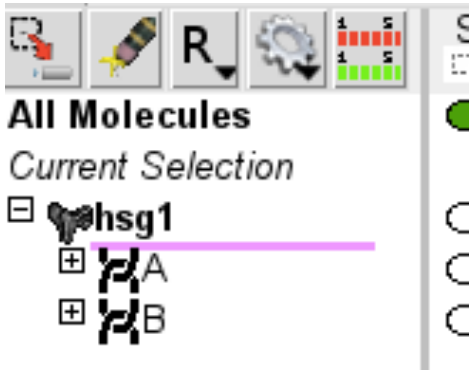
NOTES:
1 – multiple molecules can be selected in the file browser
2 – wildcards can be used on the command line (e.g. pmv –i test*.pdb)
3 – using a pdb id on the command line will fetch the protein from web unless it is in the cache

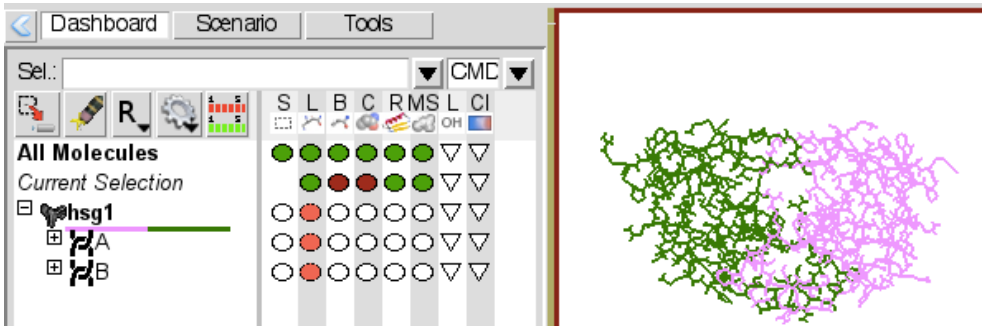
Exercise: Right click menu

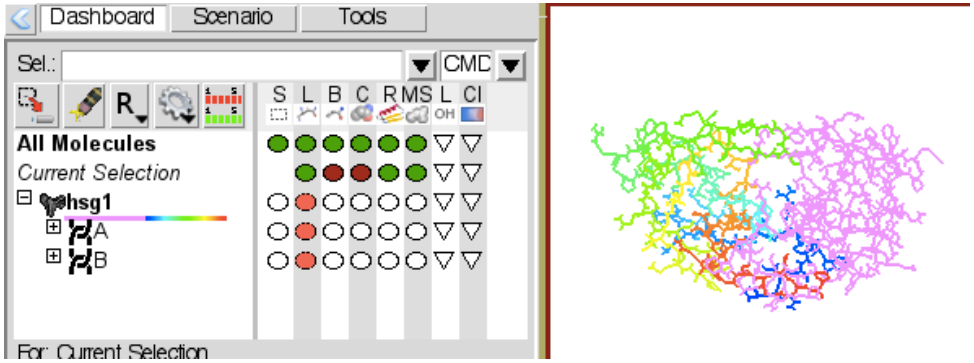
1 – Right click on elements in the dashboard usually displays a menu
2 – The "All Molecule" menu allows showing/hiding all molecules and add a colored line in the dashboard to help identify molecules
3 – Double clicking on molecule names show/hides the molecule

Task: Show the color ID of hsg1

1 – right click on "All Molecules" in dashboard
2 – Show molecules color ID







Exercise: Pmv mouse

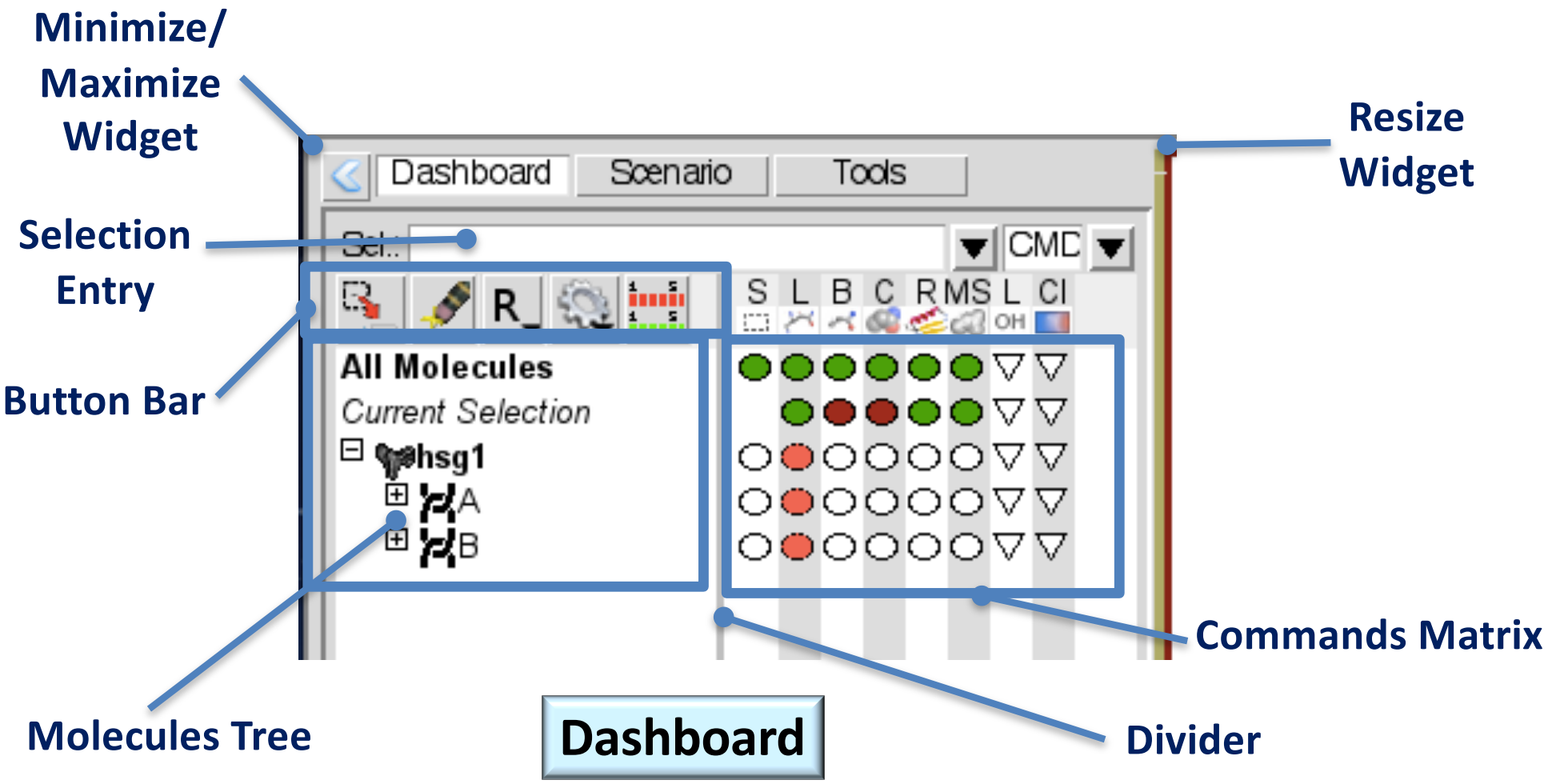
Button / Mod	Left	Middle	Right	Wheel
None	*Rotate*		*Translate left/right (X) and up/down (Y)*	*Zoom*
Shift	*Add to Selection*		*Translate in/out (Z)*	
Ctrl	*Remove from Selection*		*Center on Pixel*	

Exercise: Pmv key bindings

Task: learn PMV viewer keystrokes

Key	Action
R	***Reset*** *view*
N	***Normalize*** *– scale so all visible molecules fit in the Viewer*
C	***Center*** *on the center of gravity of all the molecules*
D	*Toggle on/off* ***Depth-cueing*** *(blends molecule into background farther away)*
T	*Toggle between* ***transform root*** *(i.e. scene) and transform the Viewer's current object*
A	***Auto Depth-cueing*** *(set fog to cover depth of the current scene)*
L	*Toggle on/off OpenGL* ***Lighting*** *(turns on/off photorealistic lighting)*
O	*Toggle* ***Ambient Occlusion***

Pmv dashboard

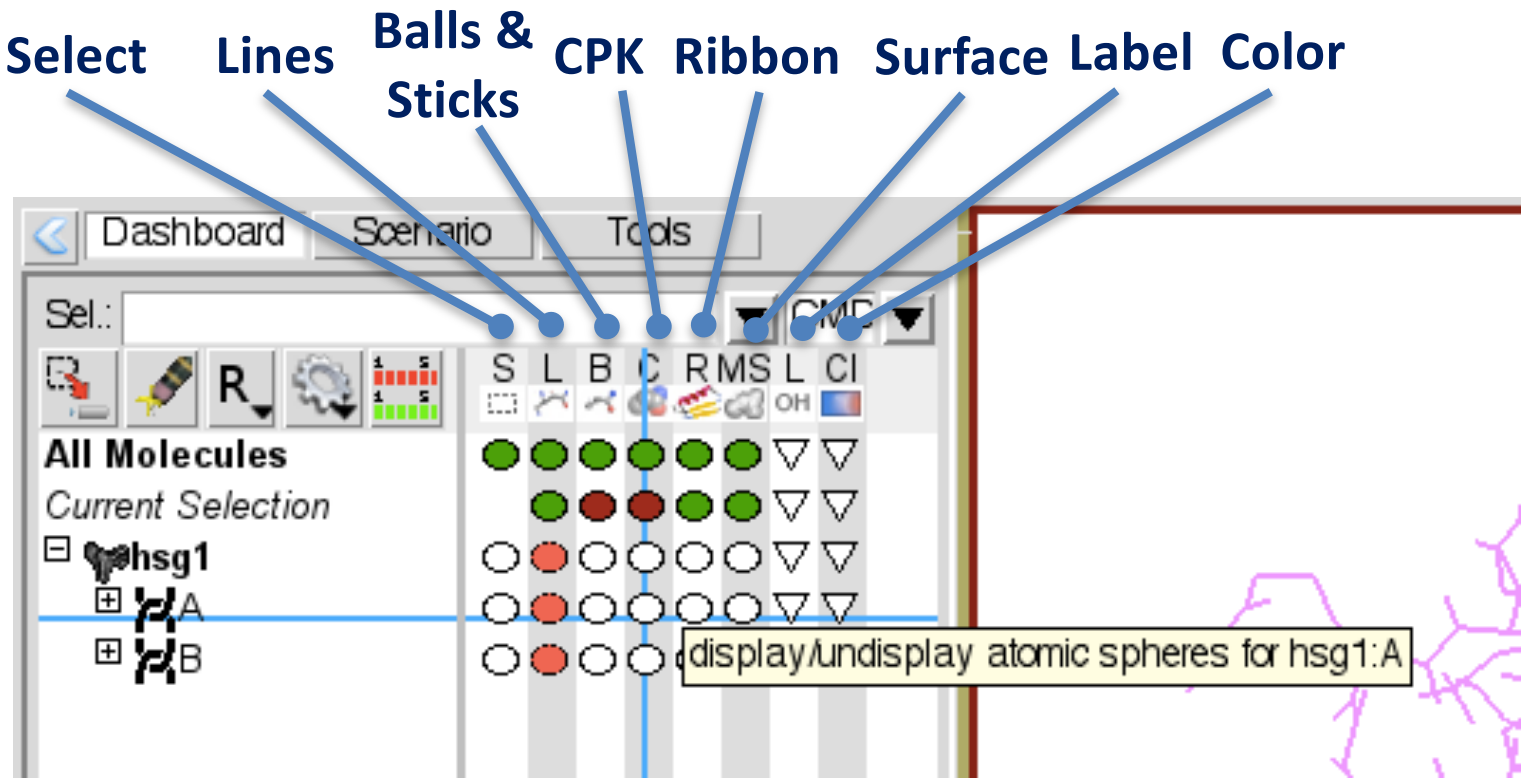


Exercise: Pmv dashboard

Task: dashboard

1 – hoover mouse over glyphs and read tool tips
2 – expand/collapse molecule tree
3 – make the dashboard wider
4 – move the divider right and left. Notice the labels in the molecule tree change upon mouse button release
5 – minimize dashboard
6 – restore dashboard
7 – find the button that sets the dashboard width to show all columns and restore dashboard's default size

Dashboard Command Matrix

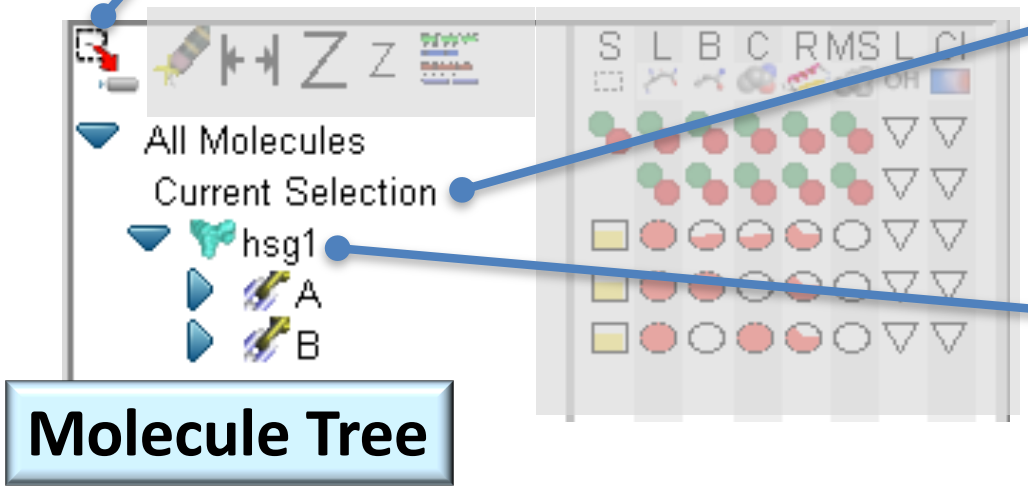


Notes:

- Tool tips on all command buttons

Dashboard Molecule Tree

Create a set using
the current selection

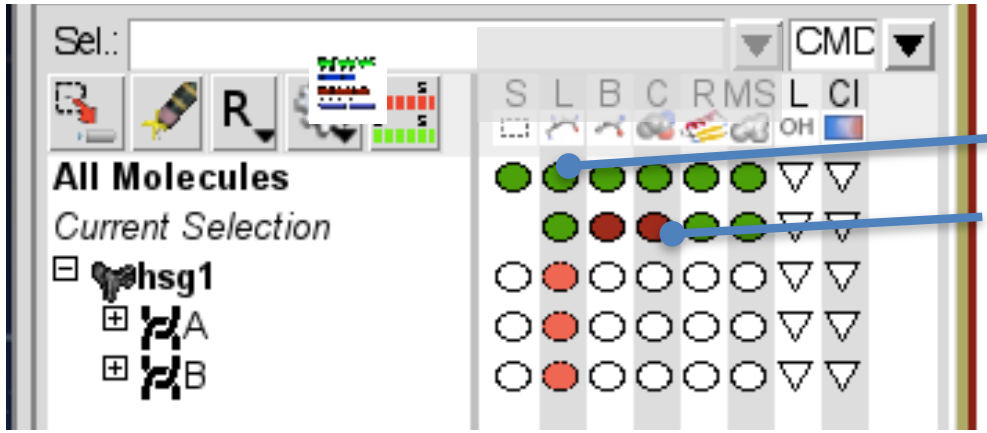


sets: cannot be expanded
represent molecular fragments
From the molecules loaded in Pmv

Molecules: can be expanded
to show chains, residues, atoms

Dashboard Command Buttons

On/Off Buttons



Left click to:

Display lines for all molecules

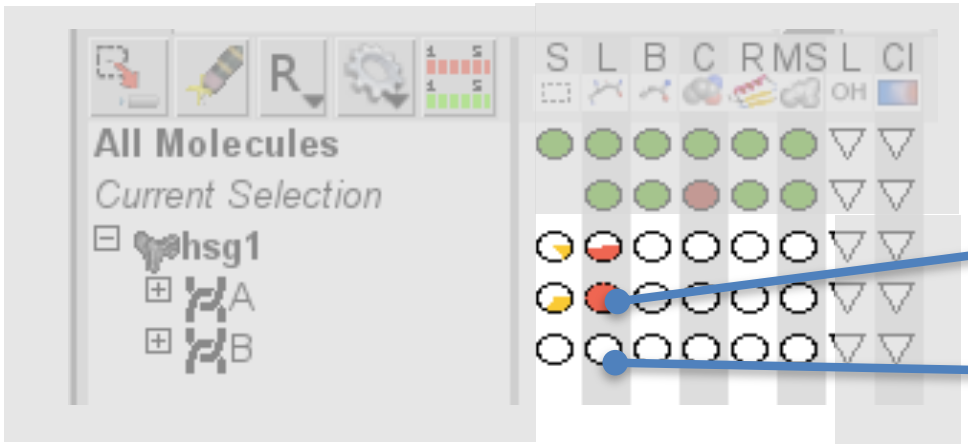
Undisplay CPK for the current selection

Notes:

- **No state**
- **Left mouse toggles on/off command mode**
- **Right mouse click to display command specific menu**
- **Green button triggers command (i.e. select, display lines, etc …)**
- **Red button triggers inverse of the command (i.e. deselect, un-display lines, etc…)**
- **Used for sets (i.e. current selection, user defined sets (see below))**

Dashboard Command Buttons

Percentage Buttons



Left click to:

Un-display lines for chain A

Display lines for Chain B

- Left mouse click to activate button
- Right mouse click on green button click to display command specific menu
- Show percentage (i.e. 50% of hsg1 is displayed as lines and part of chain A is selected)
- Buttons cycle from "partial" to "full", to "empty", to "full" etc.
- Used for molecules in tree (i.e. hsg1)

Exercise: Display Lines

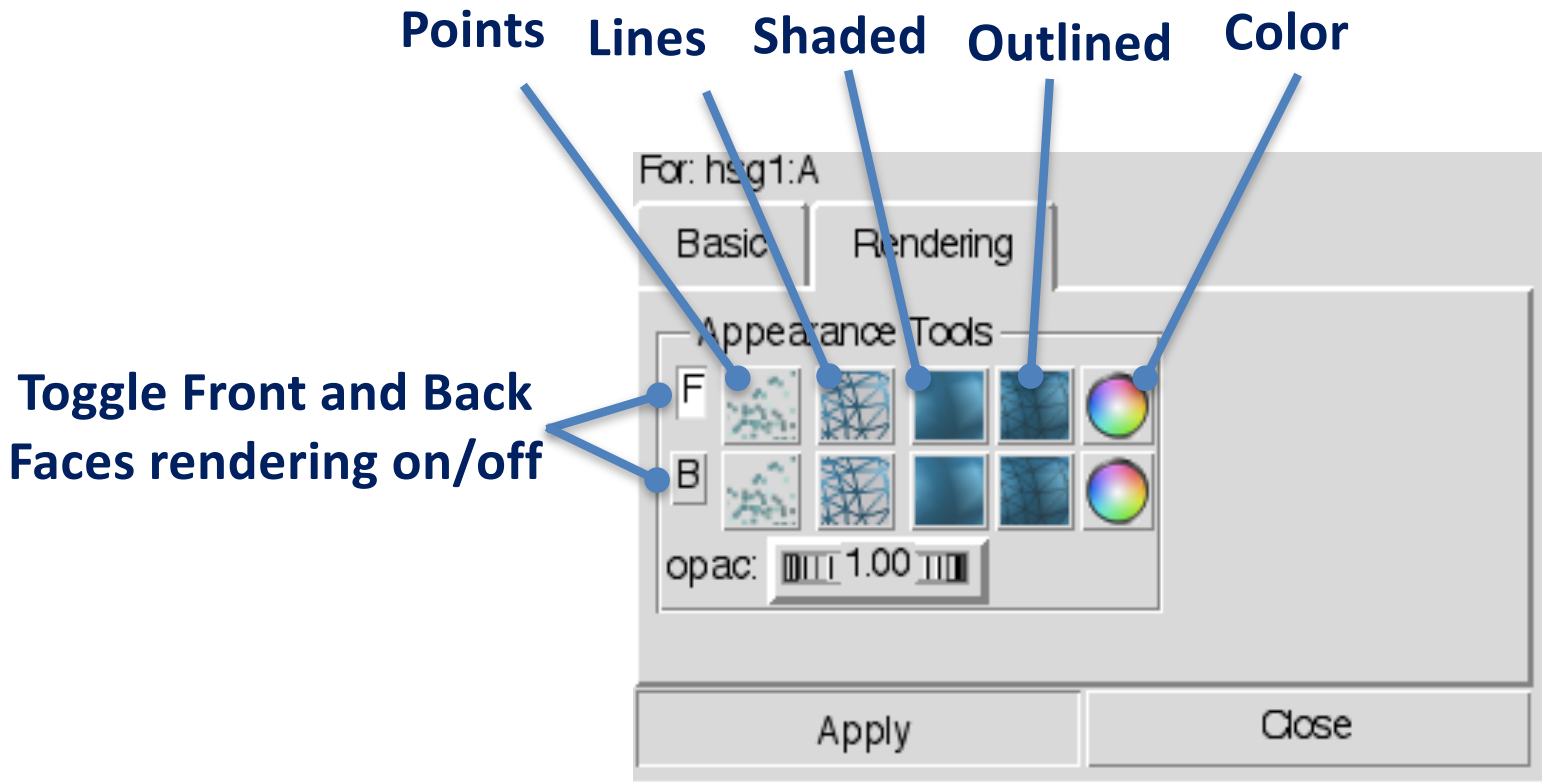
Task: display lines

1 – un-display lines for Chain A. NOTE partial line display feed back on hsg1
2 – left click 2 times on Lines for hsg1. NOTE how the button and display cycles from partial to full to empty
3 – un-display lines for chain B
4 – Right click on lines for chain B
5 – change the line width to 4

Exercise: Display Balls and Sticks

Task: geometry quality and rendering options

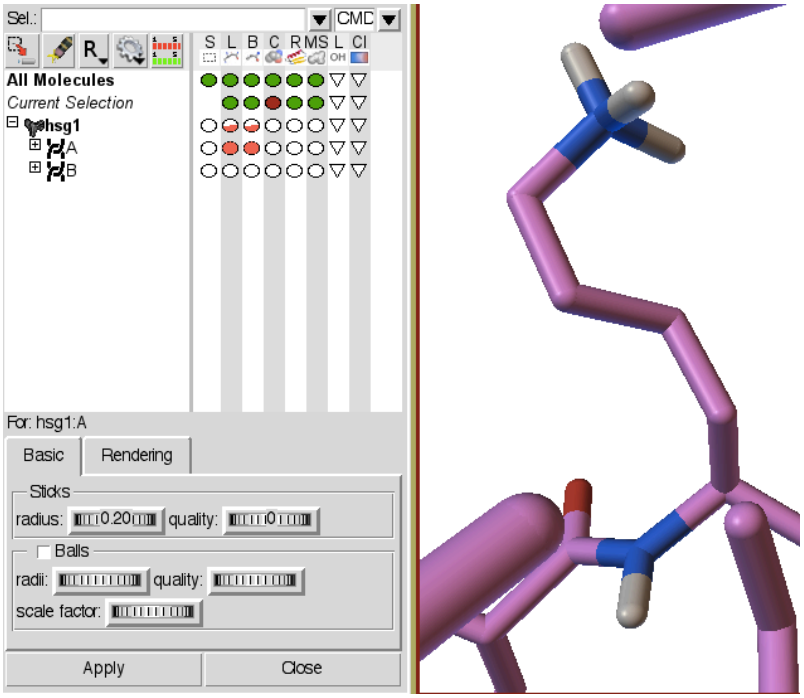
Quality changes the number of polygons used
0 automatically selects the tessellation

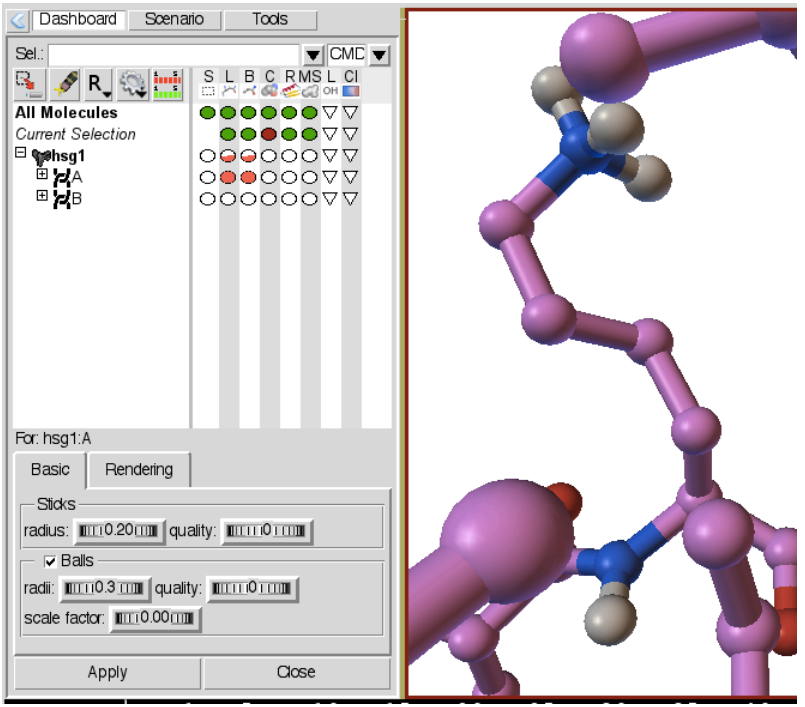


Exercise: Display Balls and Sticks

Task: display balls & sticks

1 – display B&S for chain A
2 – right click on B&S for chain B and check Balls to modify spheres radii



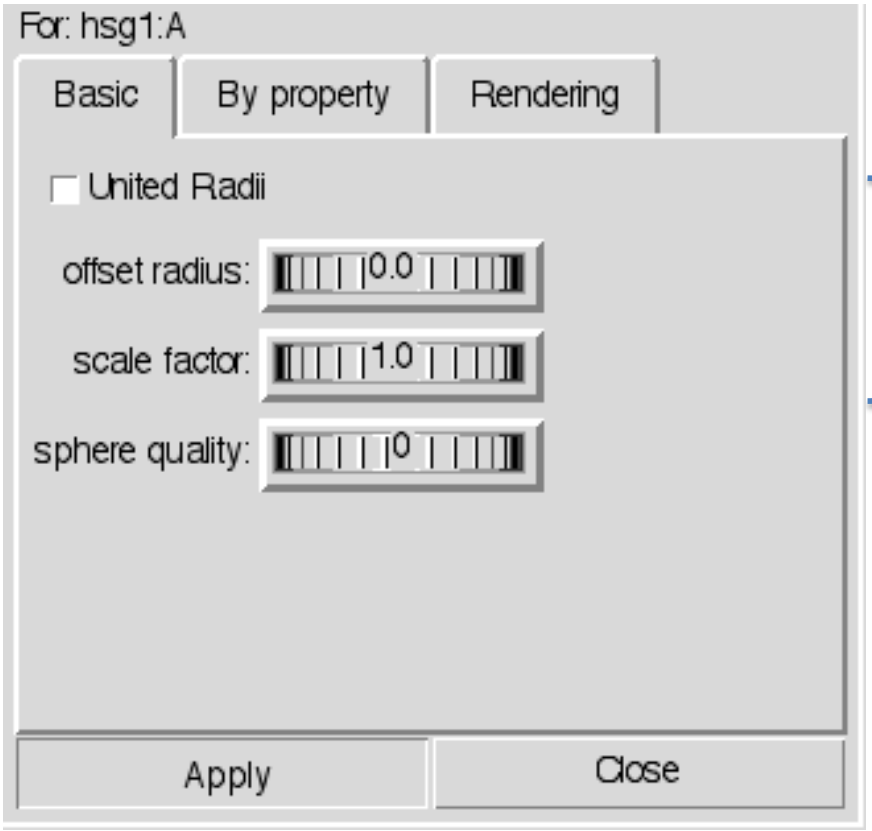


Quality changes the number of polygons used
0 automatically selects the tessellation

Exercise: Display CPK

Task: display CPK

1 – display and un-display CPK for chain A
2 – right click on display CPK for chain B to display option panel
3 – scale CPK spheres

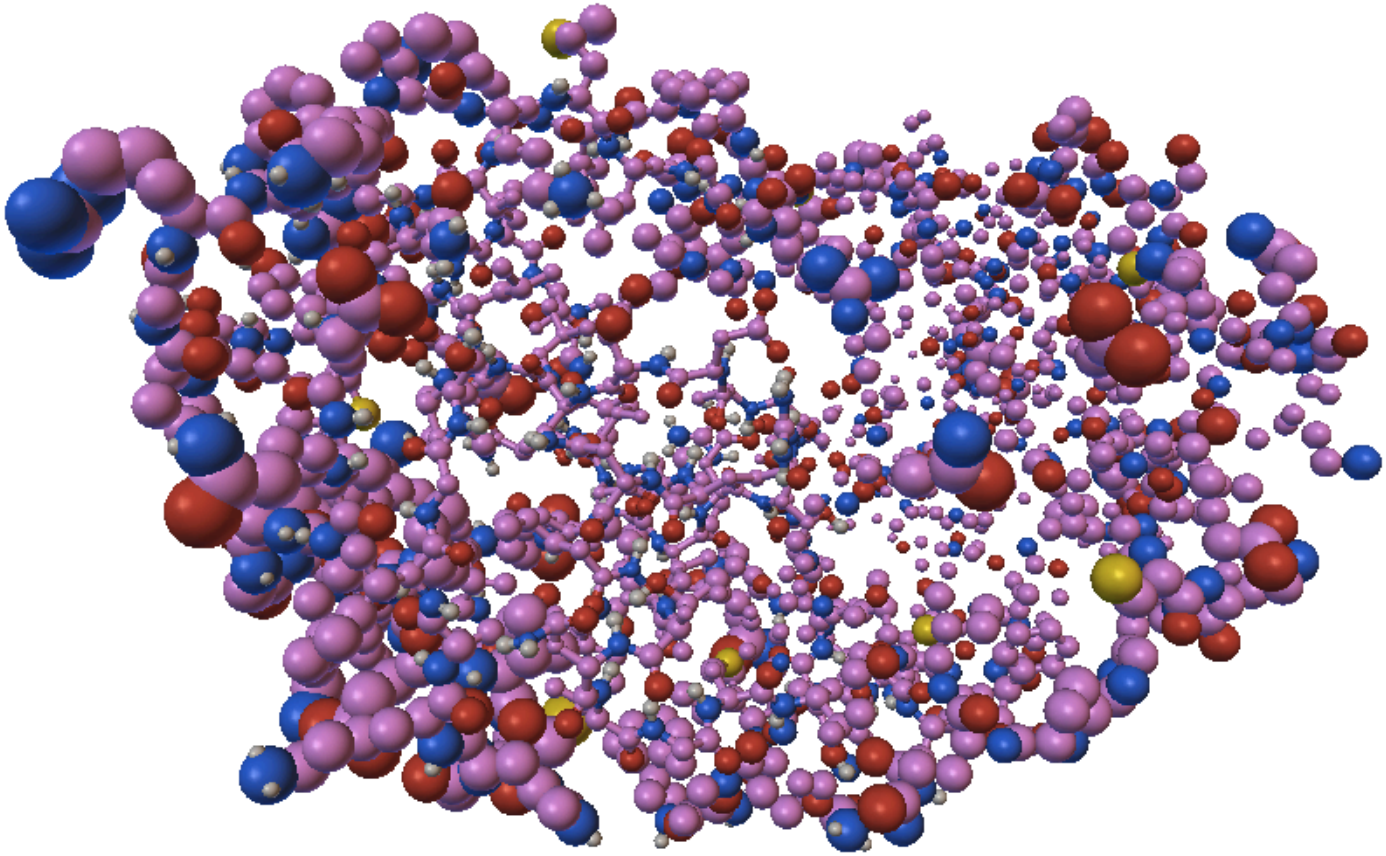


Radius = offset + atom radius*scale

Exercise: Display CPK

Task: display CPK

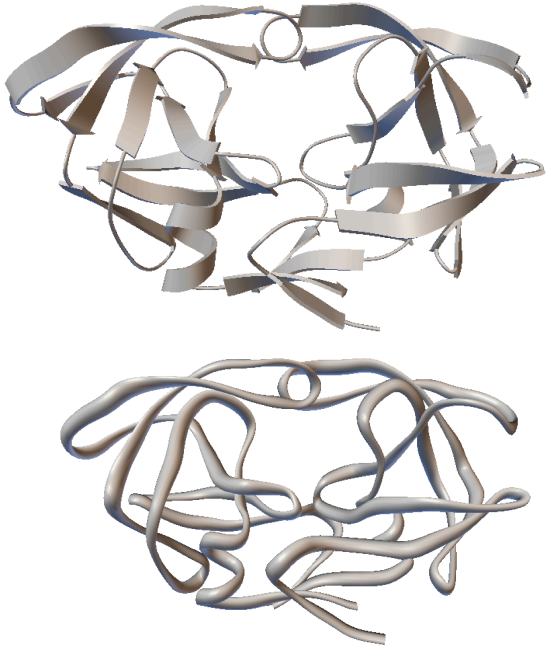
1 – Right click on CPK for hsg1
2 – check “By Property” button
3 – select atomic property temperature Factor
4 – set scaling to 0.02



Exercise: Display Ribbon

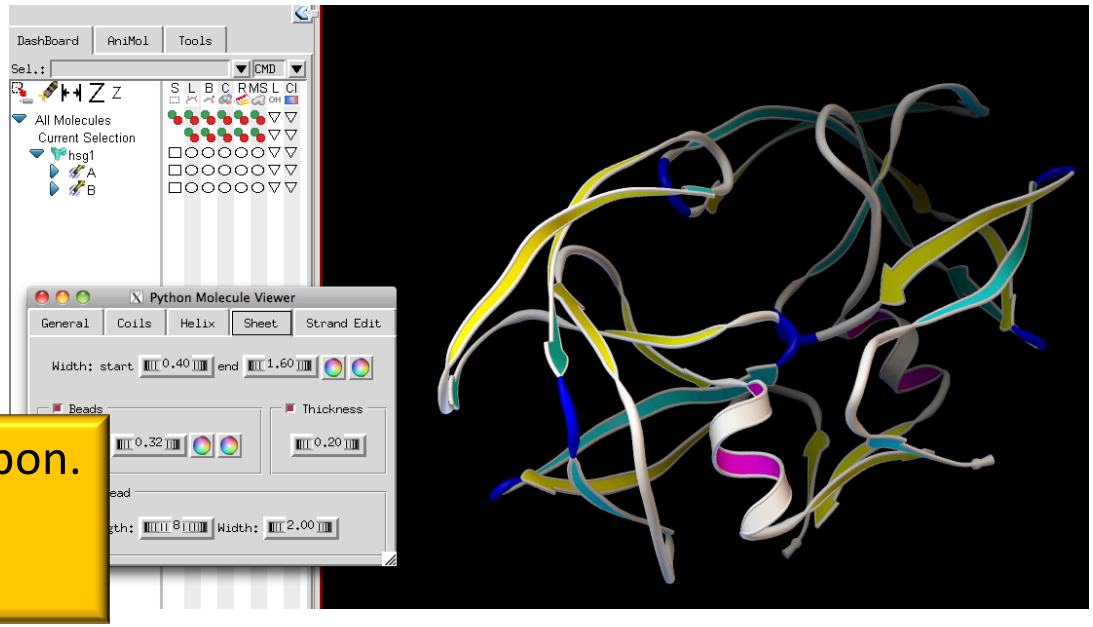
Task: display Ribbons

1 – display ribbon for Chain A.
2 – right click in ribbon for chain B
and select ‘ellipse’ for he shape
3 – un-display all ribbons



Task: Beaded Ribbons

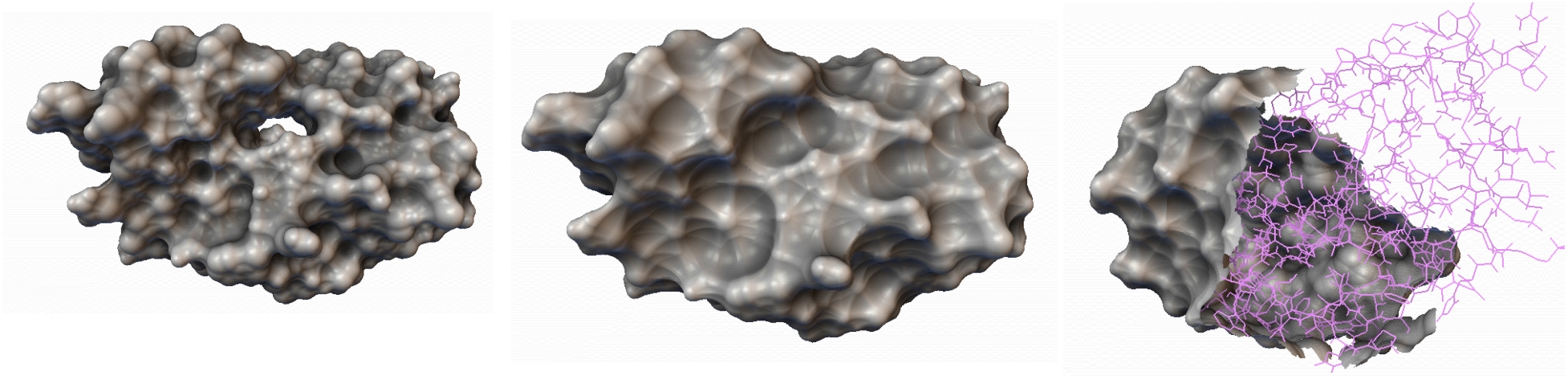
1 – use menu entry Compute -> beaded ribbon.
2 – un-display all lines
3 – un-display all ribbons



Exercise: Display Surfaces

Task: display surfaces

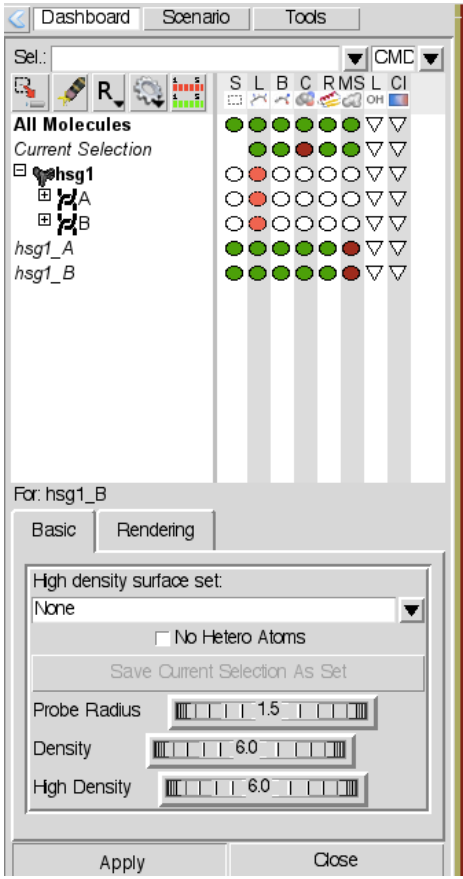
1 – display surface for hsg1
2 – un-display surface for hsg1
3 – turn ambient occlusion on ‘o’
4 – right click on surface for hsg1 and set probe radius to 3.0
5 – change rendering style of front faces to outlined
6 –compute surface with various densities
7 – display surface for chain A only (NOTE the surface is open)
8 – turn display of back faces on in rendering tab
9 – display lines for hsg1

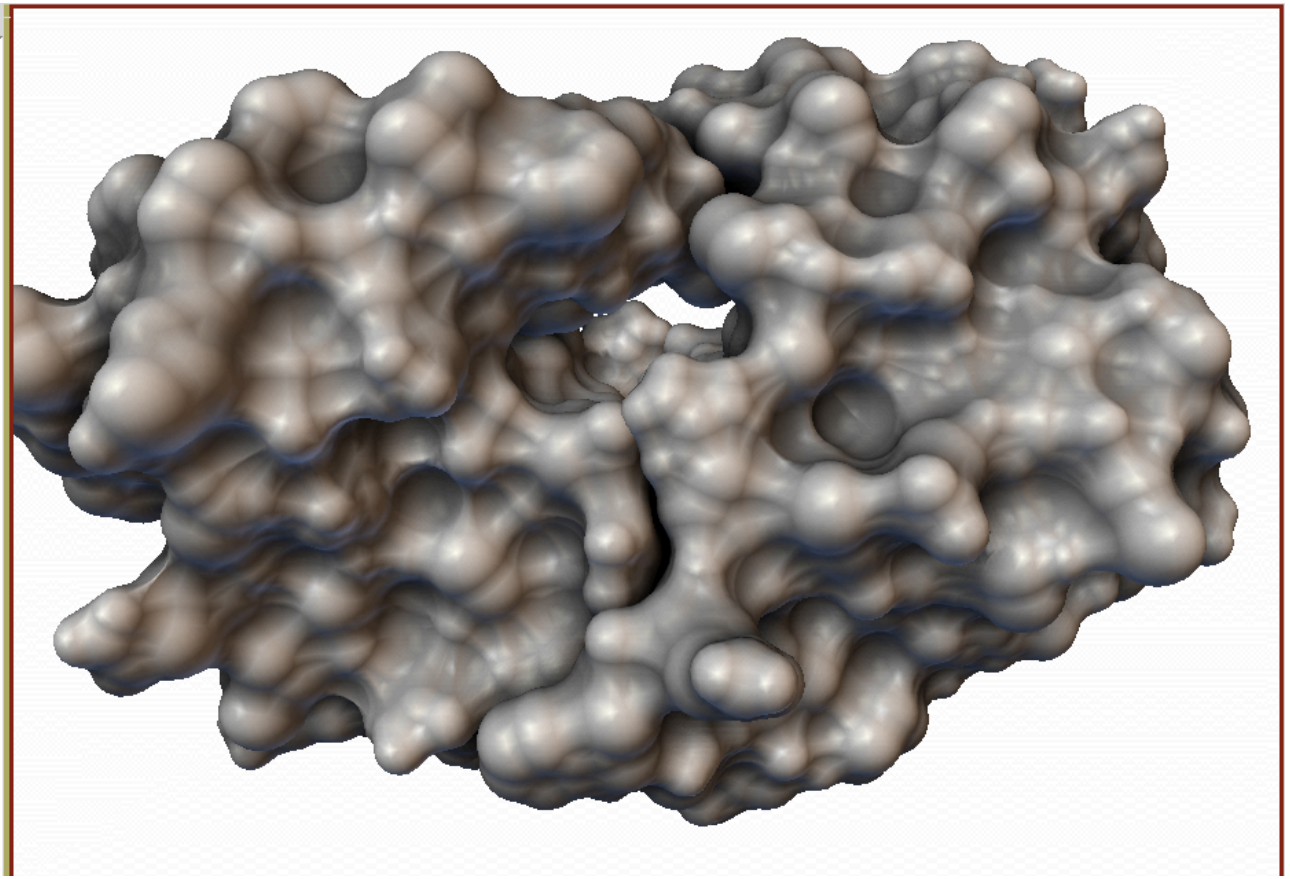


Exercise: Closed surfaces for chains

Task: display closed surfaces

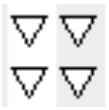
To close the surface:
1 – right click on the “hsg1” label in the molecule tree
2 – select “Make sets for chains”
3 – compute surface for the 2 created sets

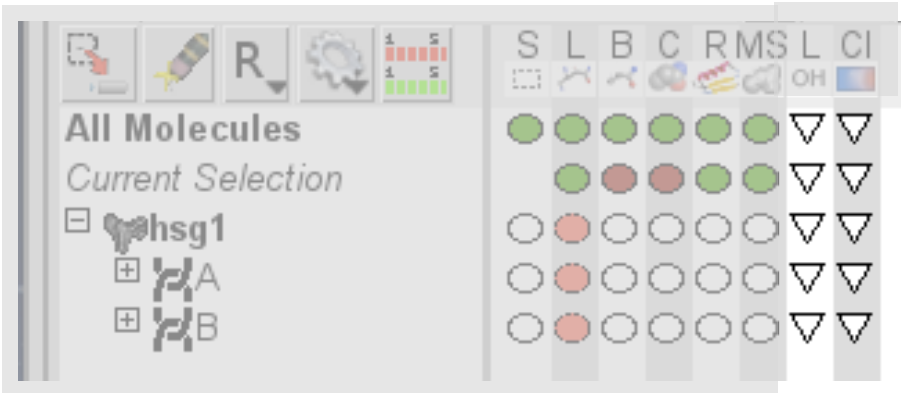




Dashboard Command Buttons

Menu Buttons

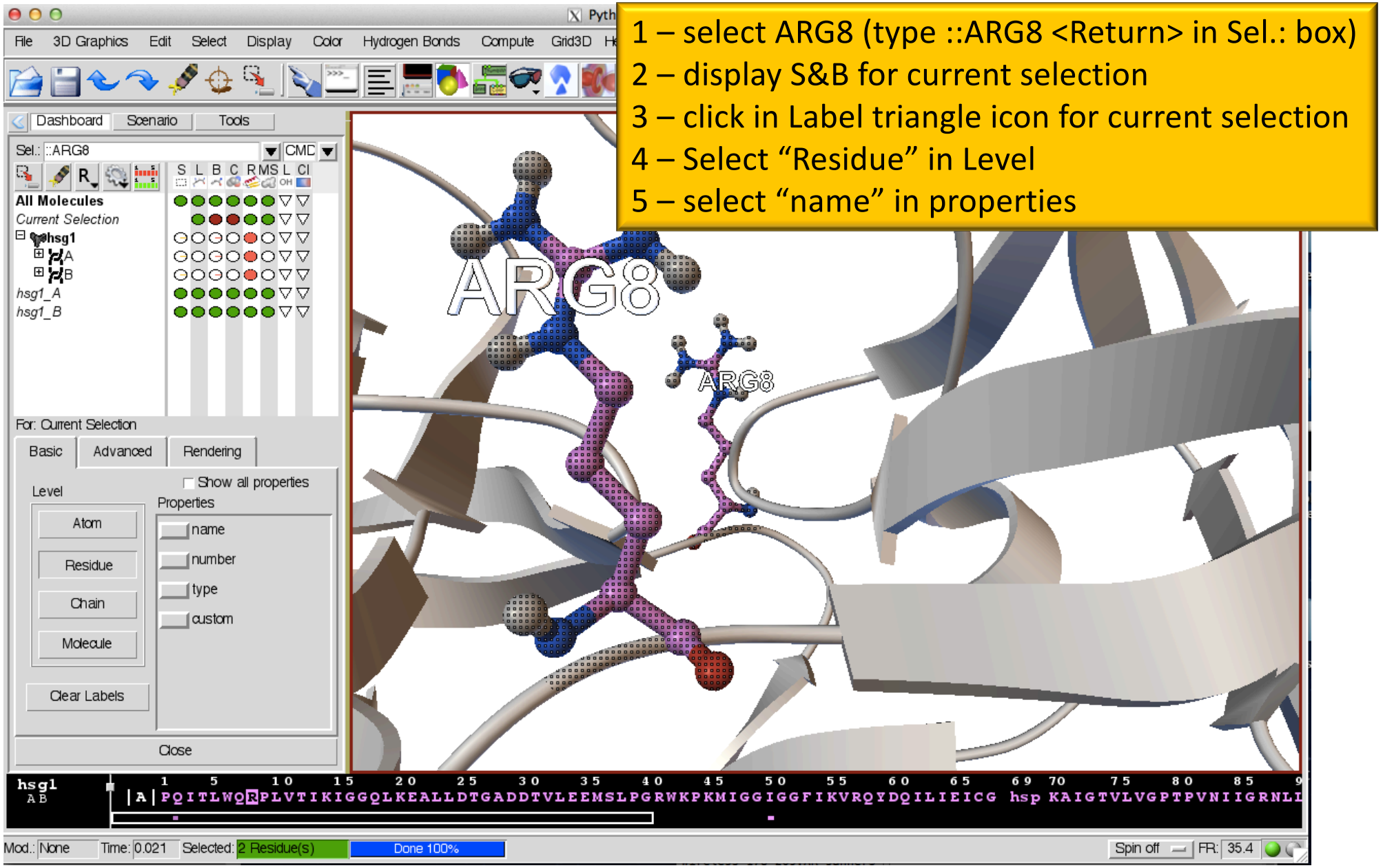




- Left mouse click to display menu

Exercise: Label Residue

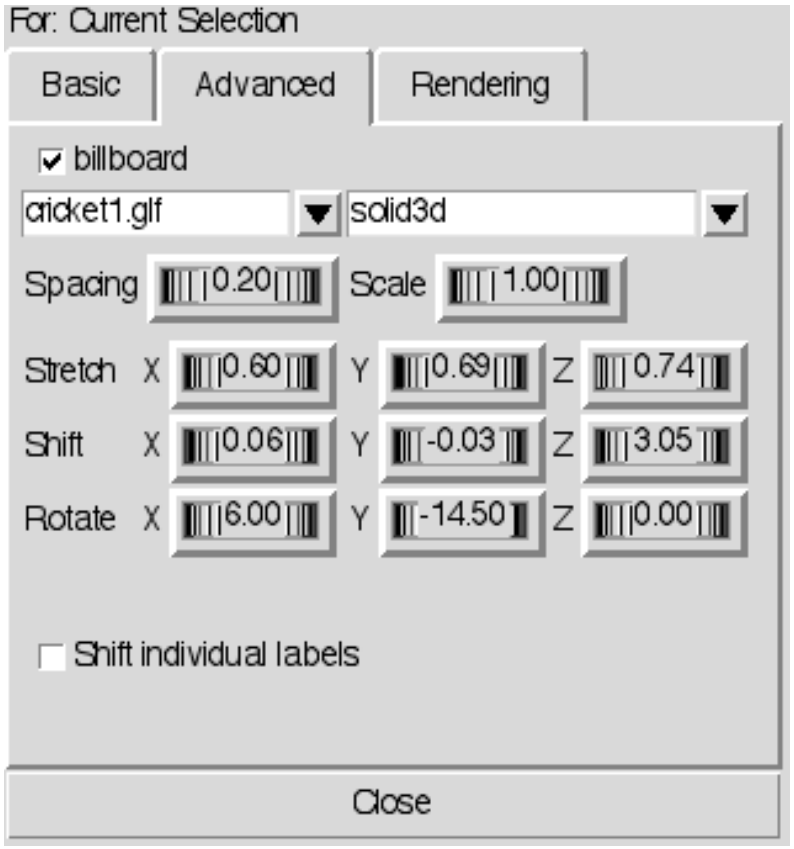
Task: use label menu on Arg8

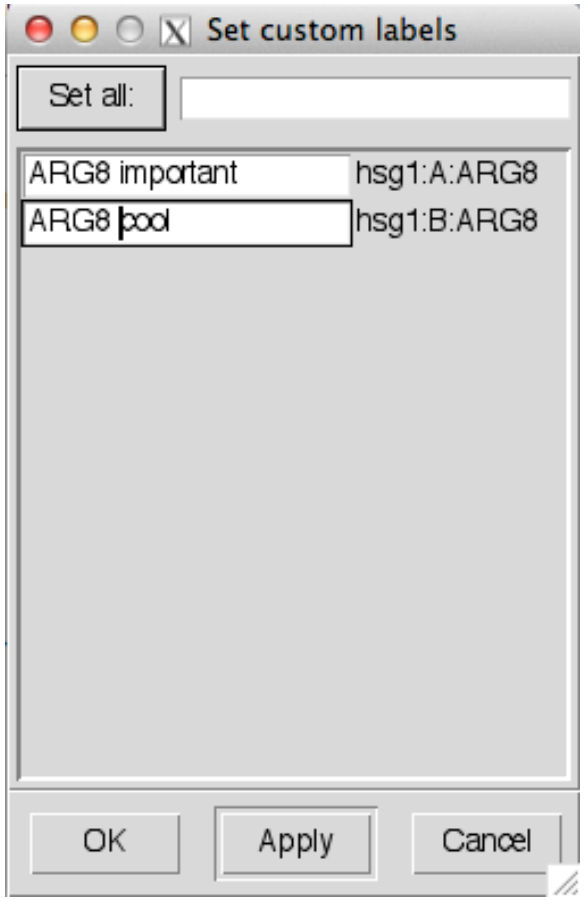


Exercise: Labeling options

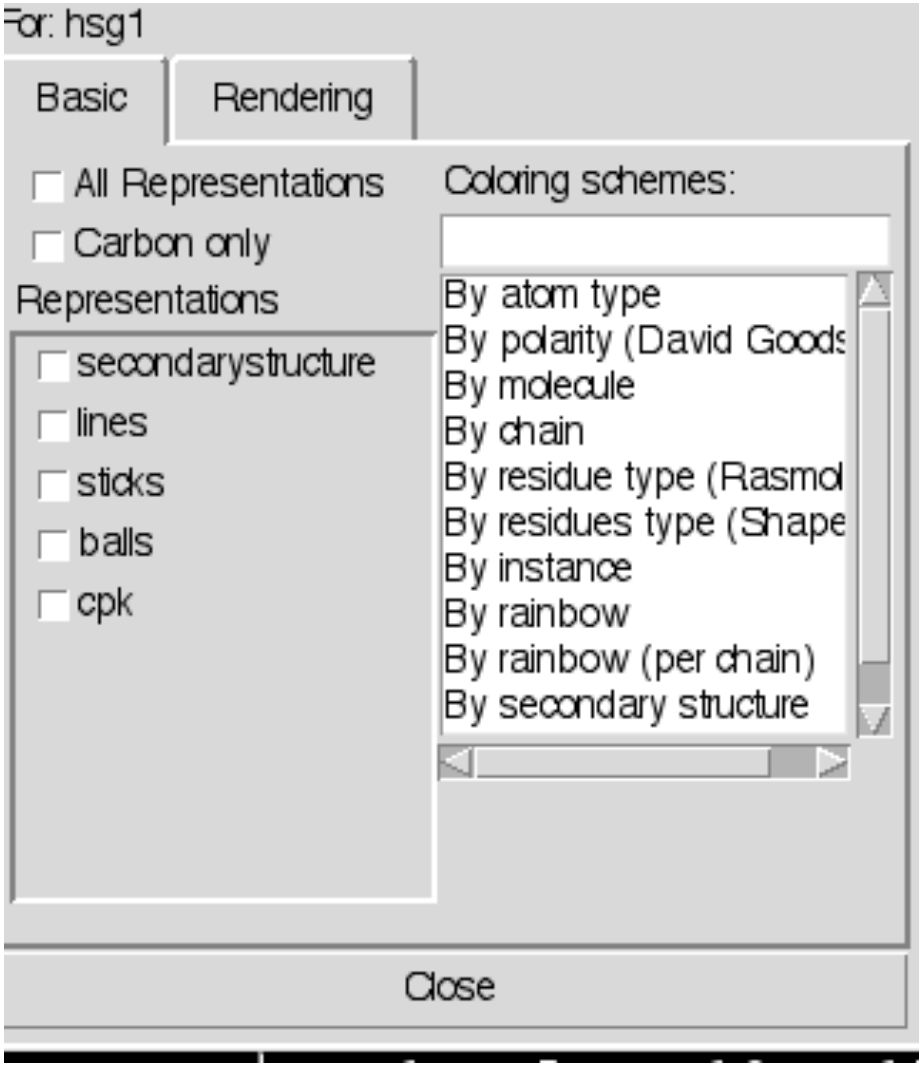
Notes:

- **If you click more properties the label is extended**
- **Use Clear labels to remove all label at the current level**
- **Use the advanced tab to modify labels**
- **Use "custom" property in Basic to customize any label**





Exercise: Color Menu



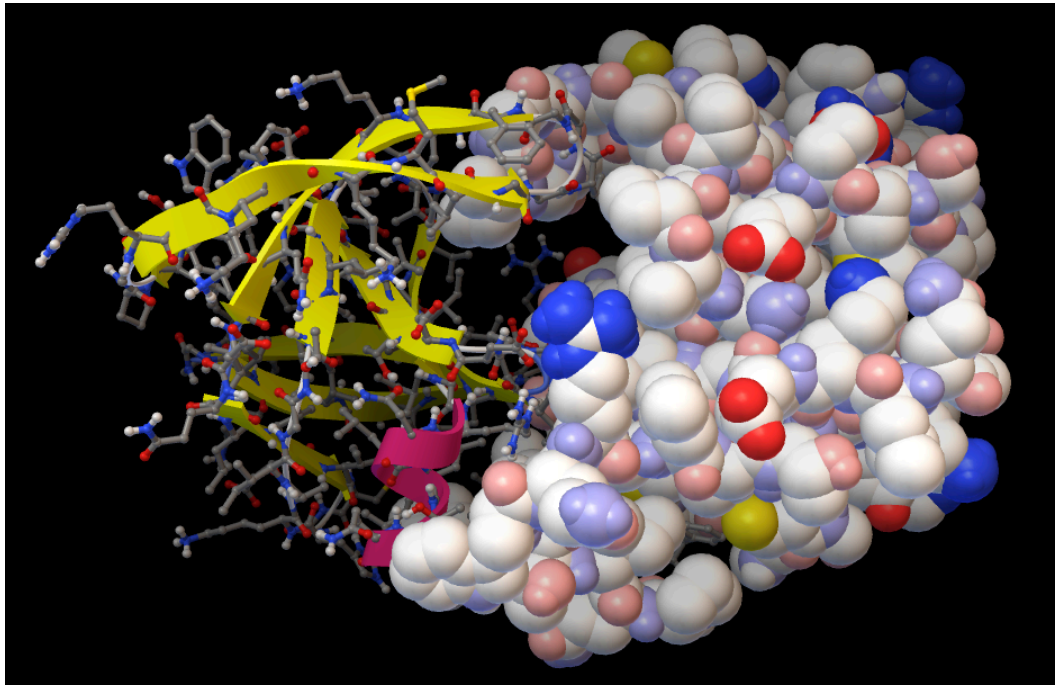
Notes:

- **Only displayed representation (lines, CPK, etc) are shown**
- **Coloring schemes are applied as they get selected provided at least one geometry is select**
- **The “By secondary structure” scheme only appears if the molecule(s) we are coloring have a ribbon**

Exercise: Color Menu

Task: Apply different coloring schemes to various representations

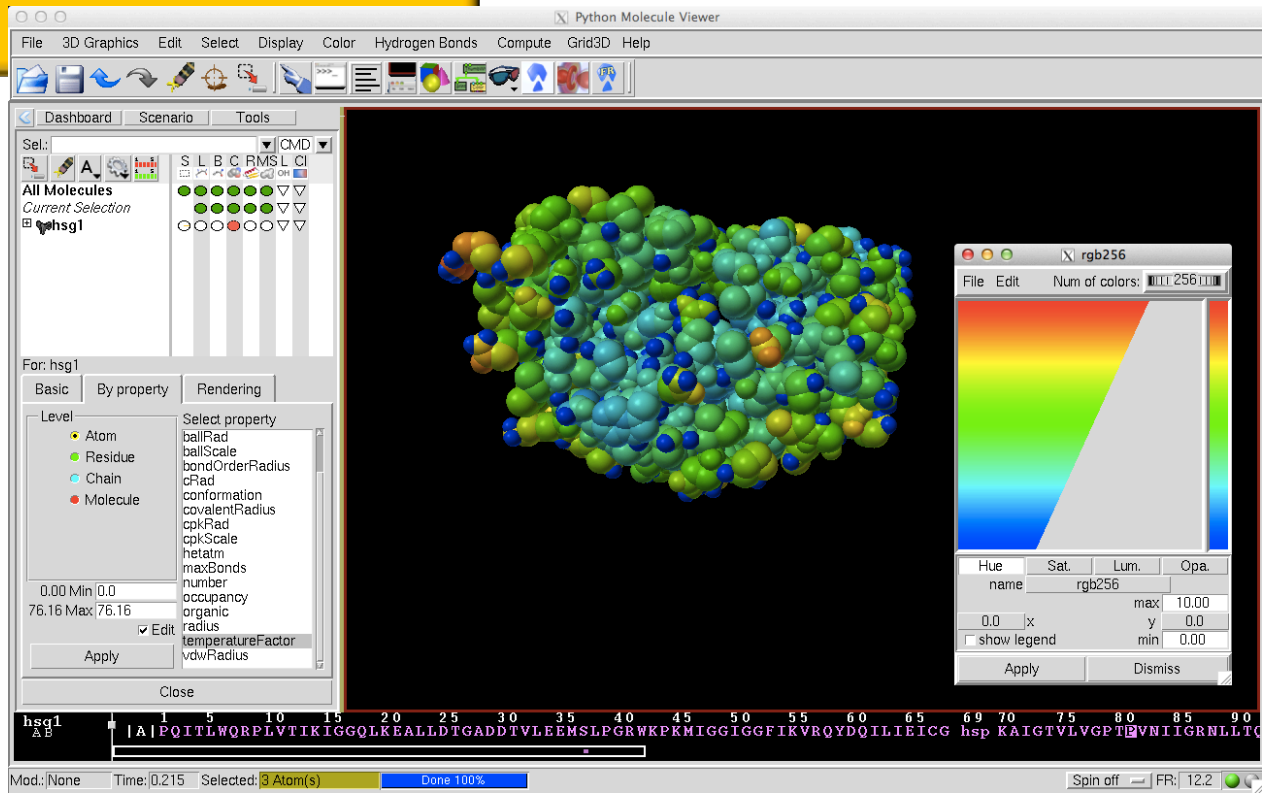
1 – display Balls & sticks for chain A
2 – display CPK for Chain B
3 – color Balls and Sticks for chain A
By atom type
4 – color CPK for chain B by Polarity
5 – display ribbon for chain A
6 – color ribbon by secondary struct.



Exercise: Color By Property

Task: color CPK by temperaturFactor

1 – display CPK
2 – Display color menu for protease
3 – check CPK in Representations in the Basic Panel
4 - Select “By Properties”
5 – select temperatureFactor
6 - Apply



Exercise: Color Palettes

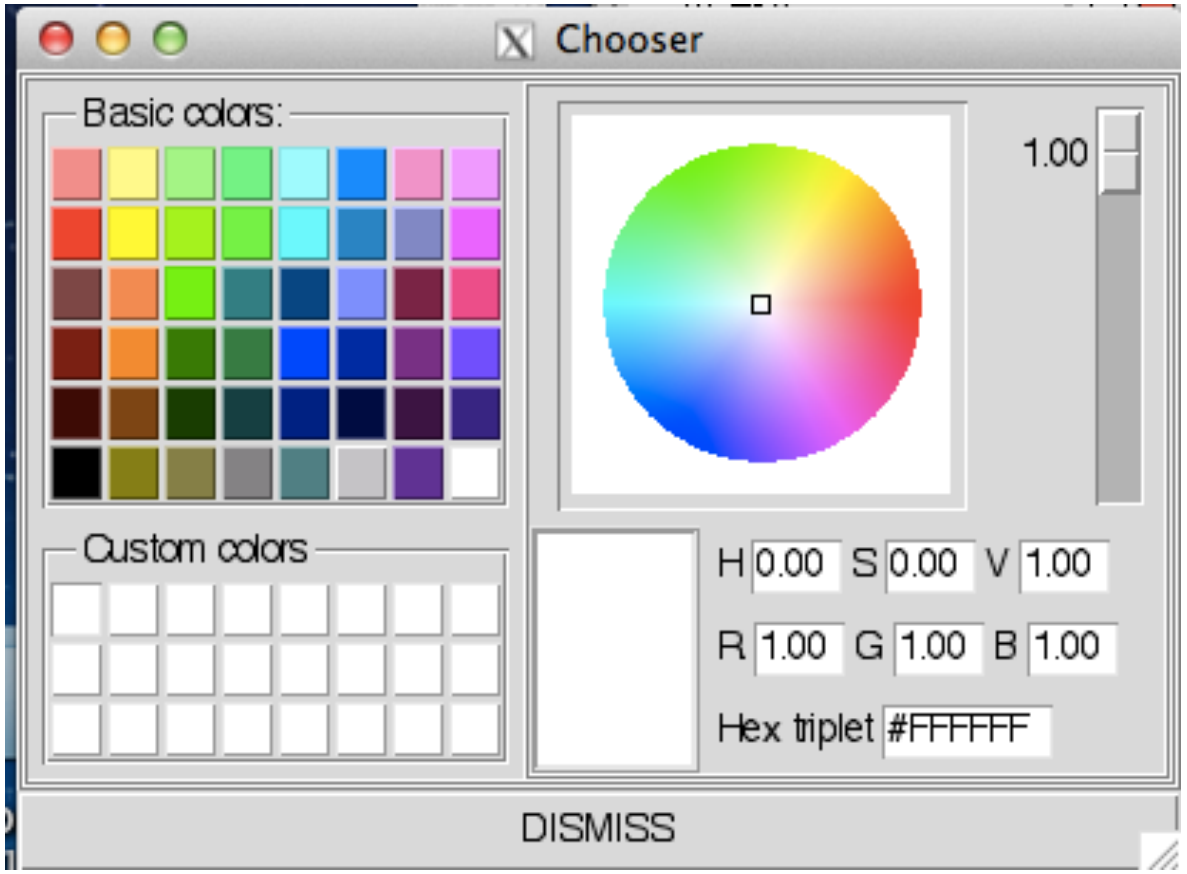
Task: Modify the first color in the color by molecule palette

1 – Edit -> Color Palettes -> Edit Color by Molecule
2 – click on color 0
3 – select new color in color chooser
4 - Restore default

Make Default would make this change permanent by writing it into the _pmvrc file

Exercise: Color Editor

Picking a custom color will extend the color editor
Custom colors survive the PMV session

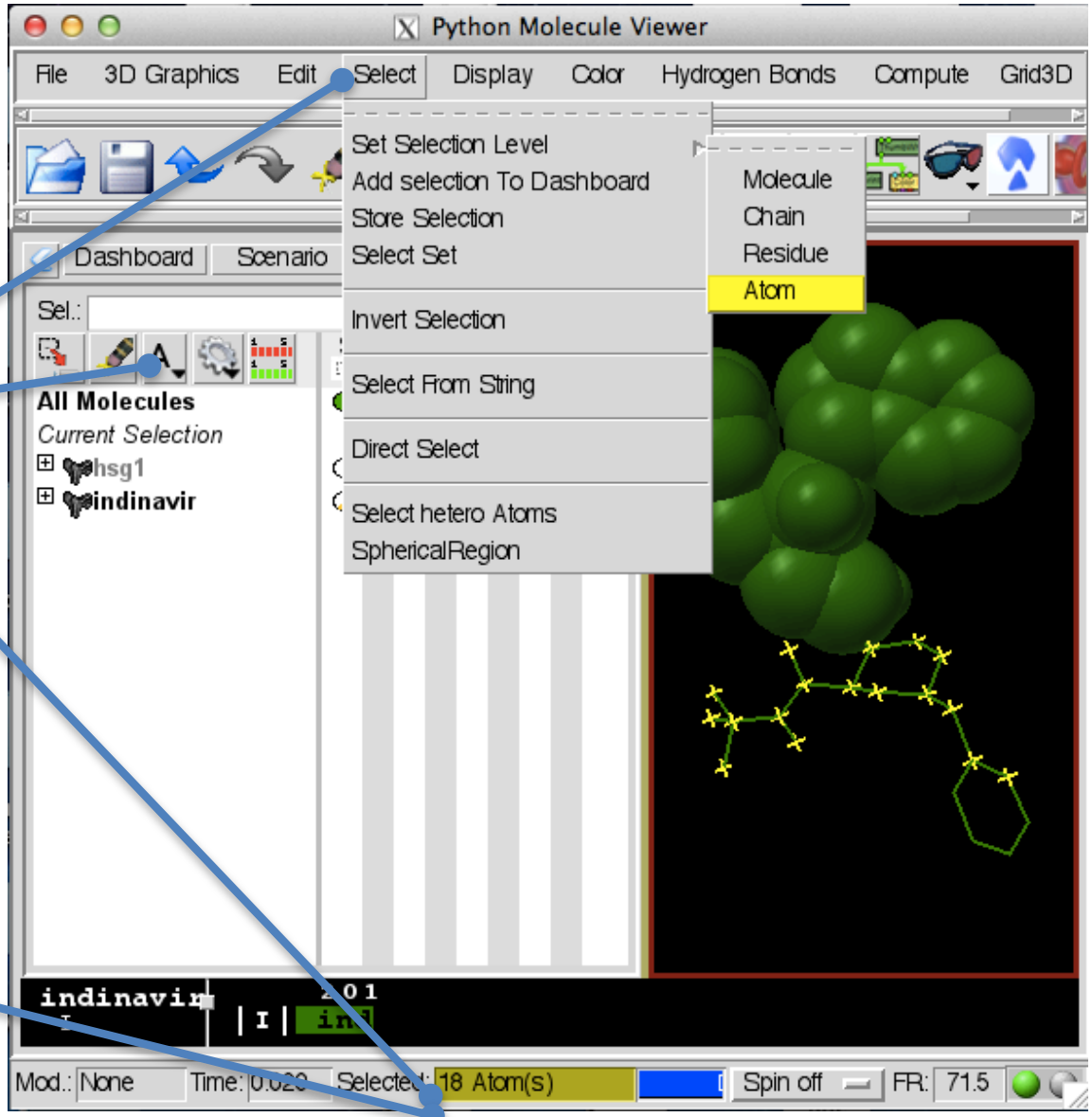


Pmv selection

Clear selection

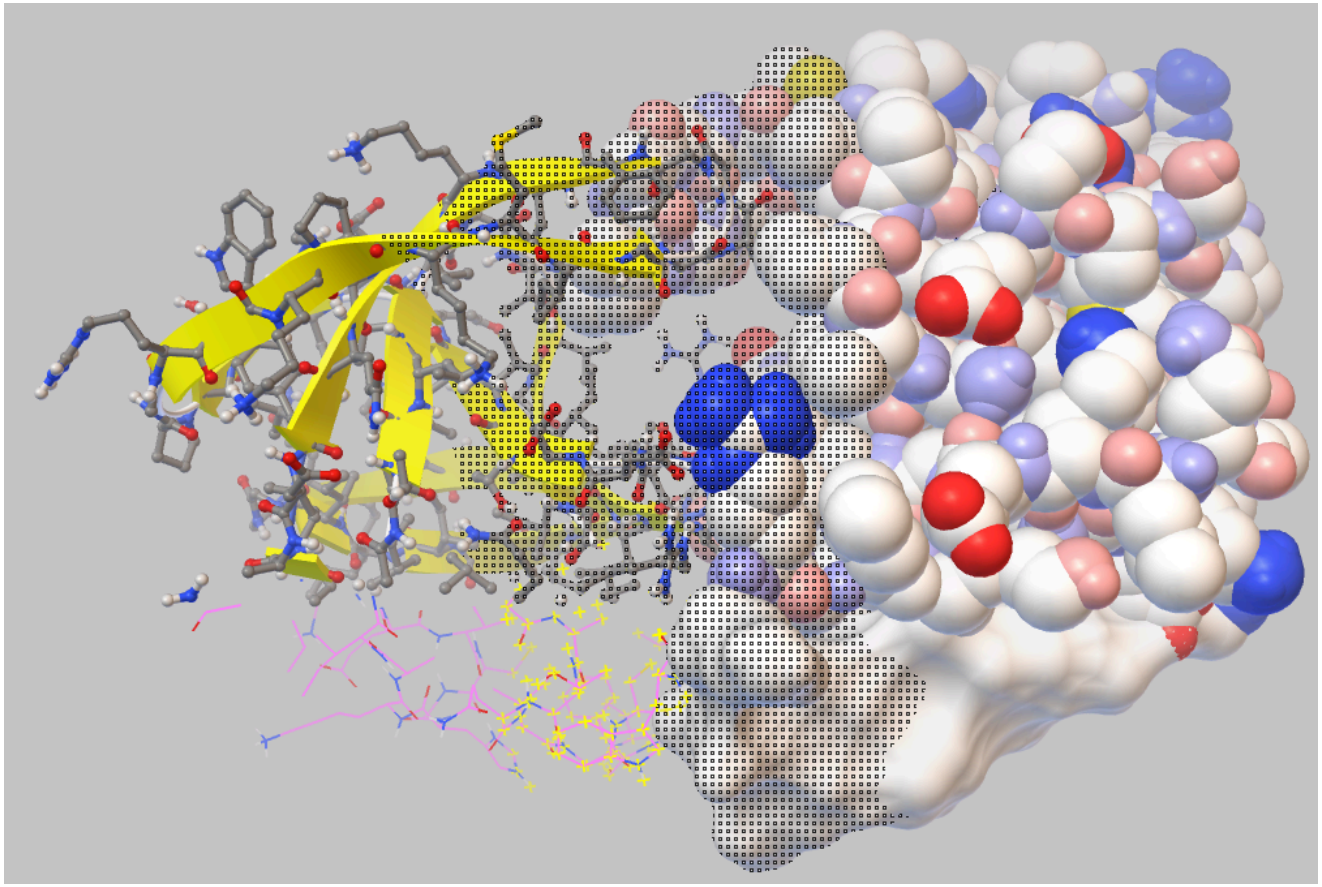
Set selection level

Current selection description



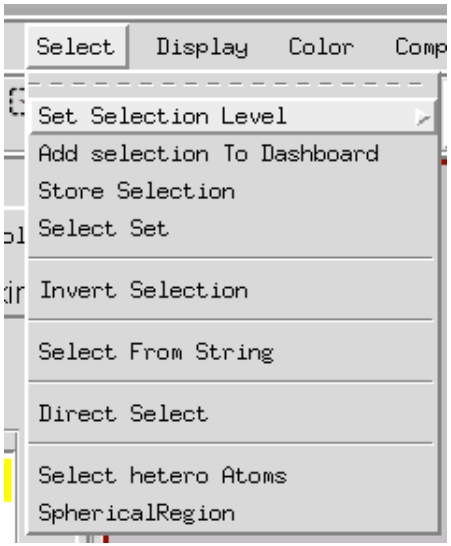
Pmv selections

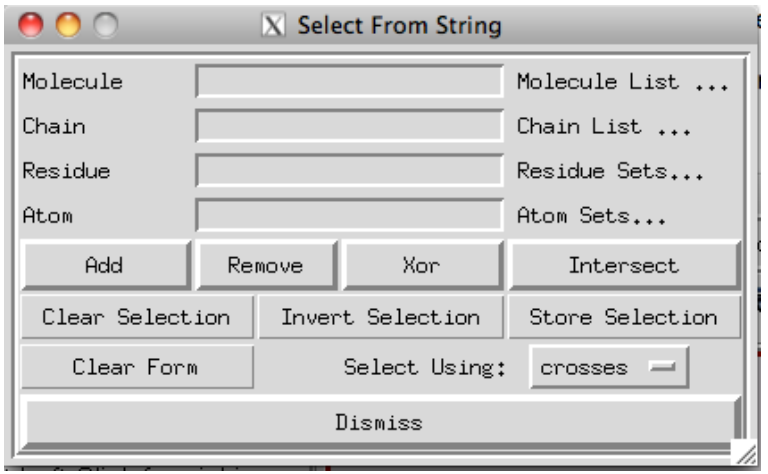
- Visual feed back of selected atoms on all representations



Creating selections

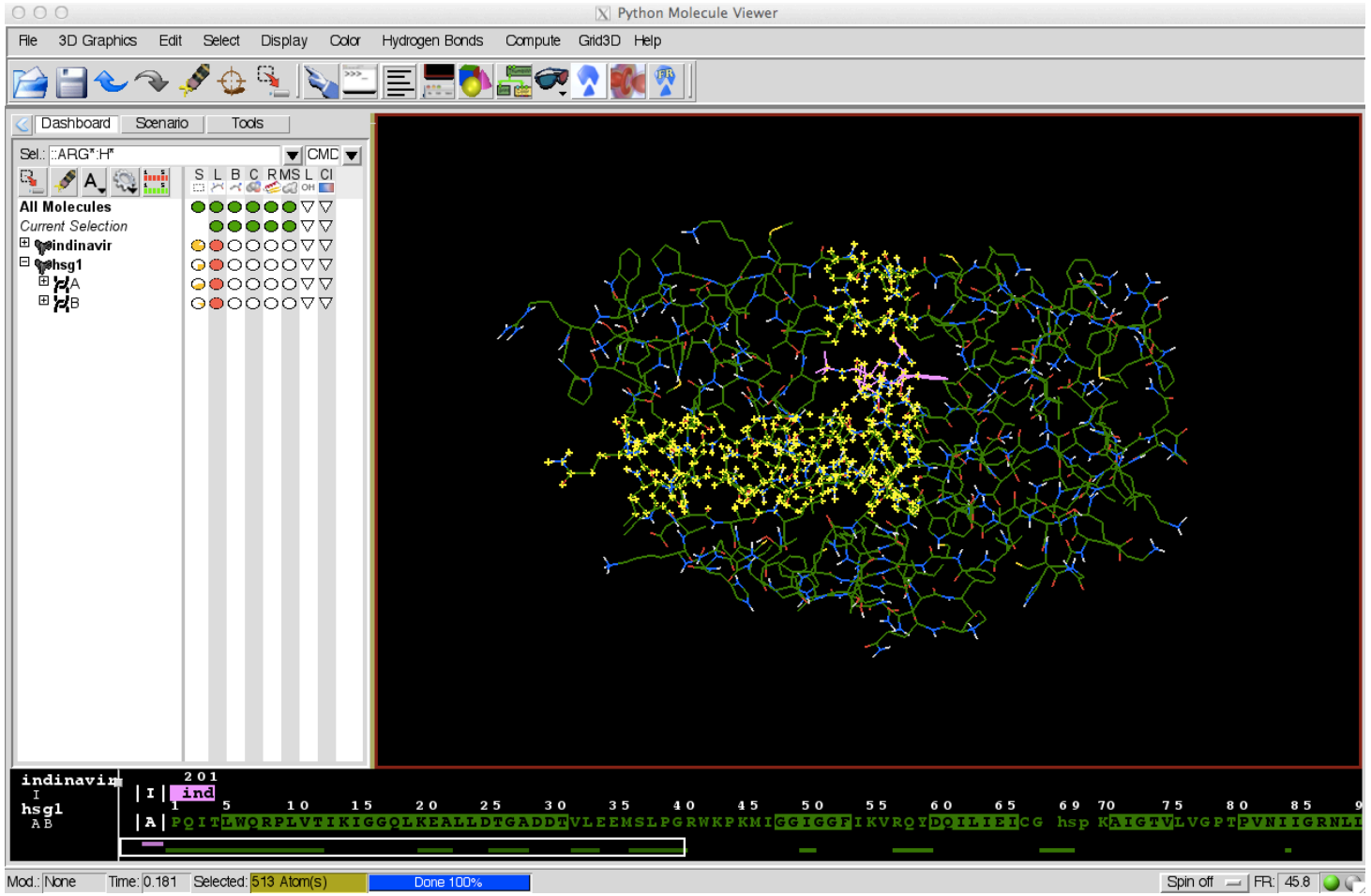
- Pmv menu commands and dashboard entry “current selection” operate on selection
- Pmv has various way to build complex selections
  - Shift left click and drag in 3D Viewer
  - Dashboard selection column and sel.: entry
  - Selecting residues in sequence viewer
  - Menu Select ->





Creating selections

- Shift Left Click an drag to add to the selection
- Ctrl left click and drag to remove from the selection



Creating selections

Notes:

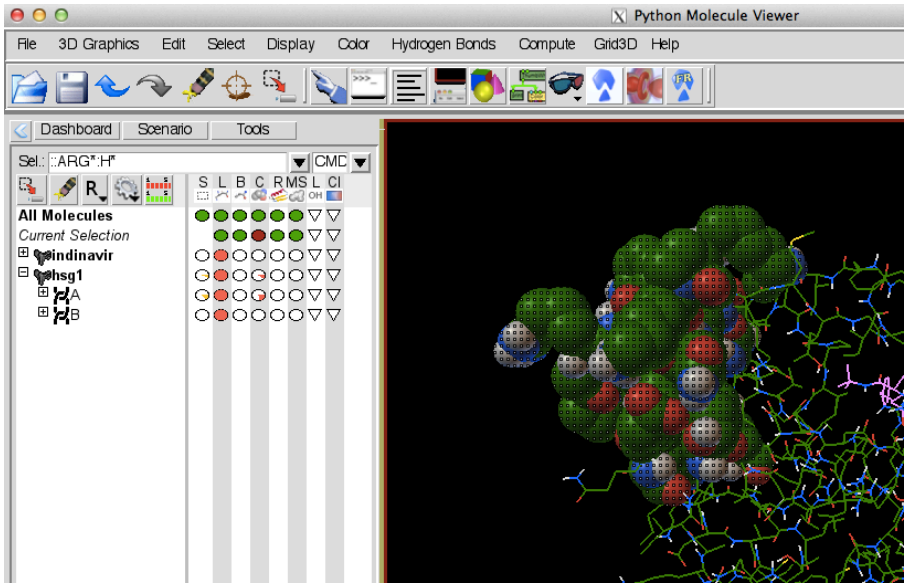
- clicking without dragging will only select the one atom closest to the viewer. Dragging will draw a rectangle and select all atoms falling inside the rectangle.
- Selection is perform at the current selection level. If the level is residue, selecting a single atom will select the whole residue

Creating selections

- Left click in Selection column of the Dashboard
  - Toggle selection state for the item

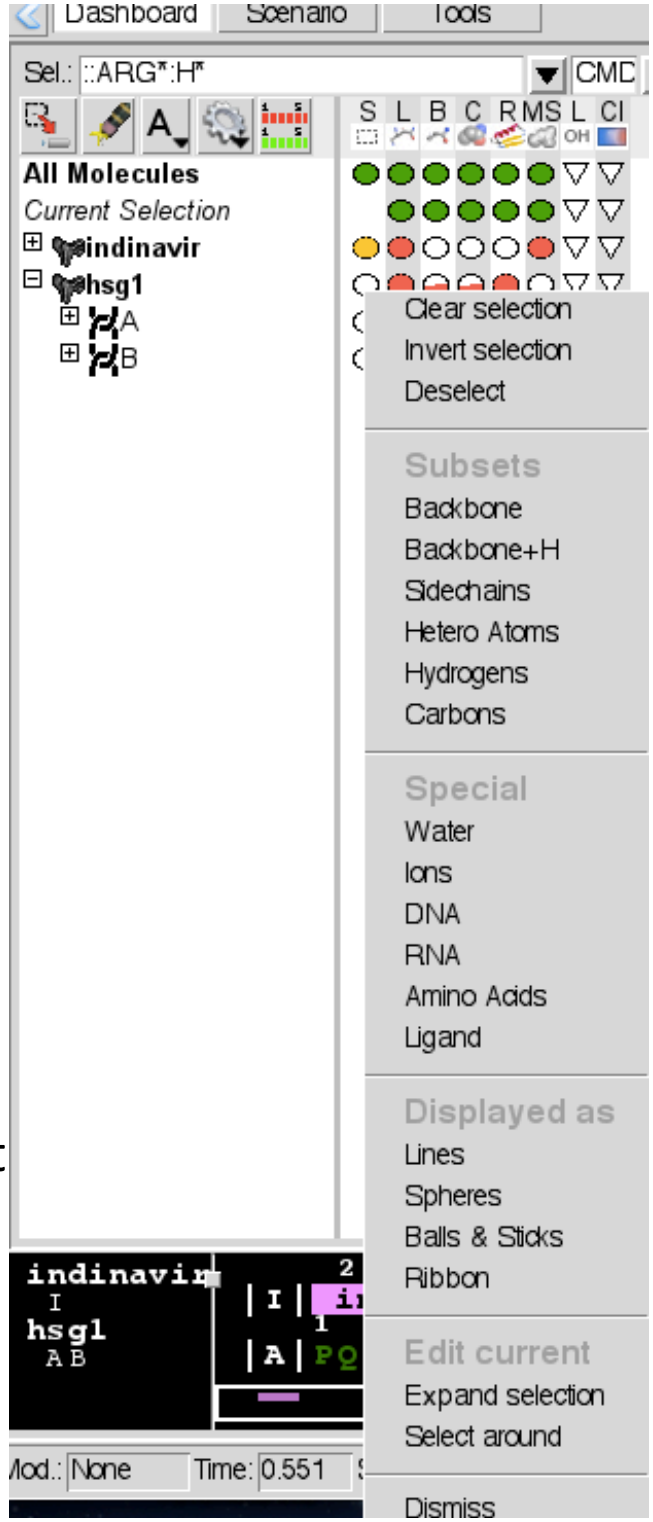
Task: create selections using the dashboard at various levels

1 – select hsg1
2 – deselect chain B
3 – clear the selection
4 – set the level to Atoms
5 – Shift click drag a box over part of a chain
6 – change the level to residues
7 – use the current selection entry to display CPK



Pmv selections

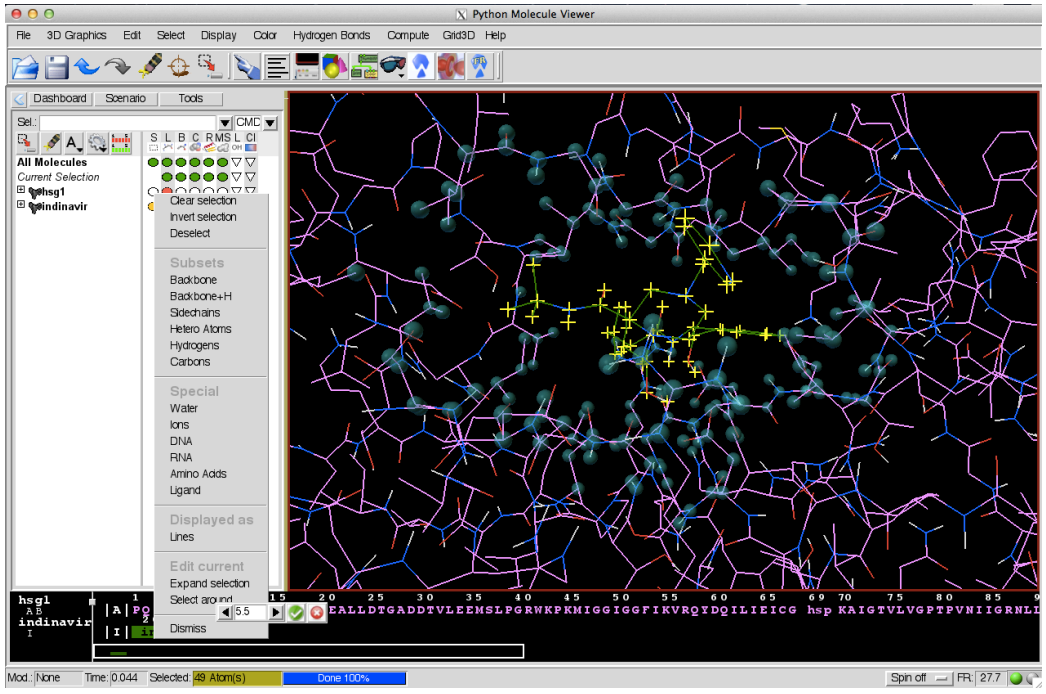
- Dashboard selection menu
  - ***Clear*** selection
  - ***Invert*** selection within fragment
  - ***Deselect*** fragment
  - Select ***subsets*** of atoms
  - Select ***special*** residues
  - Select atoms ***Displayed as***
  - Edit selection:
    - Expand selection within fragment
    - Select around selection within fragment

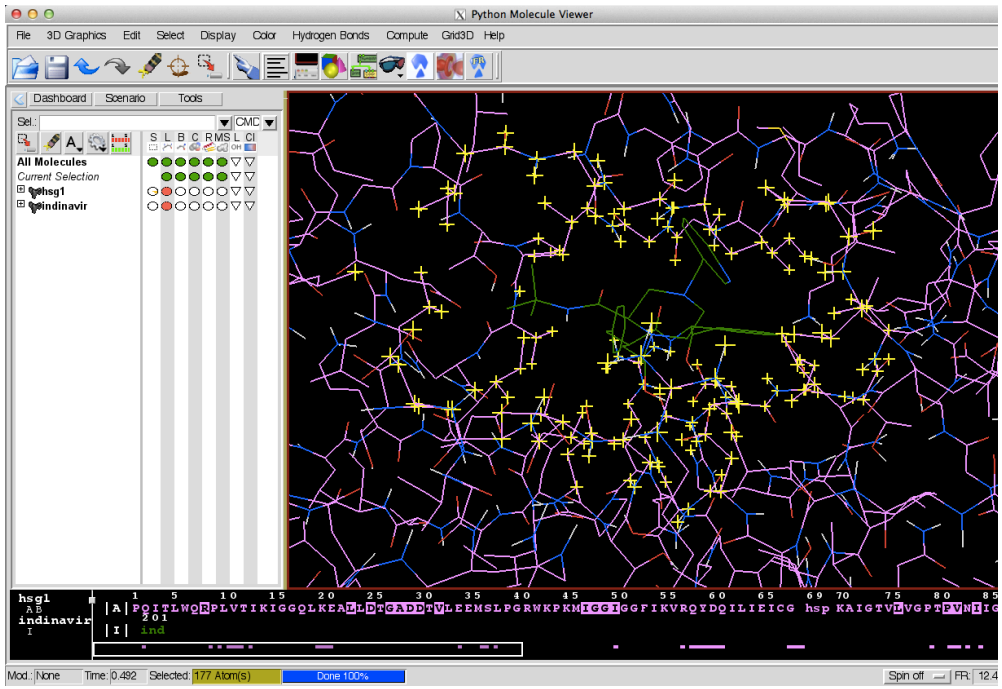


Pmv selections

- Expand selection and select around

1 – load molecule indinavir.pdbq
2 – clear selection
3 – display lines only
4 – right click on select hsg1 -> Select Around
5 – increase the range to 5.5 (more blue spheres appear)
6 – accept





Pmv selections

- Powerful selection mechanism using regular expressions:
  - moleculeRE:ChainRE:ResiduesRE:AtomsRE
  - wildcards such a (e.g. *) and ranges (e.g. PRO1-ARG8)
- Available in the Python shell and dashboard
  - Examples:

"::" will select all Atoms in all Residues in all Chains in all Molecules in Pmv

"Mol1::" will select all Residues in all Chains in molecule Mol1

"Mol2:B::" will select all atoms in Chain B in molecule Mol2

"Mol1, Mol2:::C,N,CA,O" selects backbone heavy atoms in molecules Mol1 and Mol2

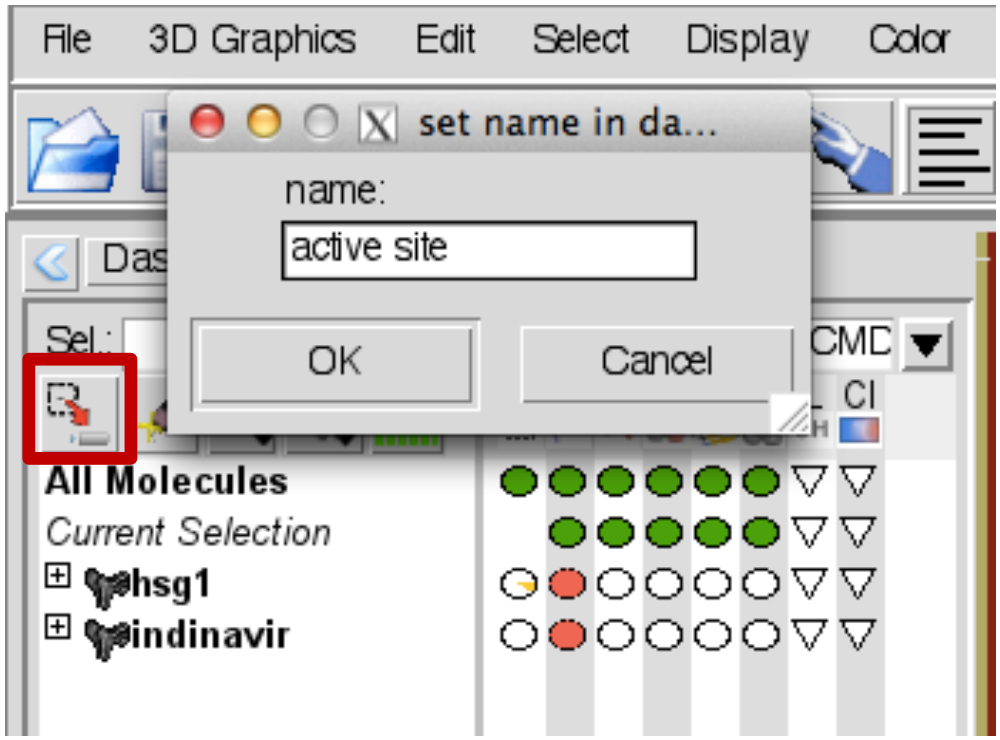
"::ALA35-THR45" selects a range of residues

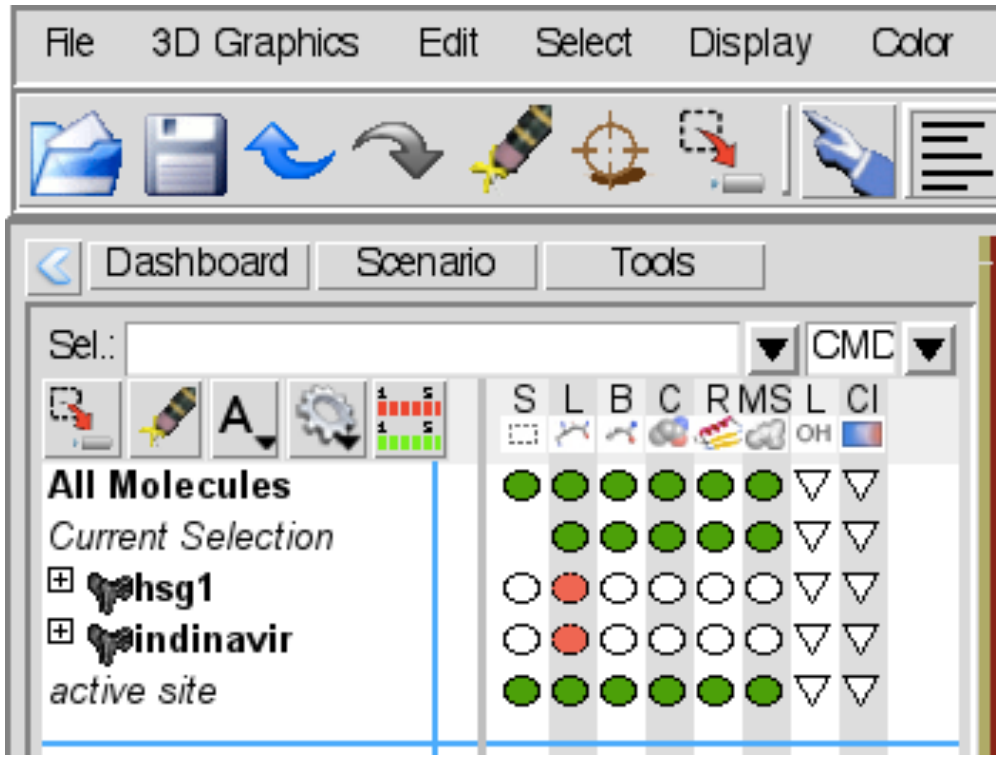
"::ARG*:H*" all the Hydrogen atoms in Arginine

http://mgldev.scripps.edu/docs/mgltools/1.5.6/Selection%20Strings.htm

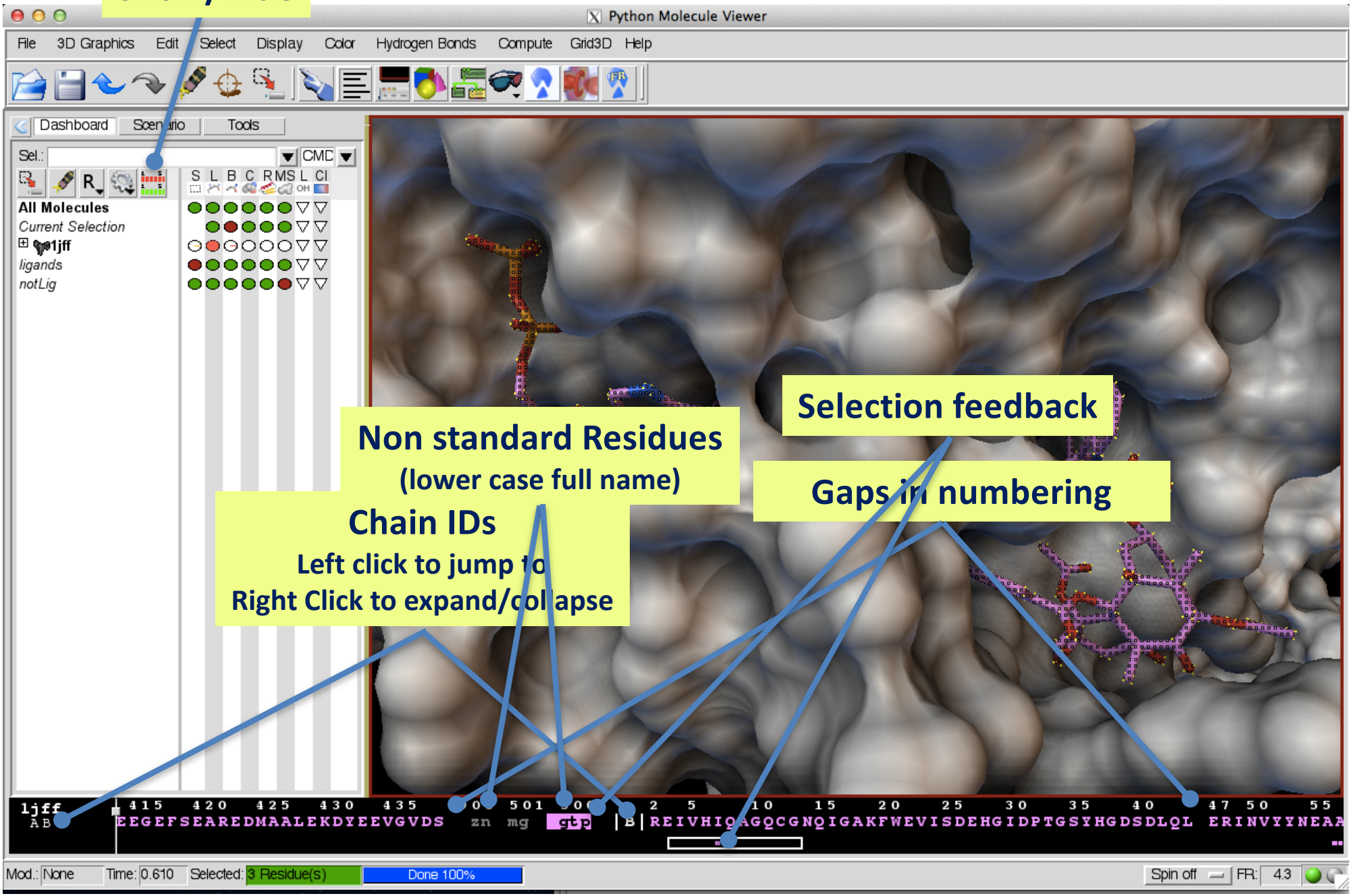
Dashboard User Sets

- Shortcut for operating on selections





Sequence Viewer



Exercise: selections

Task: explore sequence viewer

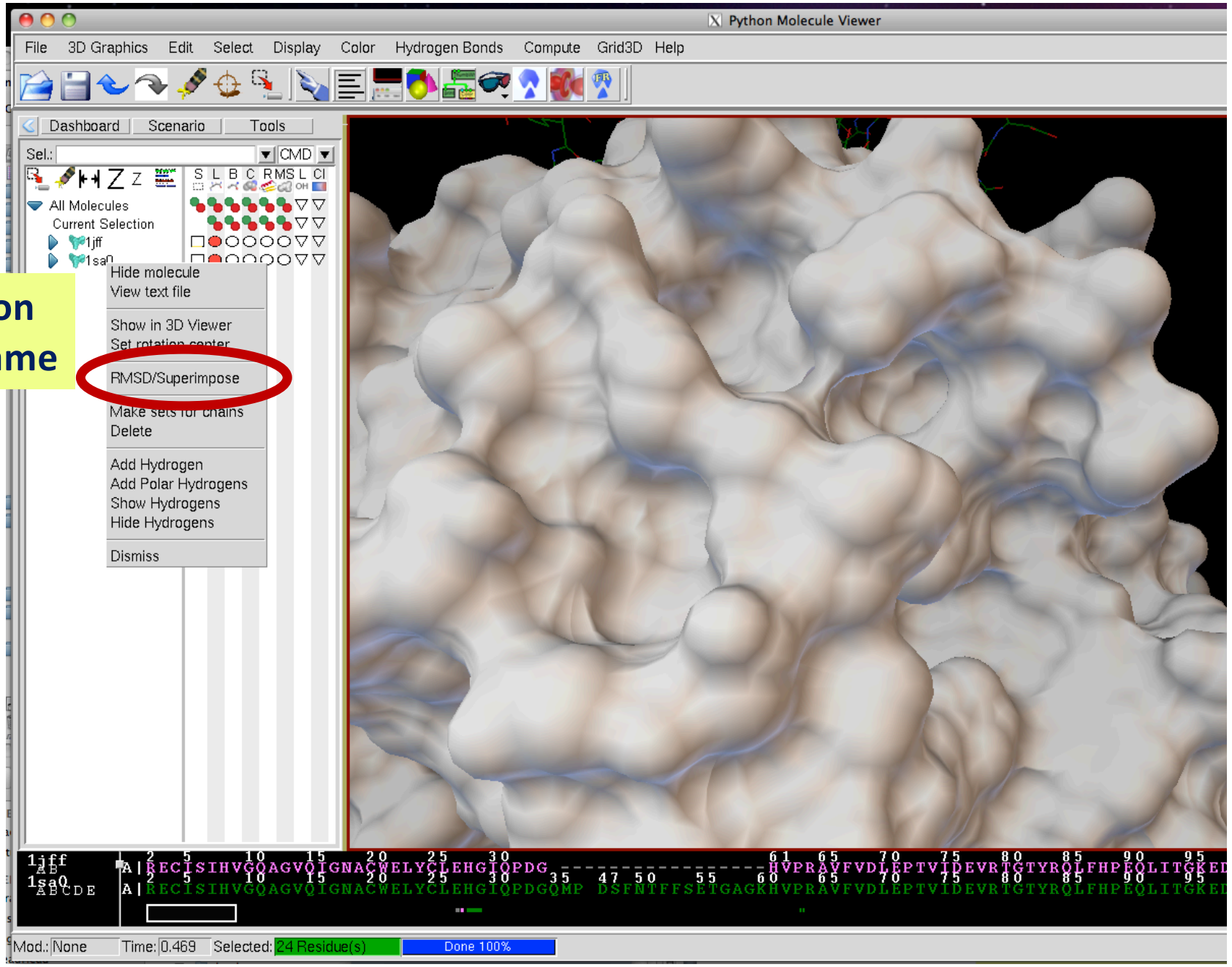
1 – load 1jff.pdb
2 – collapse chains and expand them
3 – select amino acids using sequence viewer
(Left click on un-selected residue and drag)
4 – de-select amino acids in sequence viewer
(Left click on selected residue and drag)
5 – select in 3D Viewer

Task: manual alignments

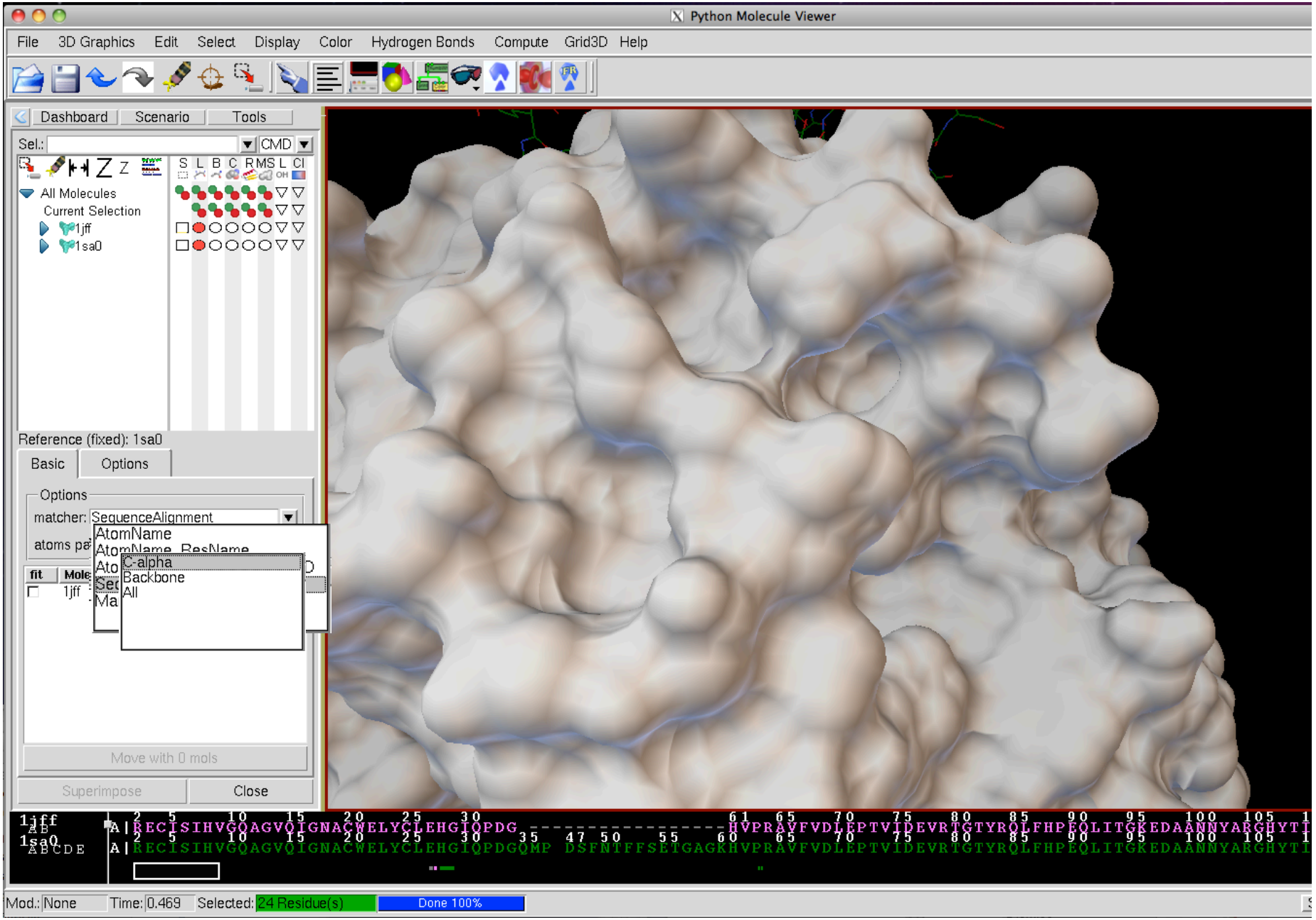
1 – load 1sa0.pdb
2 – Ctrl-Shift-Left click on Residue 1jff:A:61 and drag to the right
to align with residue 1sa0:A:61
3 – Left click on amino acid and drag a box to select across proteins

RMDS/Superimpose

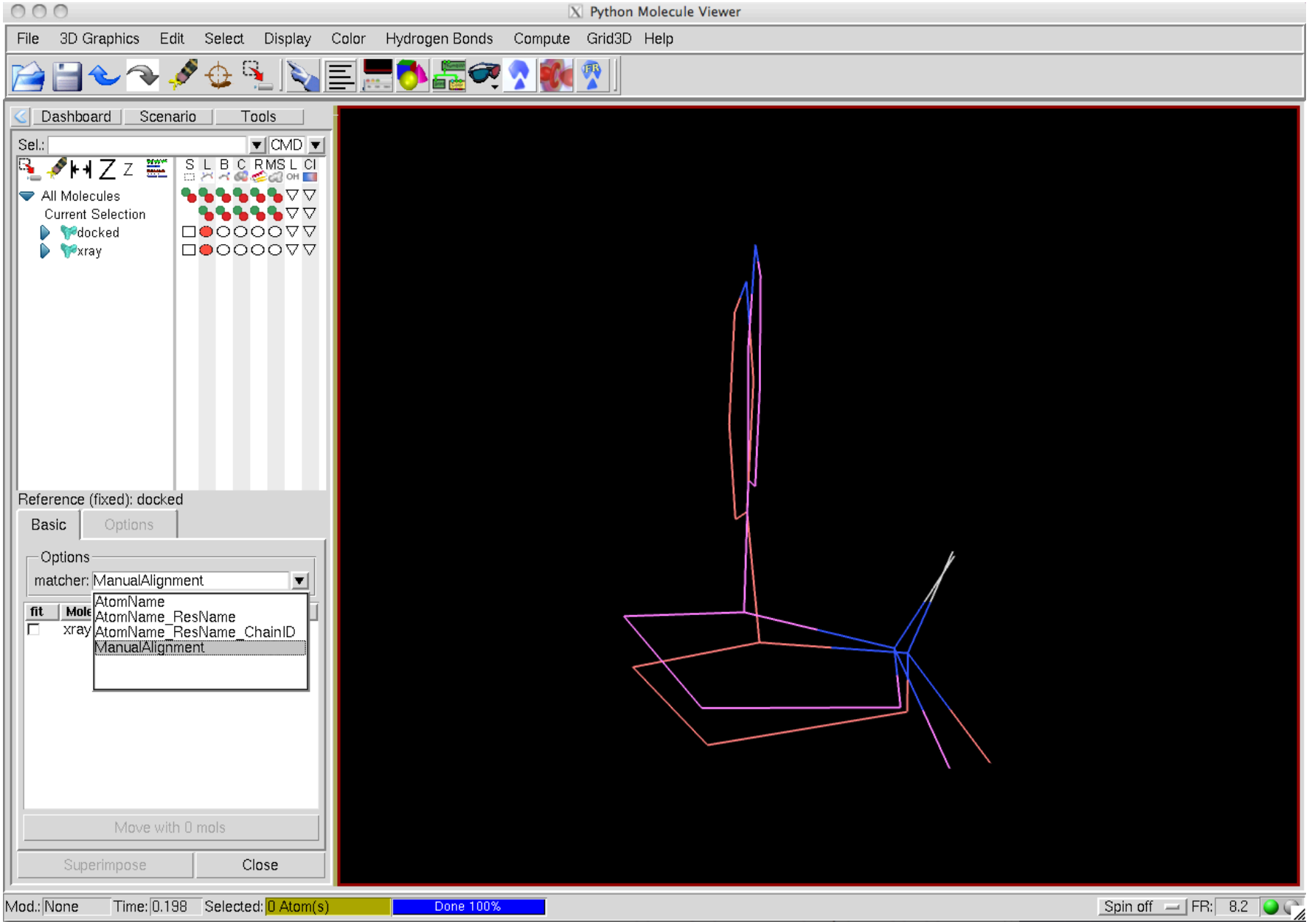
Right click on molecule name



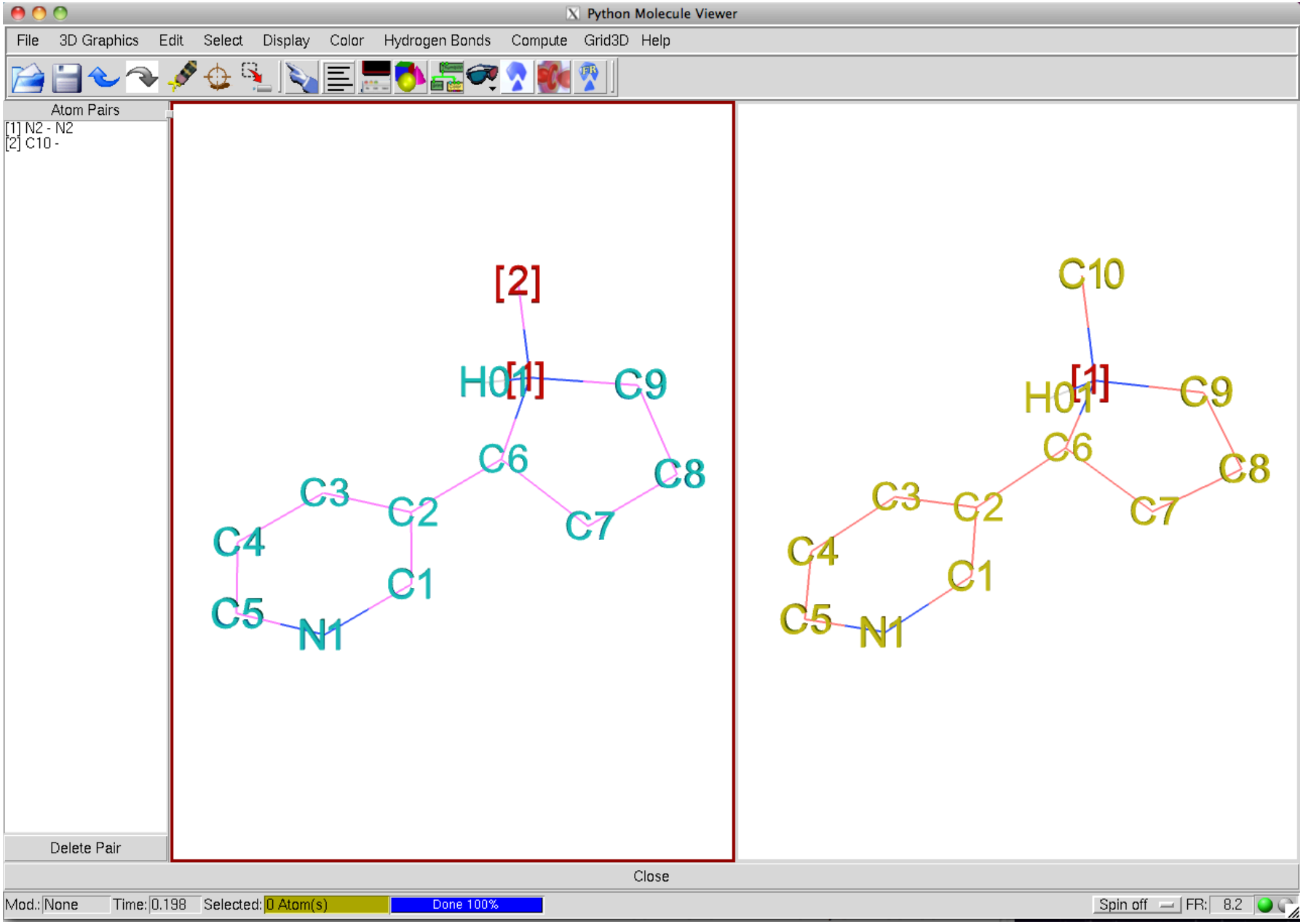
RMDS/Superimpose



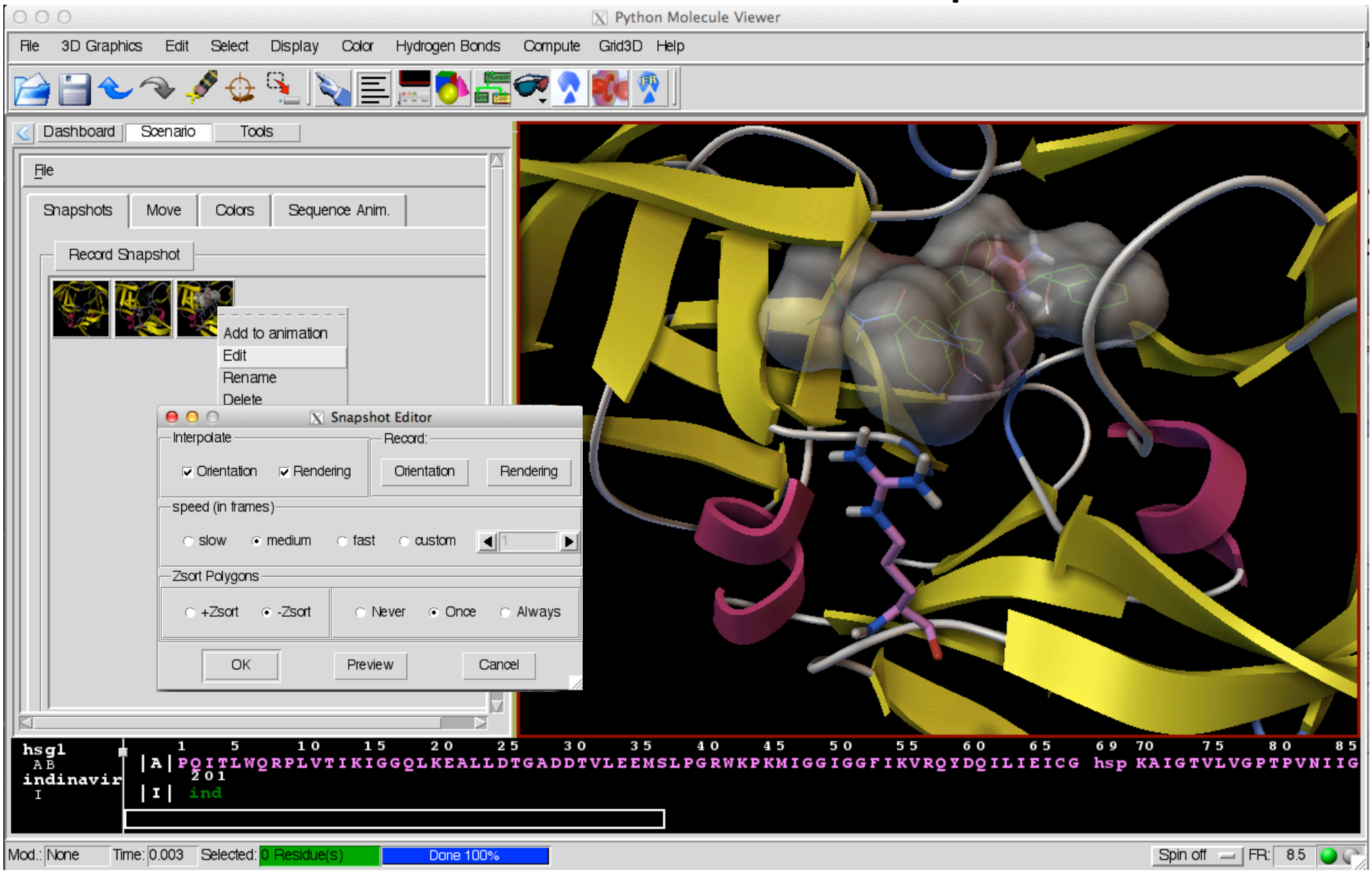
RMDS/Superimpose



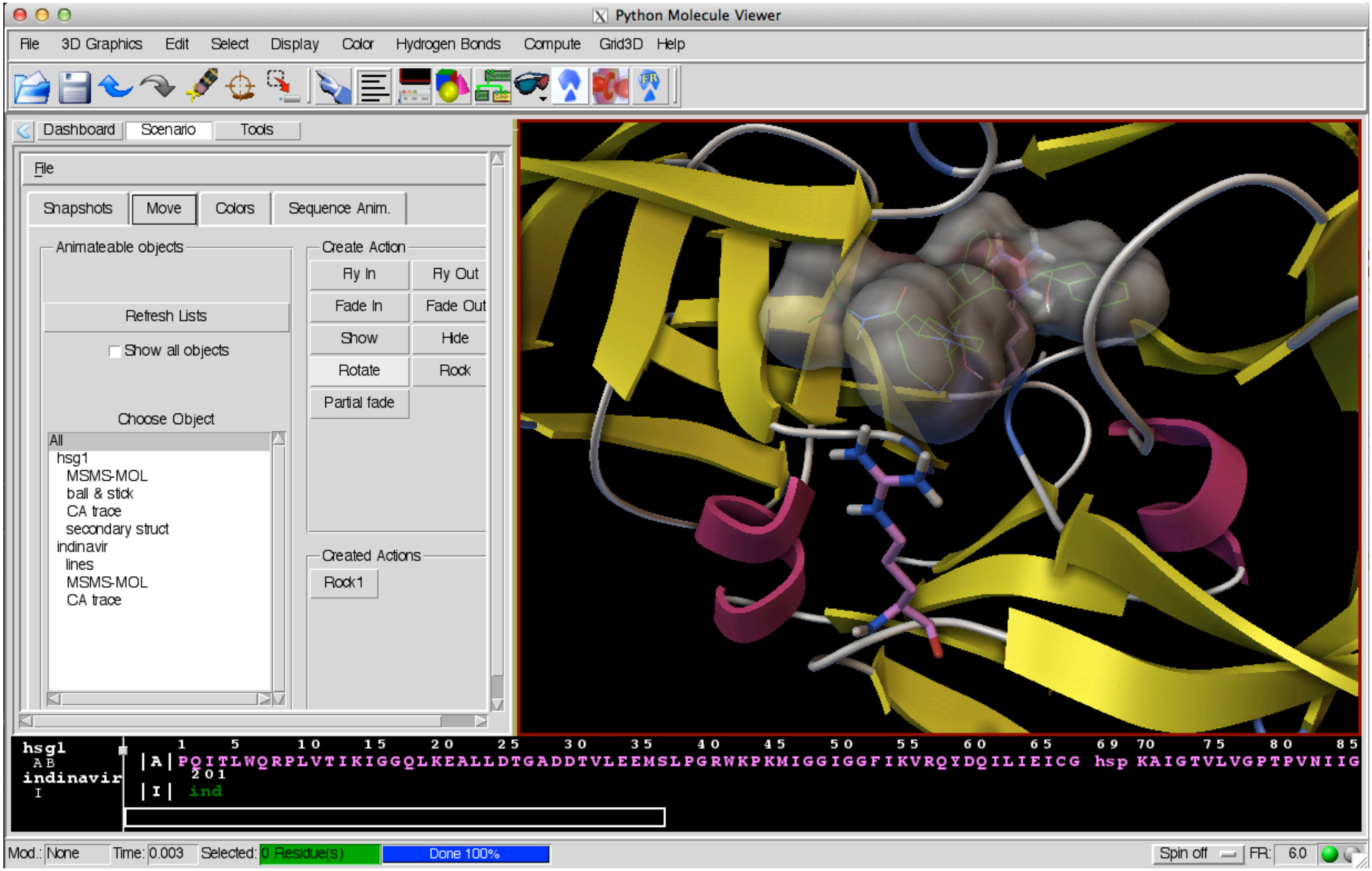
RMDS/Superimpose



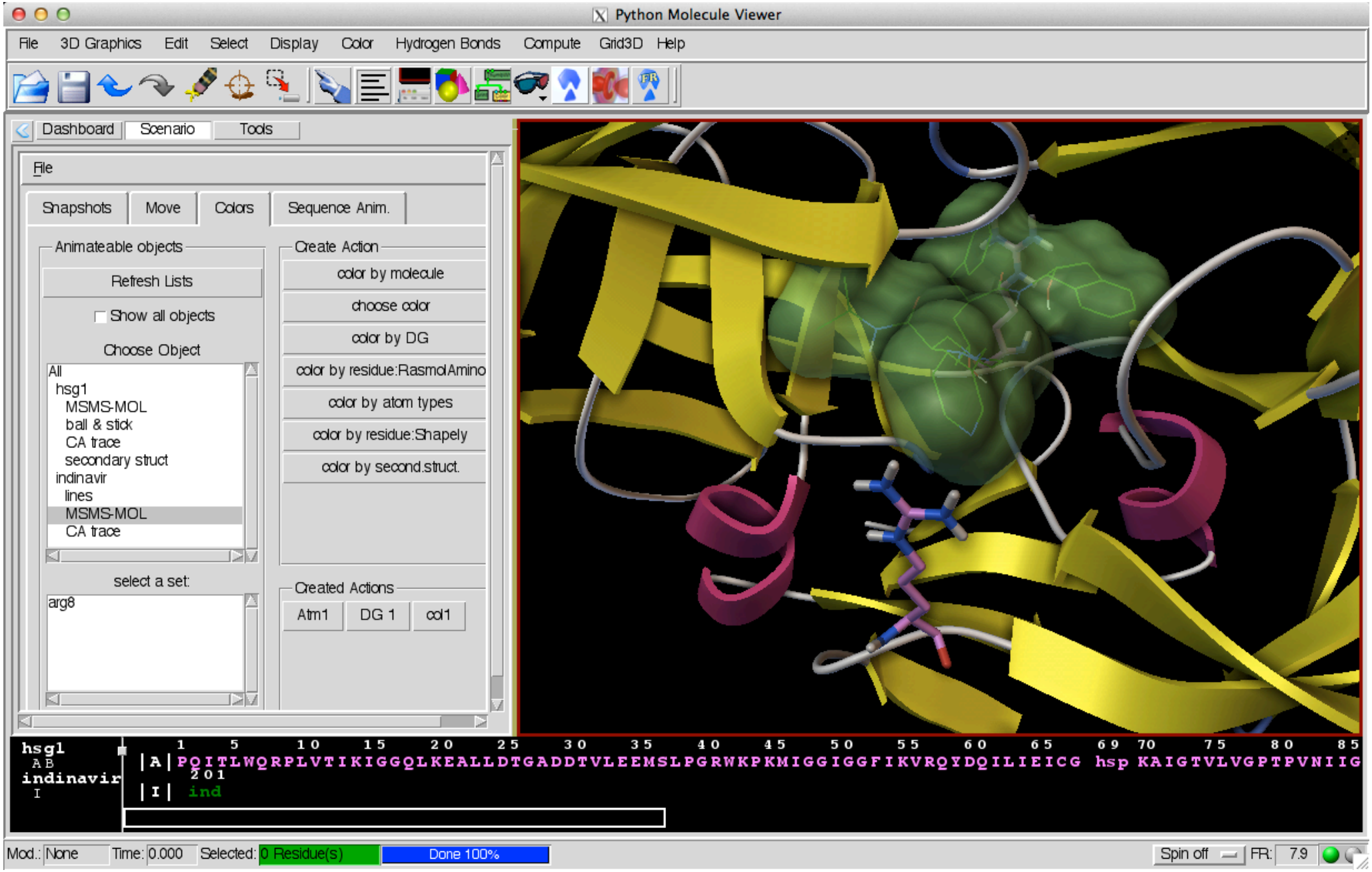
Scenario Animations: snapshots



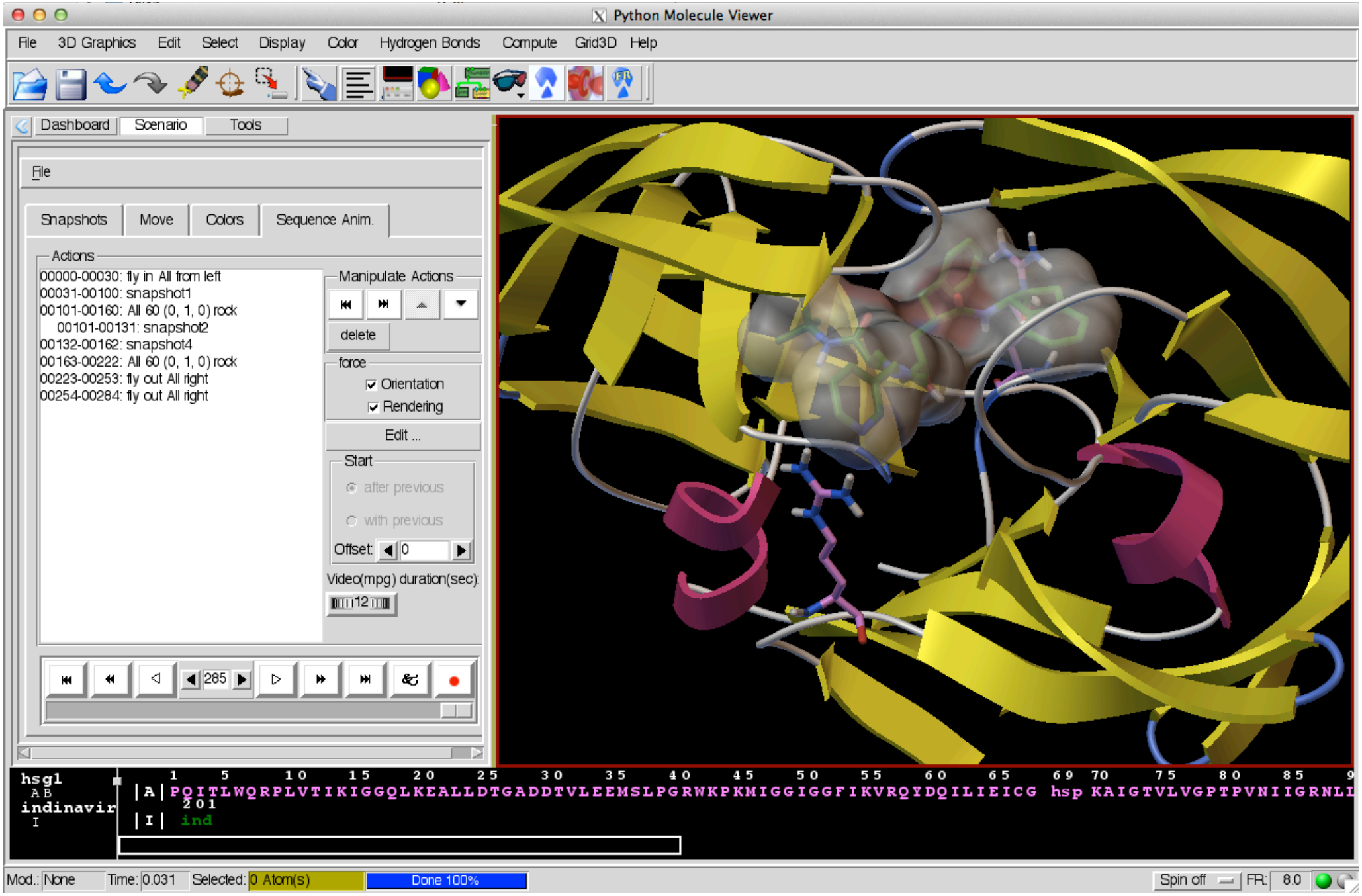
Scenario Animations: moves



Scenario Animations: color



Scenario Animations: sequence

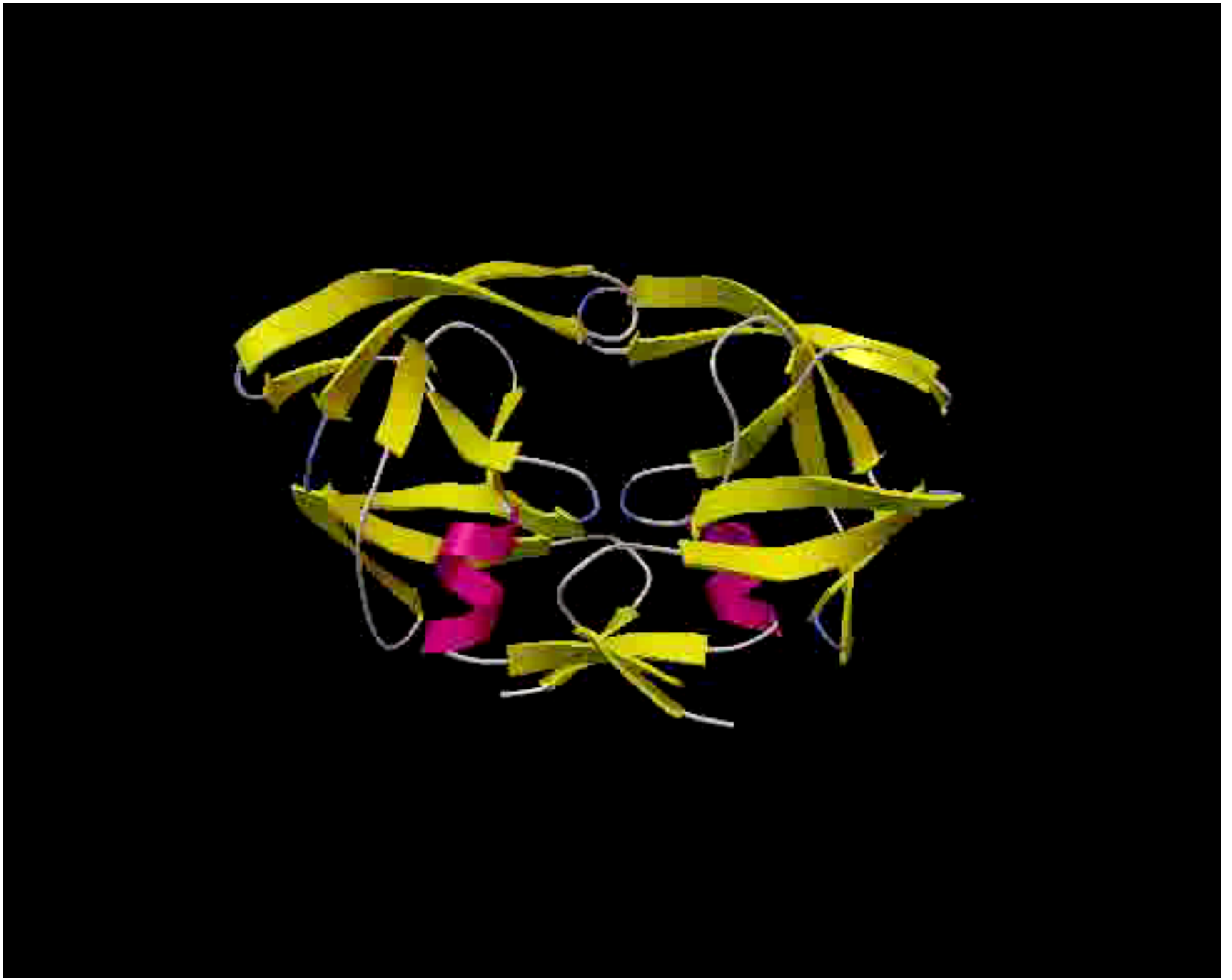


Scenario Animations: sequence

Task: create an animation

1 – load hsg1 and indinavir
2 – hide indinavir
3 – display hsg1 as ribbon colored by secondary structure
4 – create a snapshot of only 1 frame add it to the sequence
5 – create a fly-in from the left add it to the sequence
5 – zoom in to active site create a snapshot and add to sequence
6 – create a rock and add to sequence
7 – create a snapshot with arg8 visible as S&B (rendering only) and make it start with previous
8 – add a rock while fading in indinavir as a surface
9 - fly out
10 – record the animation

NOTE: Scenario animation snipets get saved in the session file

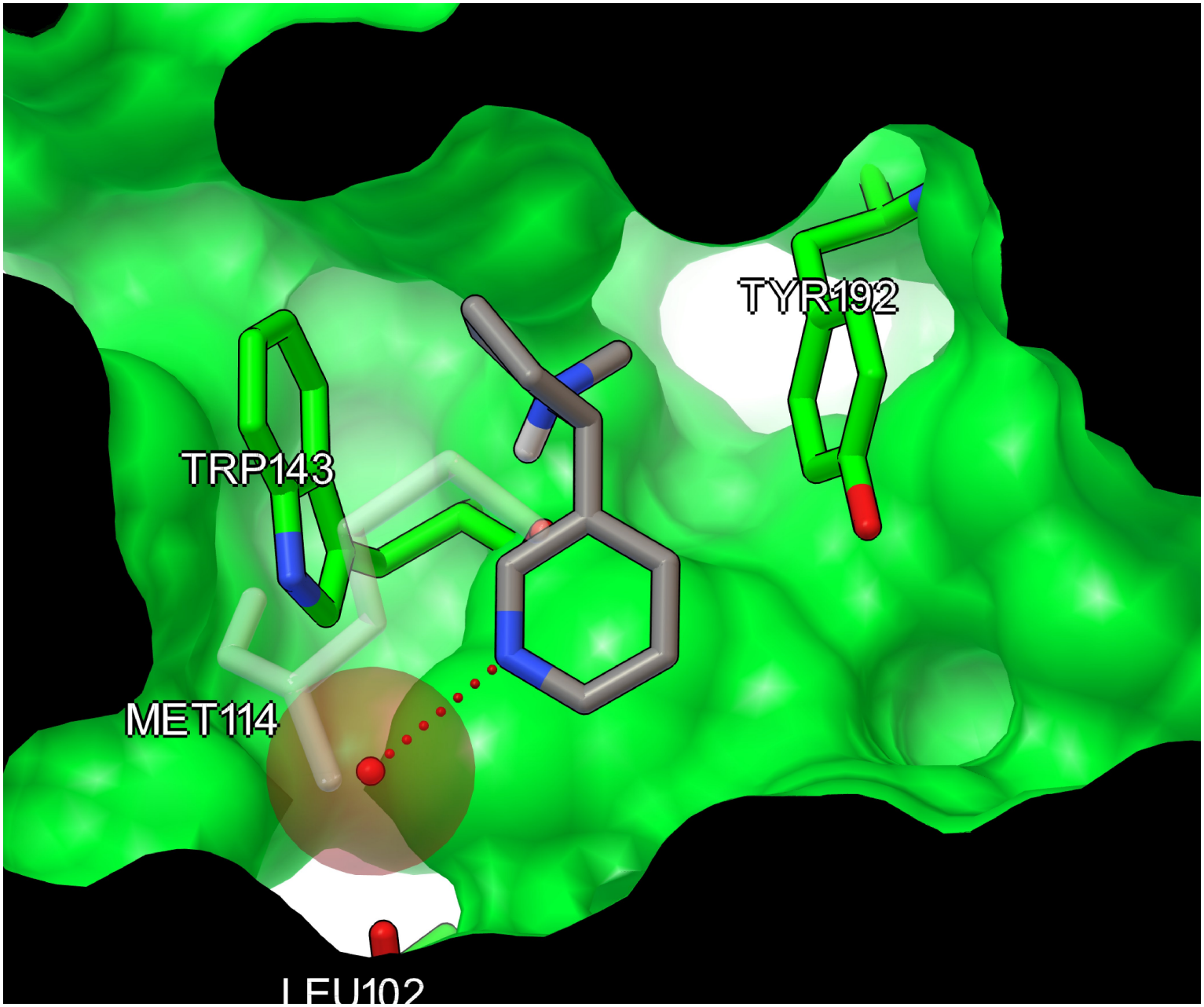


Scenario Animations

Task: create a simple animation using scenario

1 – load hsg1.pdbqs from Desktop/TutorialData
2 – undisplay lines
3 – display ribbon and color bur secondary structure
4 – center molecule and take snapshot
5 – edit snapshot to use 1 frame
6 – add snapshot to animation
7 – create fly in motion and add to animation
8 – Load indinavir and display S&B
9 – create snapshot with zoom on indinavir and add to animation
10 – create rock motion and add to animation
11 – create snapshot to zoom back out and add to animation
12 – create fly out motion and add to animation

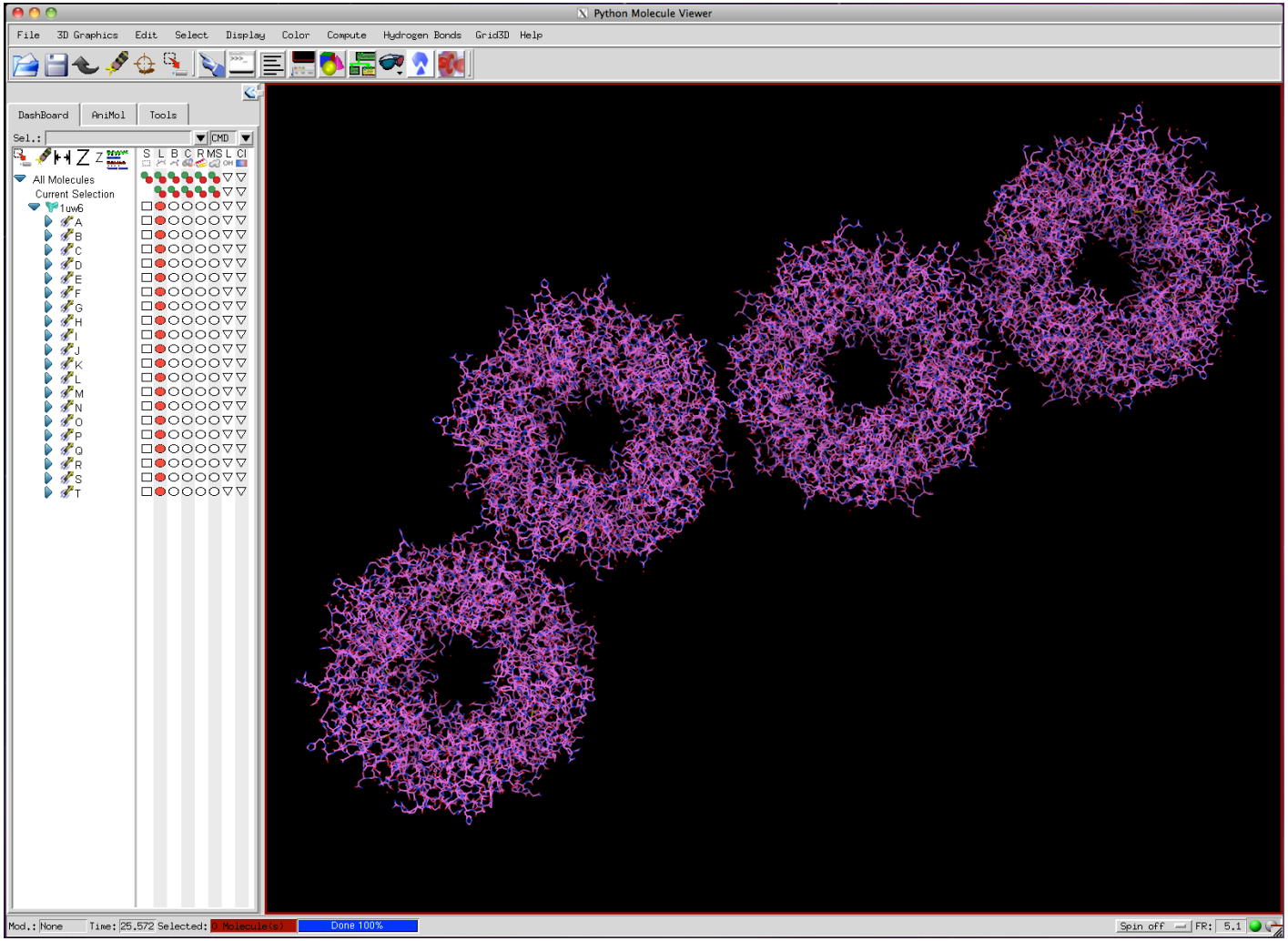
Example: 1uw6



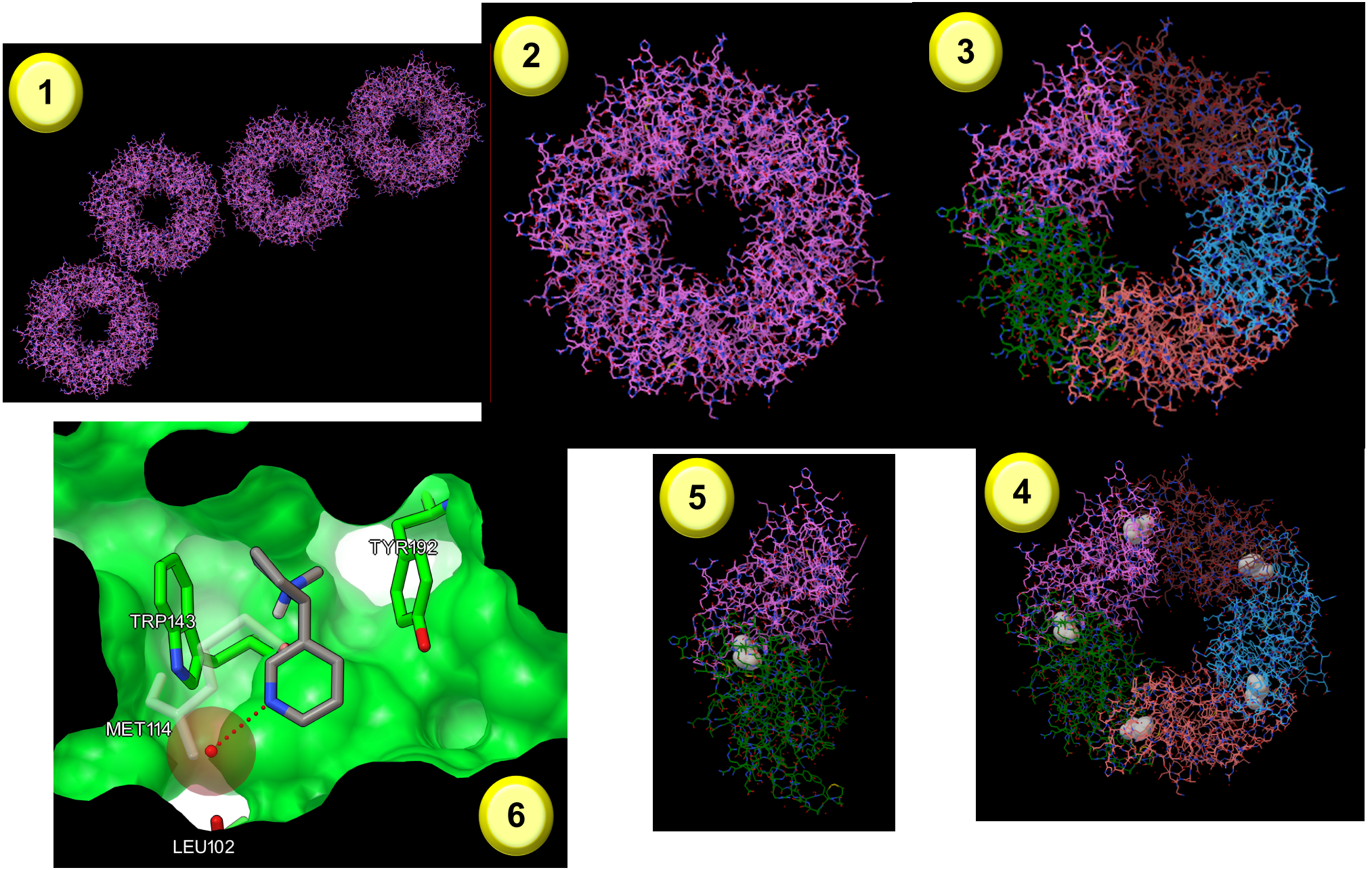
Exercise: selections

Task: get structure and get familiar with it

1 – get pdb file 1uw6 from web (File -> import -> fetch from web)



Exercise: selections



Exercise: selections

Task: Keep a single ring by deleting the 3 others

1 – select chains A-E in dashboard
2 – invert selection on the molecule
3 – right click on current selection and “delete selected atoms”

Task: visualize 5 chains in the ring and show ligands

1 – color molecule by chain (carbon only)
2 – select ligands in molecule
3 – display CPK for ligands

Exercise: selections

Task: keep only chain A and B

1 – select chains C-E in dashboard
3 – right click on current selection and “delete selected atoms”

Task: delete ligand in chain B

1 – suggestions ?

Task: focus on ligand in chain A

1 – select ligand in Chain A
2 – create user set
3 – Right click on set name and “Show me in 3D Viewer”

Exercise: selections

Task: make sets for neighboring side chains and interface water

1 – select ligand set
2 – “select around” in protein with cutoff 4.0
3 – create “binding with water” set

4 – select “binding with water” set
5 – de-select water
6 – create “binding” set

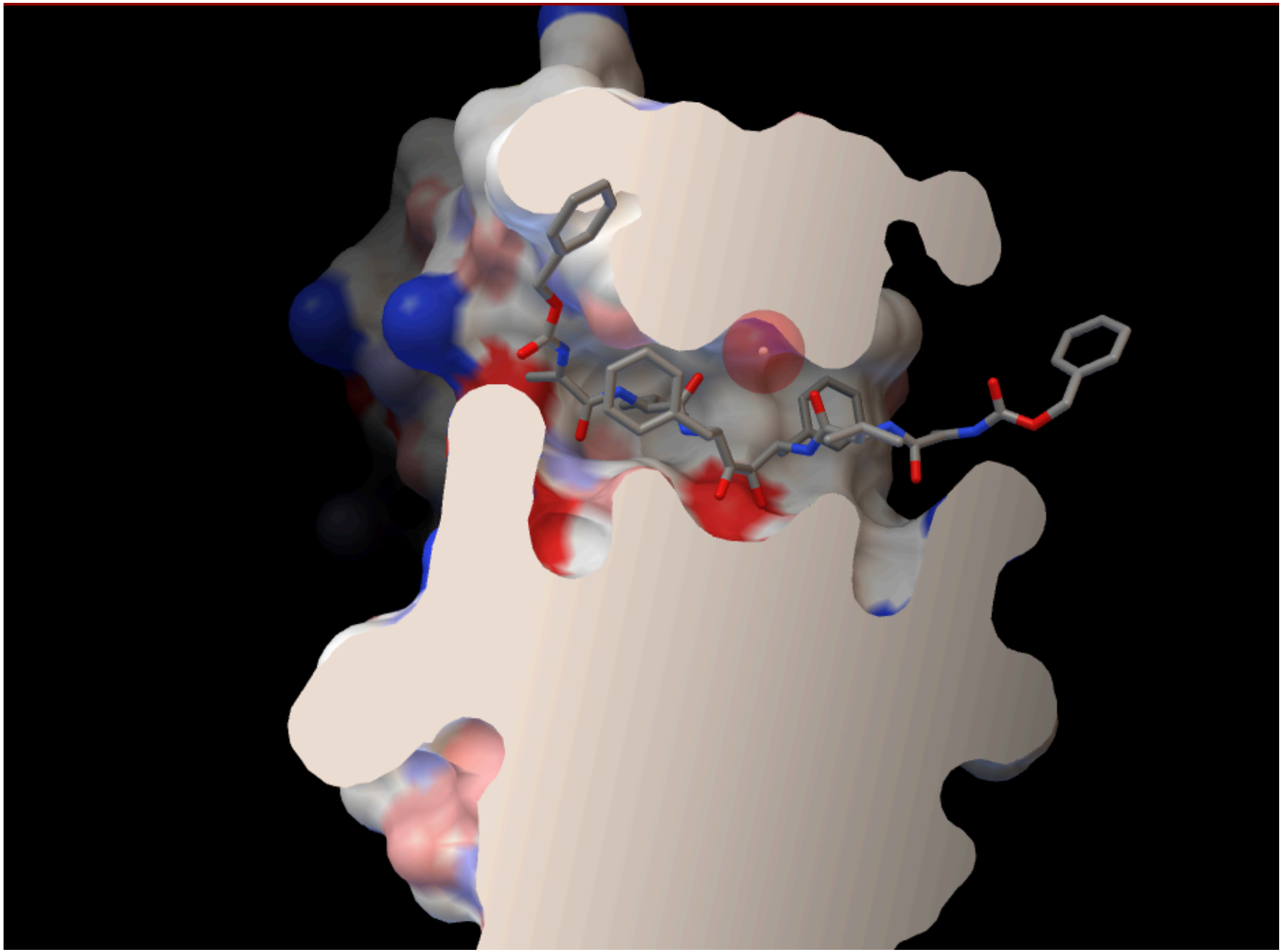
7 – select “binding with water”
8 – de-select “binding” set
9 – create “water” set

Exercise: selections

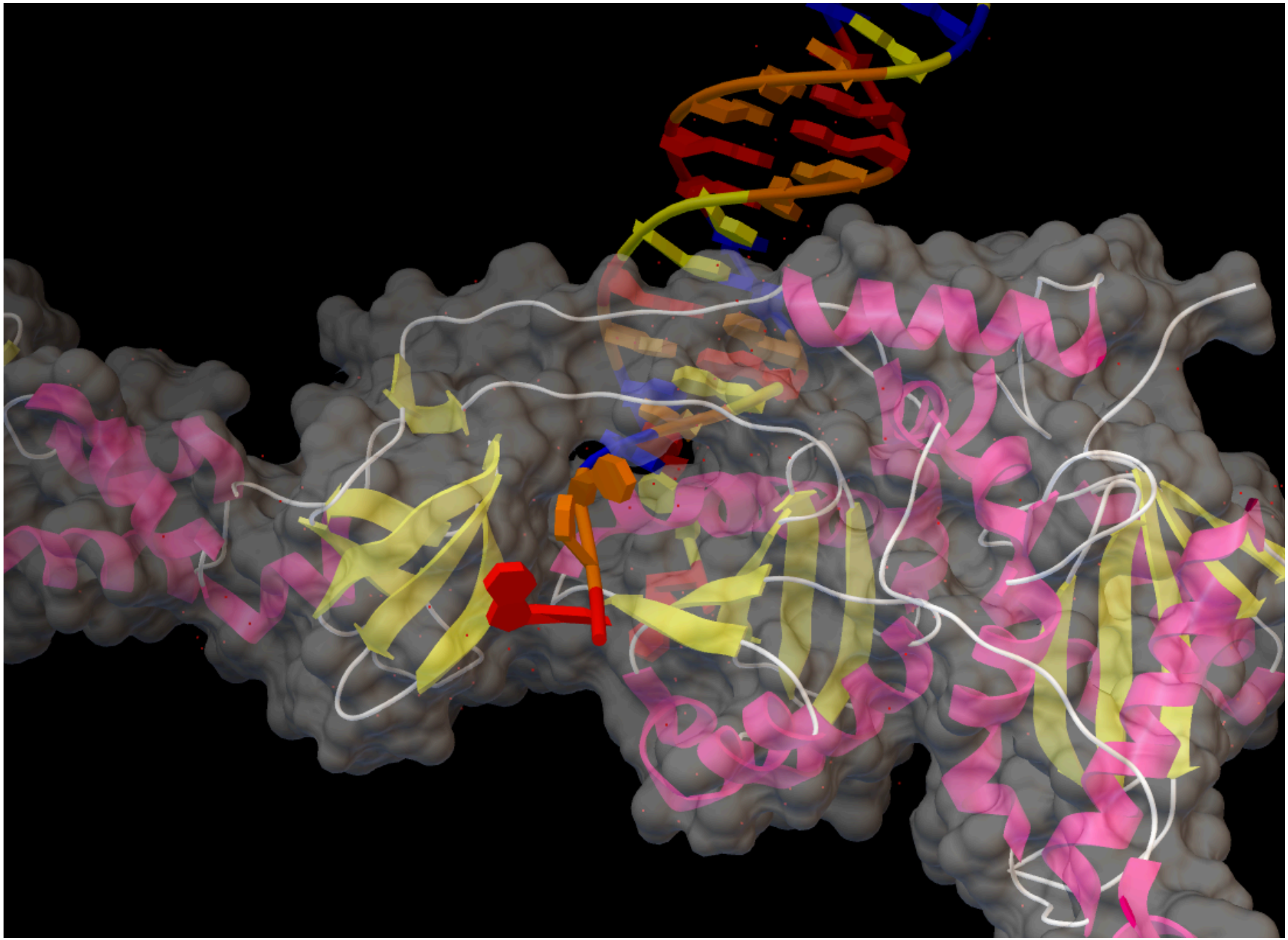
Task: compute surface

1 – select protein
2 – de-select ligand
3 – de-select binding with water
4 – de-select water
5 – make set “bulk”
6 – compute surface for bulk set

Example: 3kfr



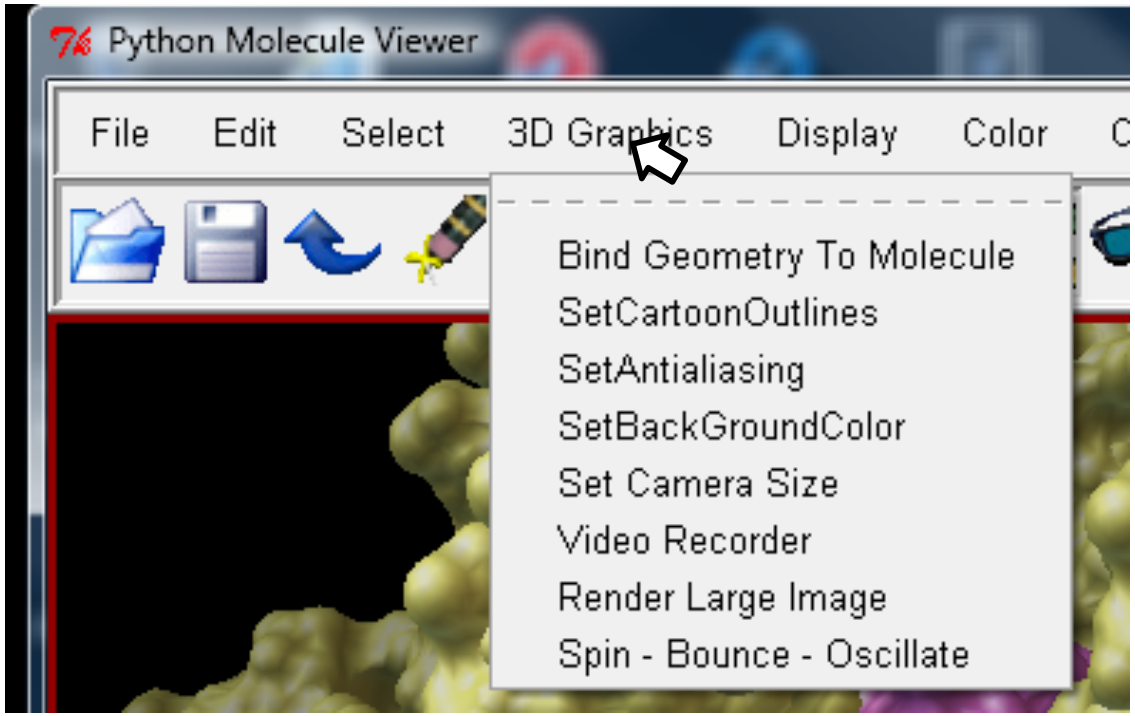
Example: 3oya



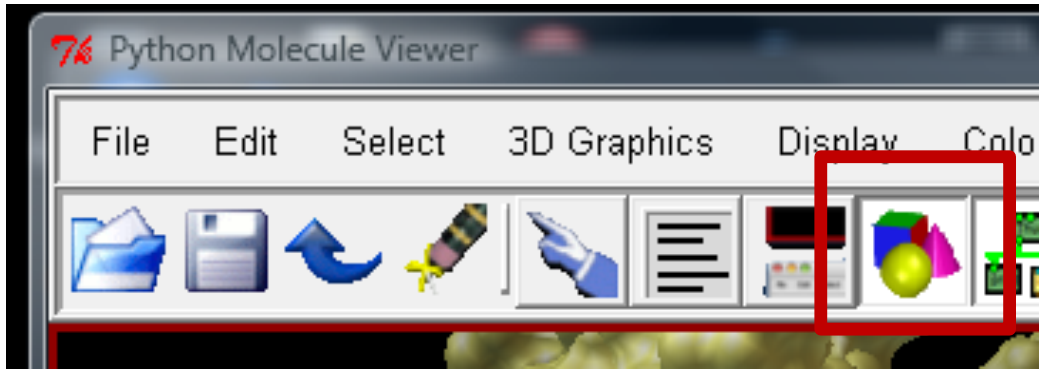
Feedback

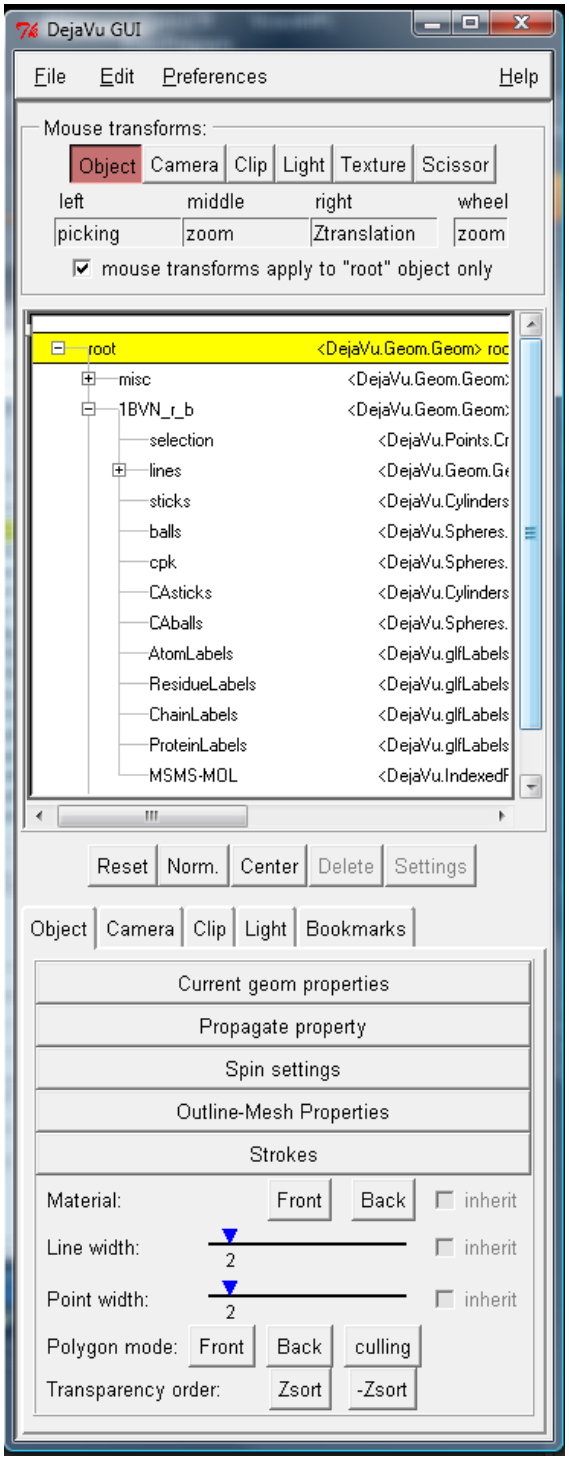
email: sanner@scripps.edu

3D Visualization

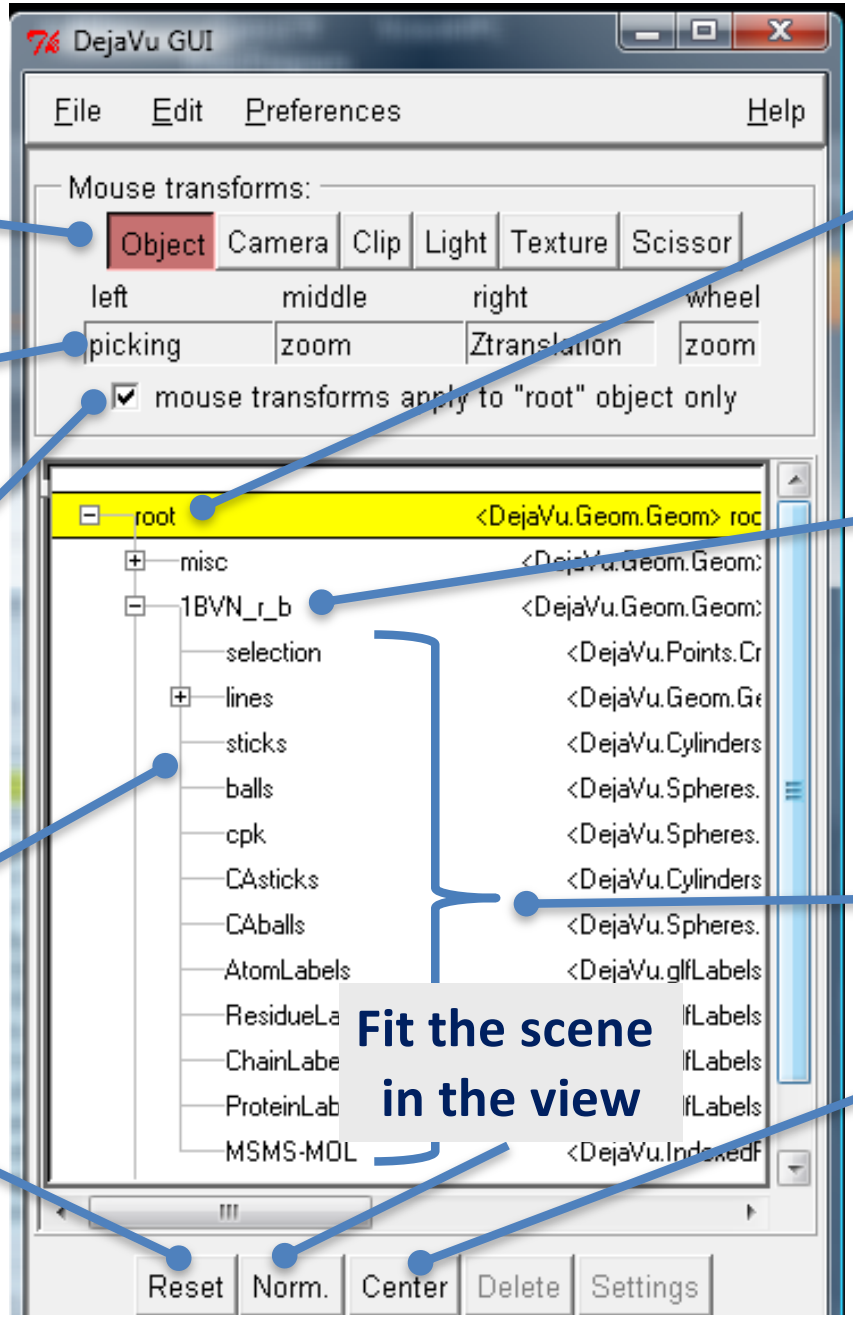


3D Visualization





3D Visualization: GUI overview



Bind Mouse to transform

Operations assigned to mouse buttons (changes with modifiers)

When checked 3D Xforms apply to root

Root geom parent of all geometries and current object

Master geom for all geoms of a given molecule

Geometry objects hierarchy

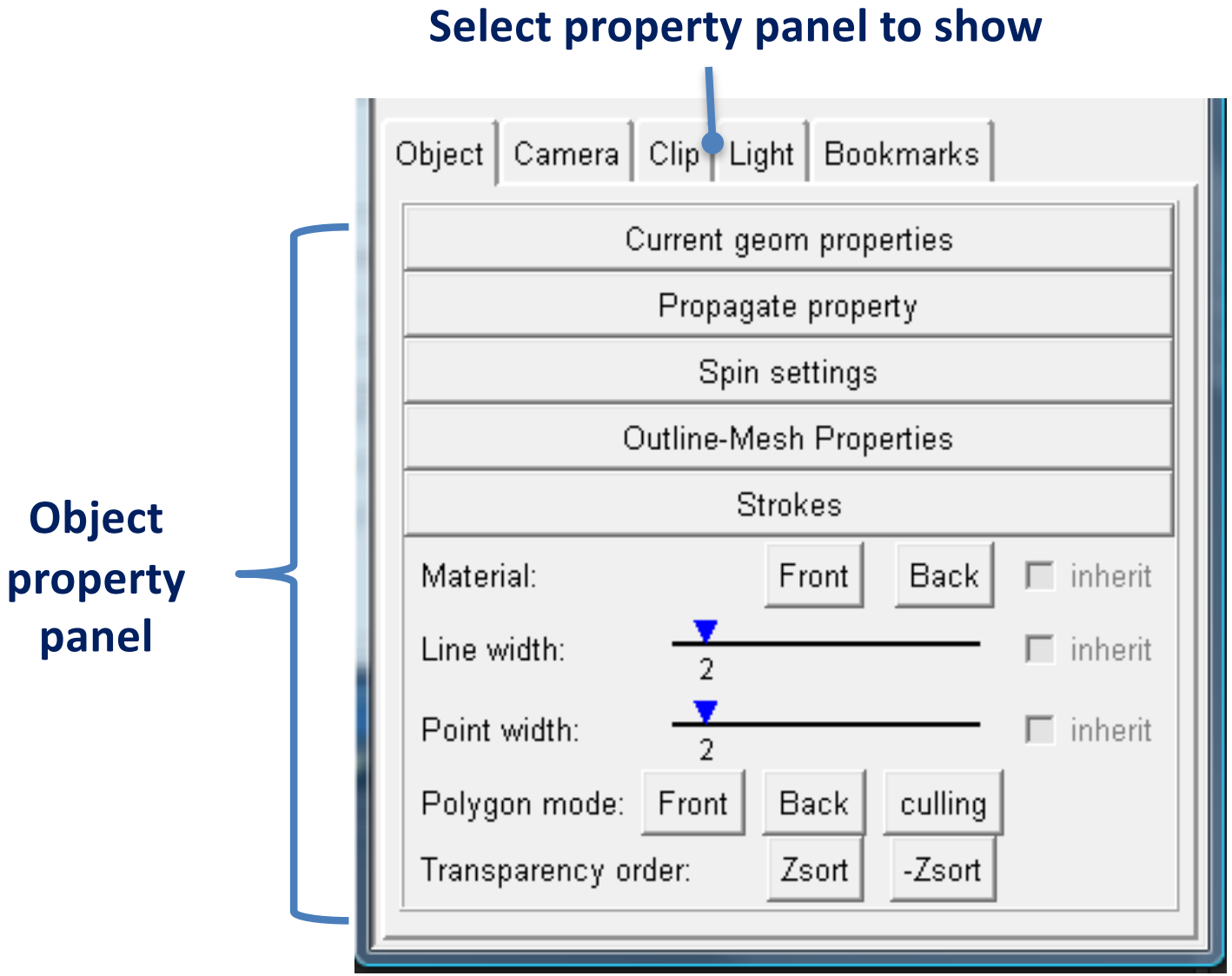
Reset Xform of current object

Fit the scene in the view

Geoms created by Pmv cmds for that molecule

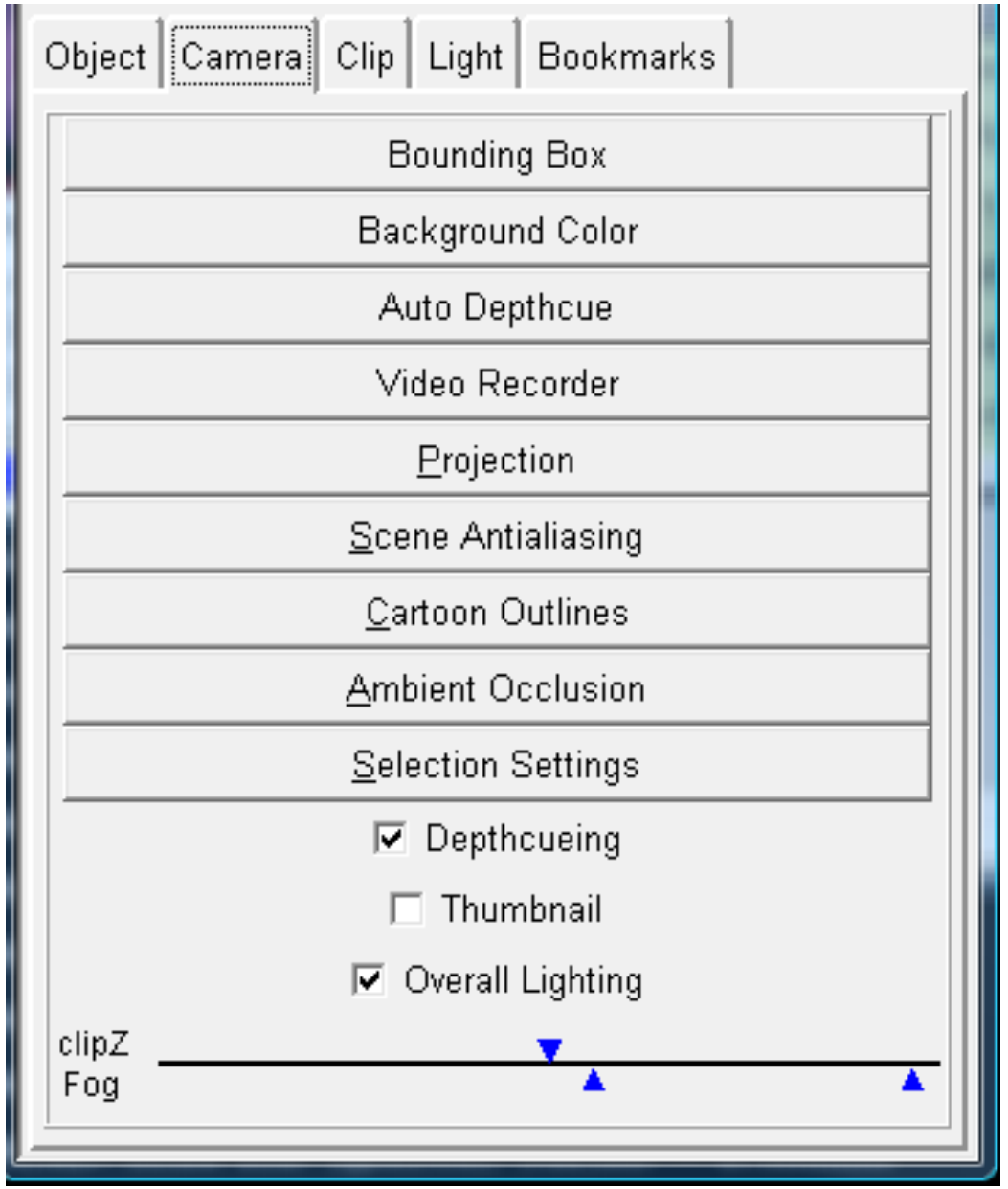
Set rotation center to center of the scene

3D Visualization: GUI overview

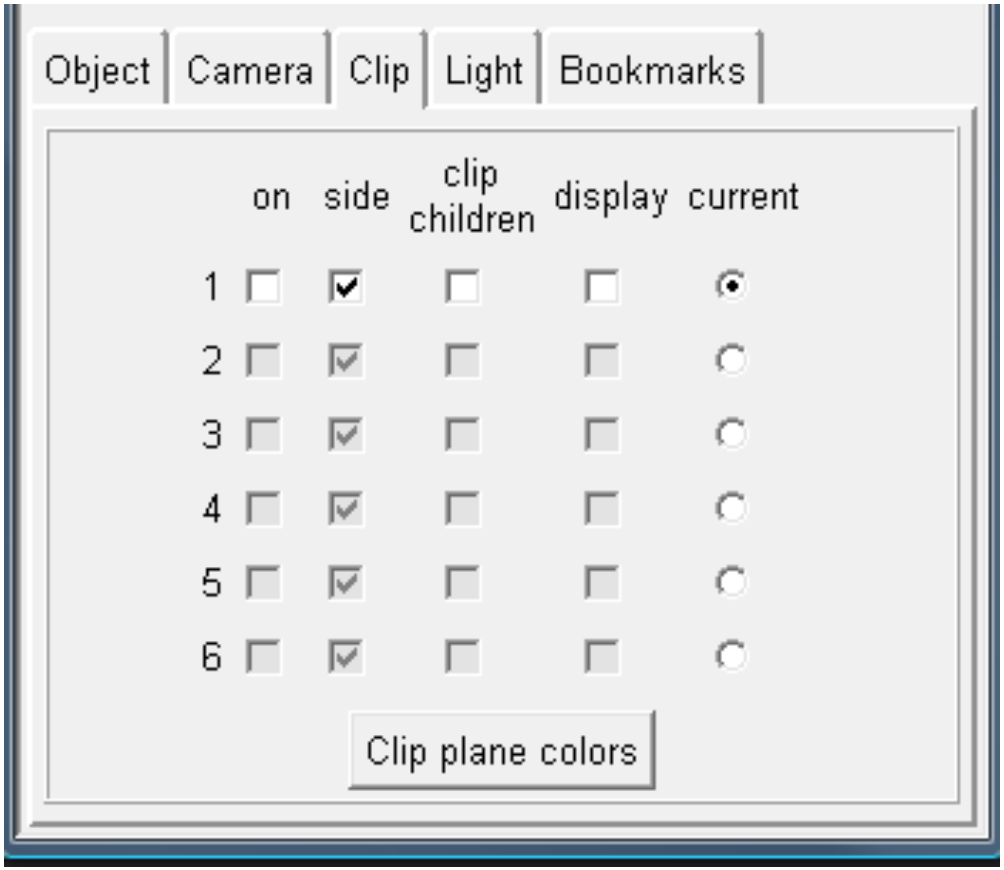


3D Visualization: GUI overview

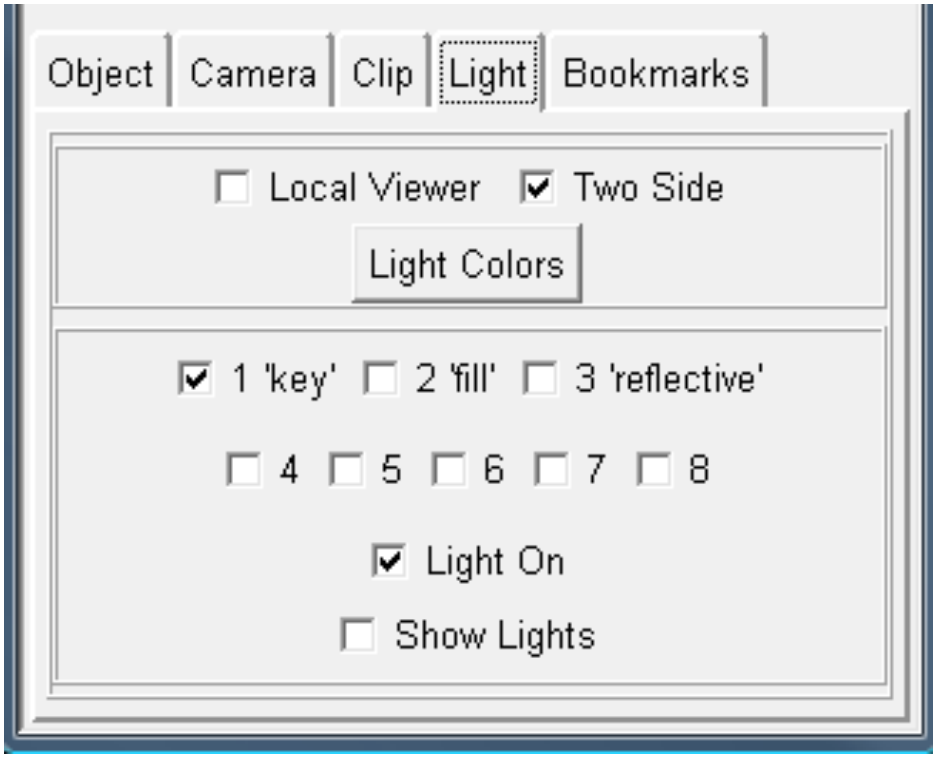
Camera property panel



3D Visualization: GUI overview



Clipping planes property panel



Lights property panel