

# Advanced Visualization with Pmv

## Instructors:

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TSRI

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

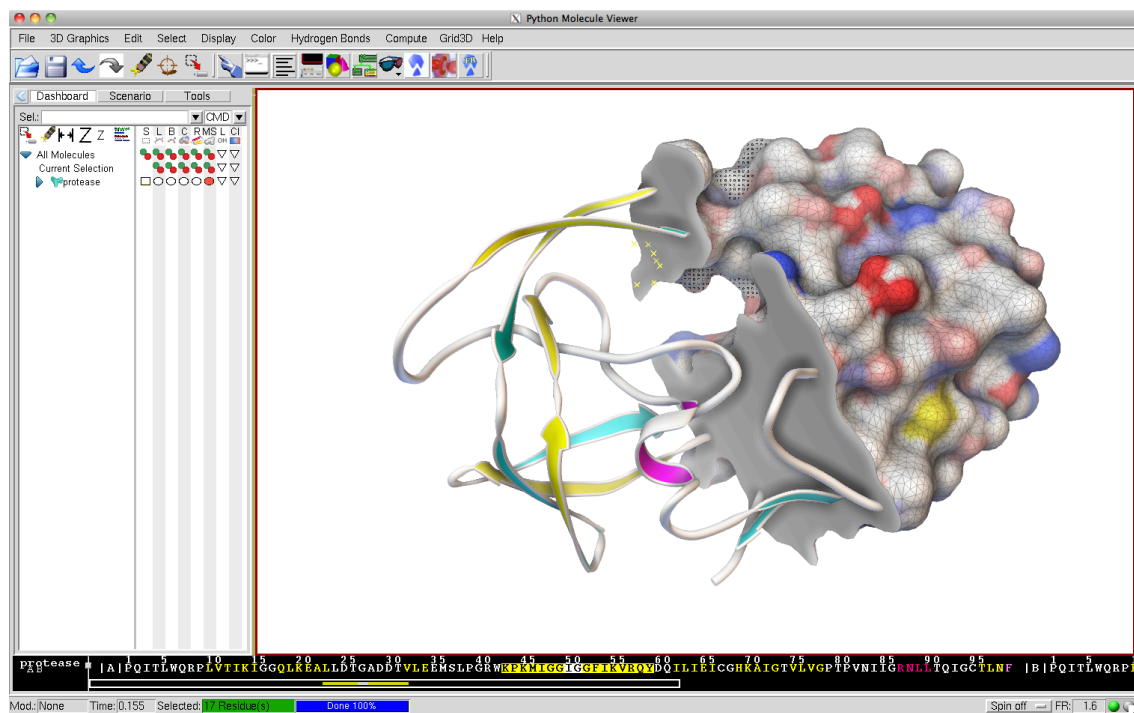
# Overview

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



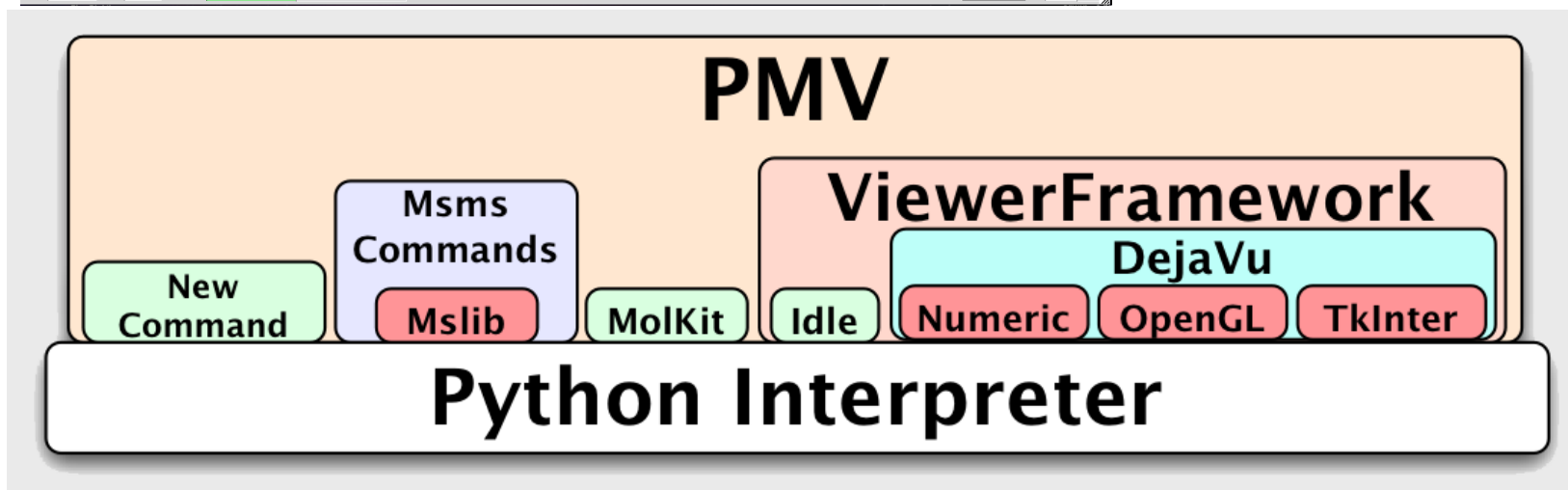
# Not Yet Another Molecular Viewer

- Component based architecture



Pmv is underlying:

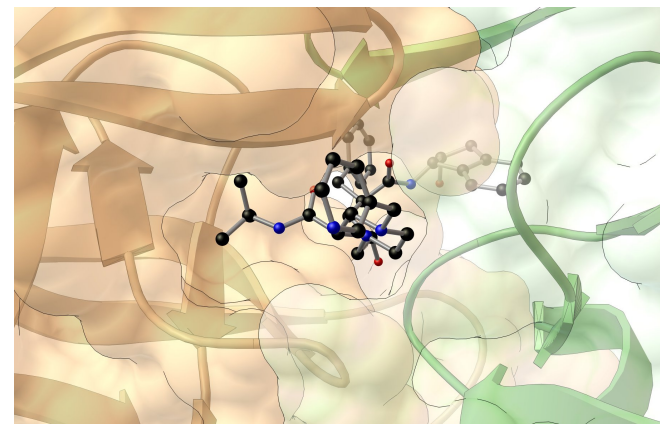
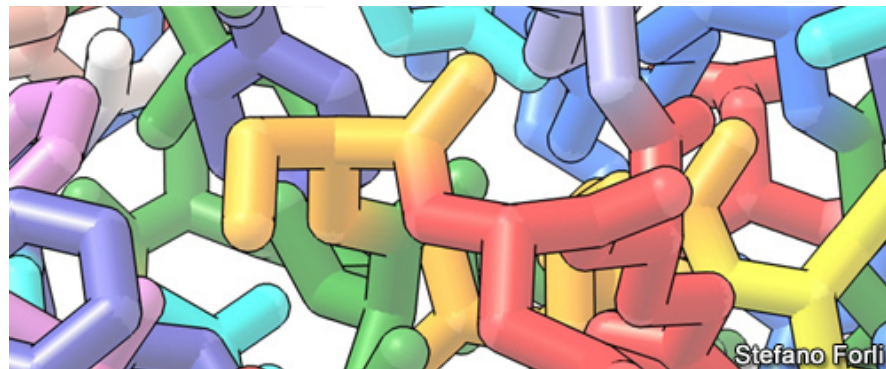
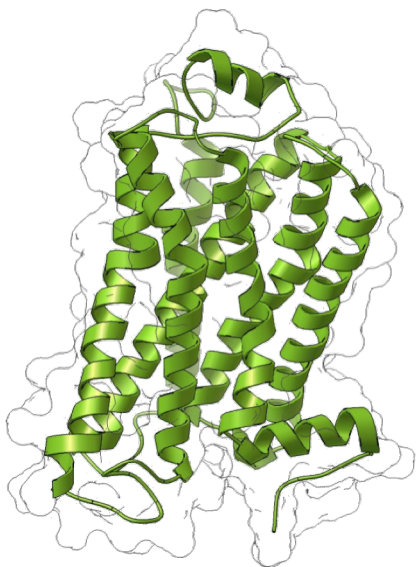
- ADT
- Raccoon
- PyARTK
- ePmv
- Continuity GUI



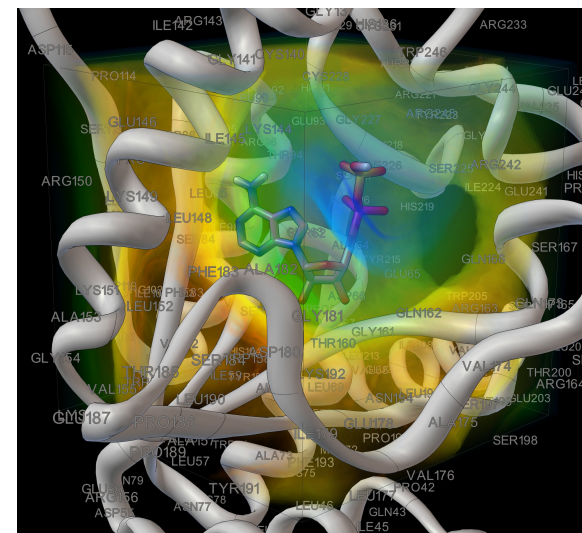
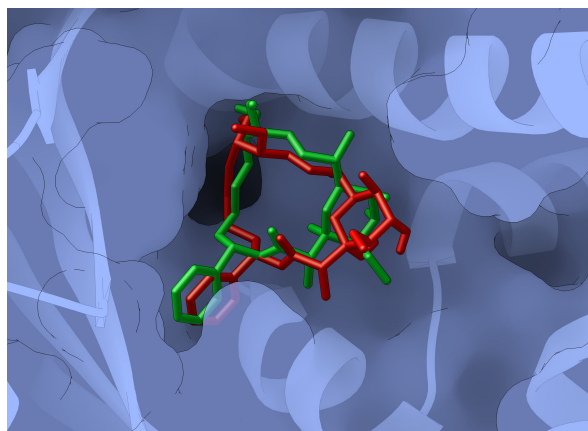
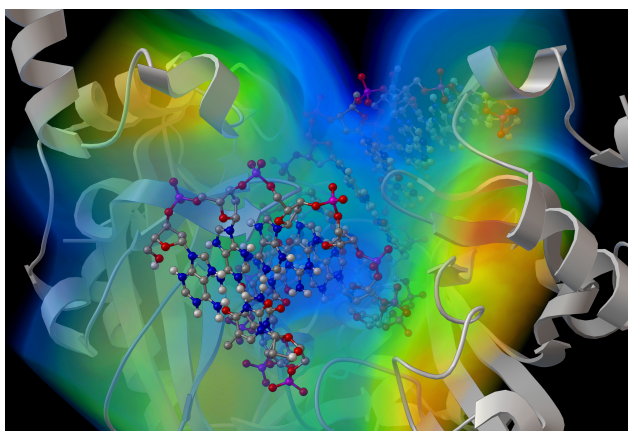
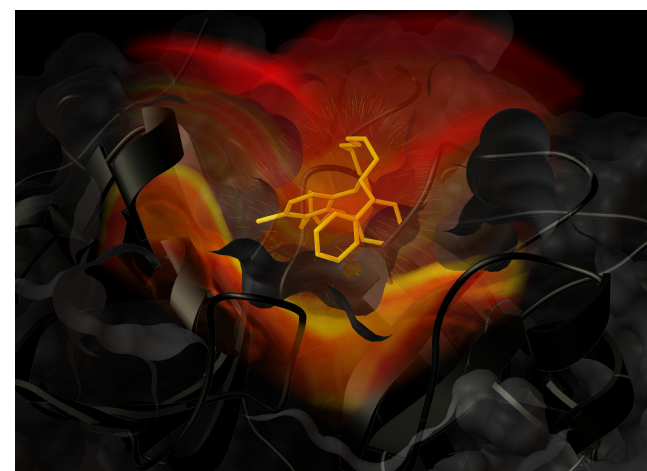
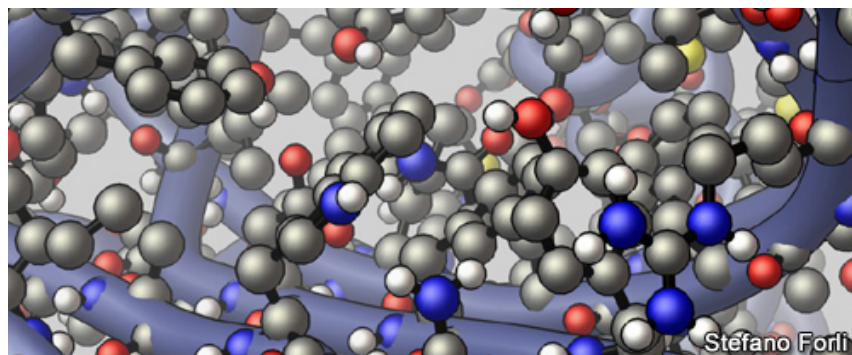
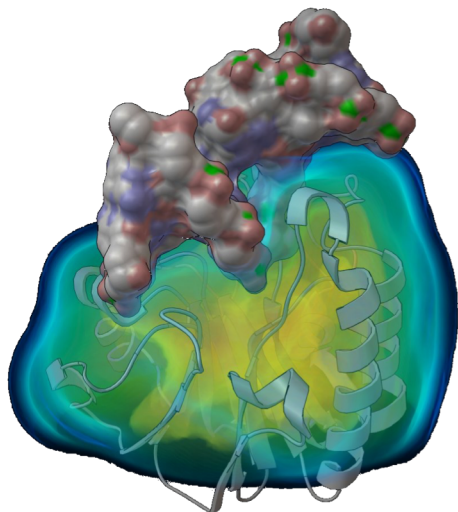
# Unique Design Features

- 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
- Animation capabilities

# Powerful 3D graphics



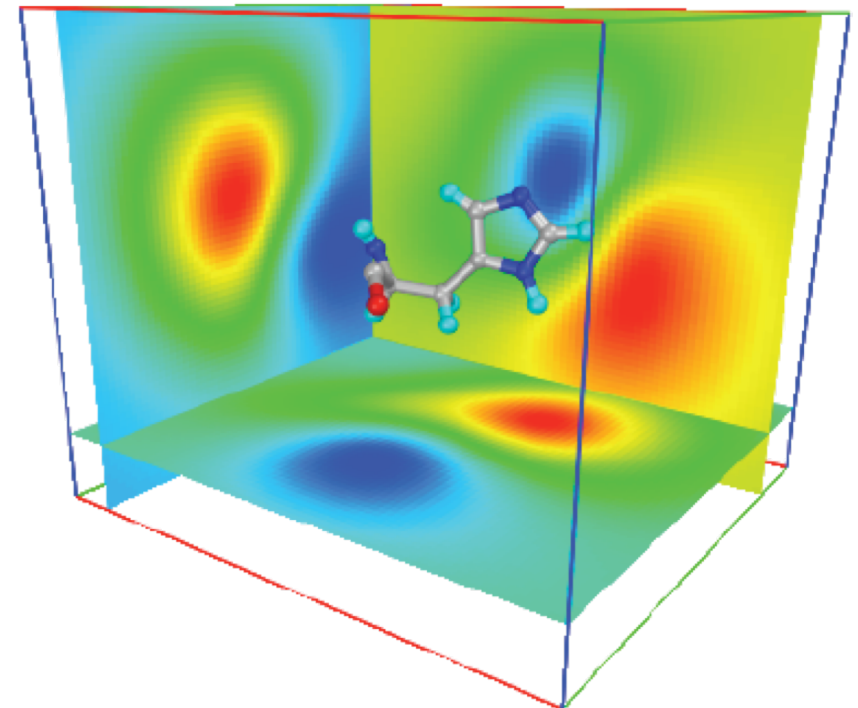
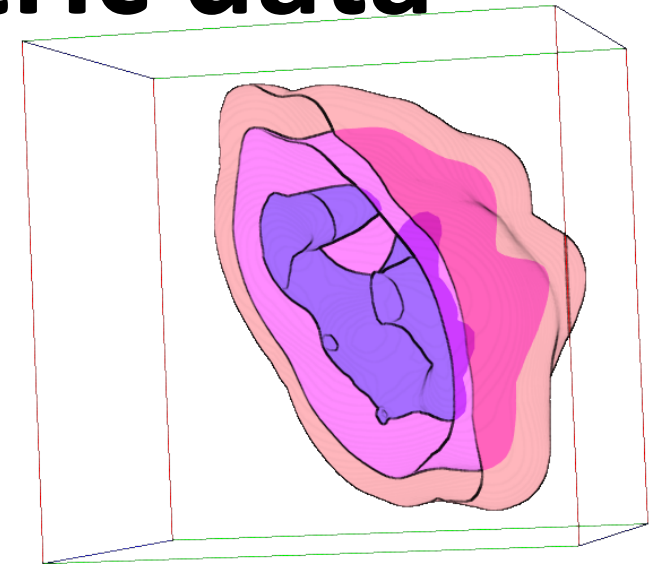
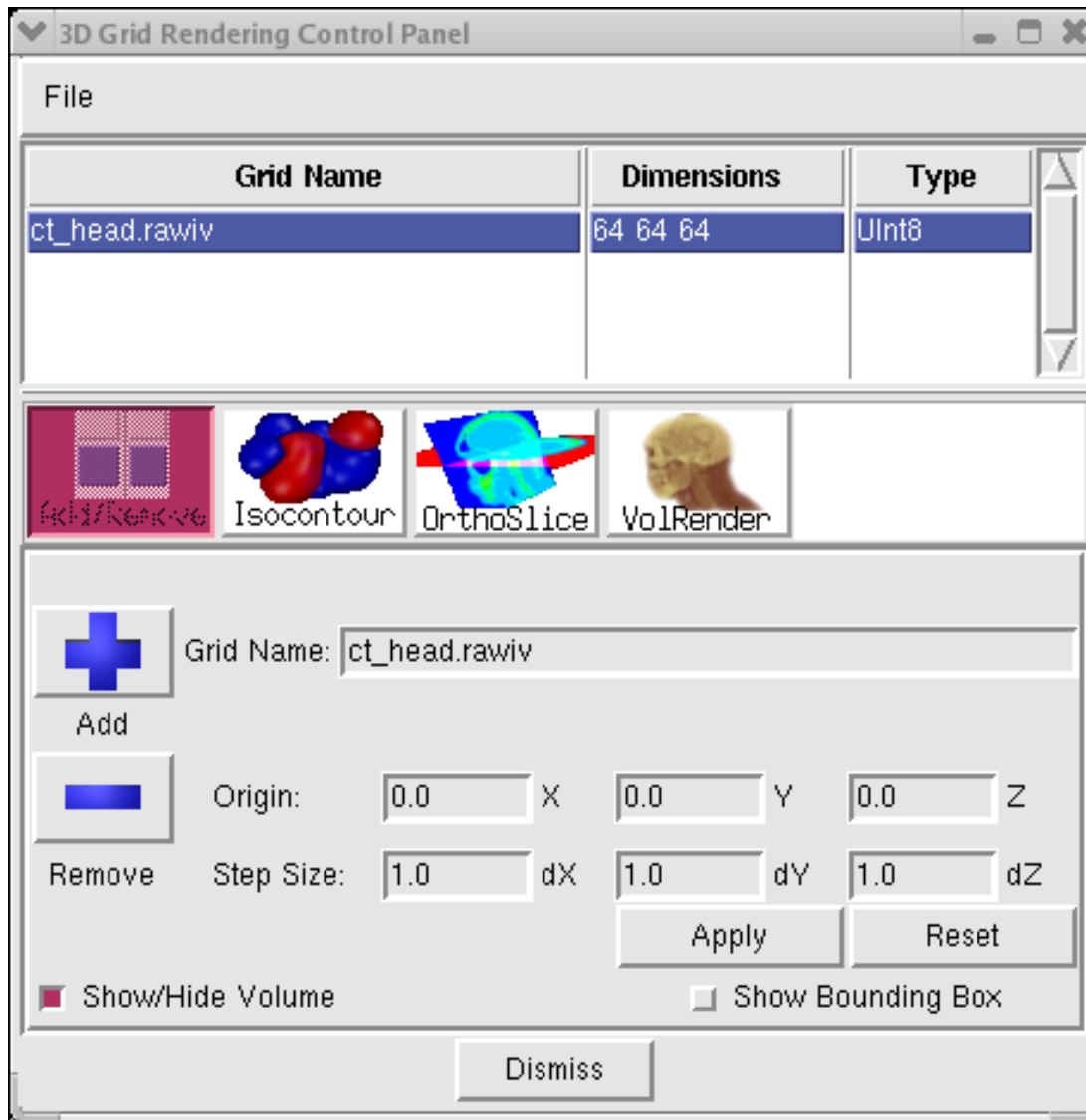
A protein structure with a yellow ribbon and a green surface representation. A small molecule (black, white, blue, red) is bound to the protein.





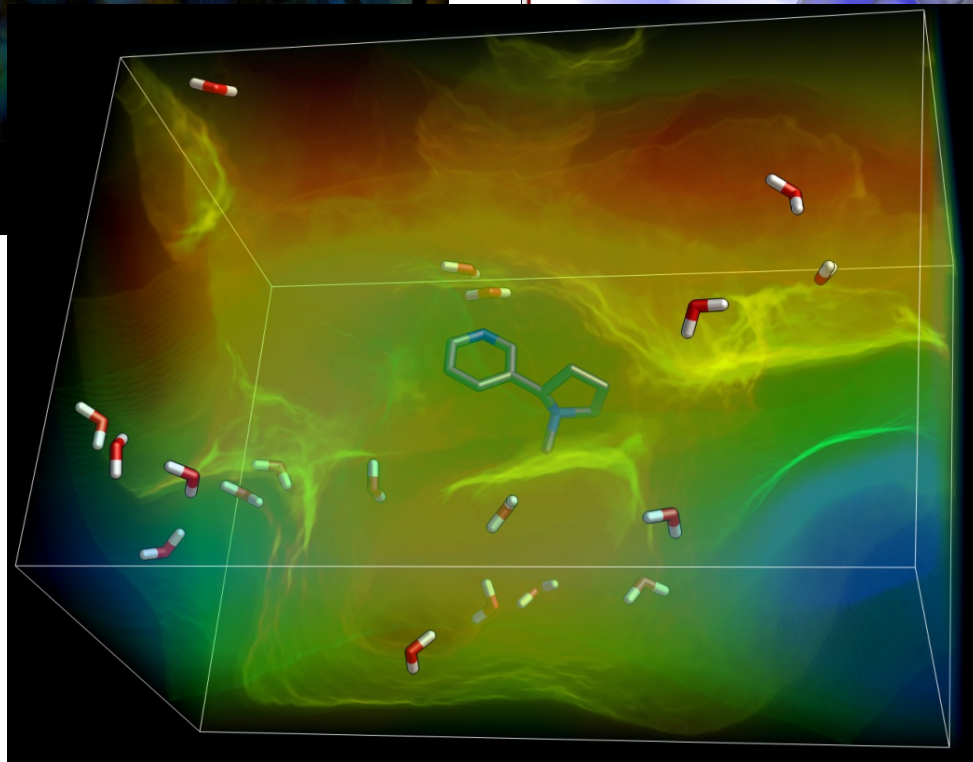
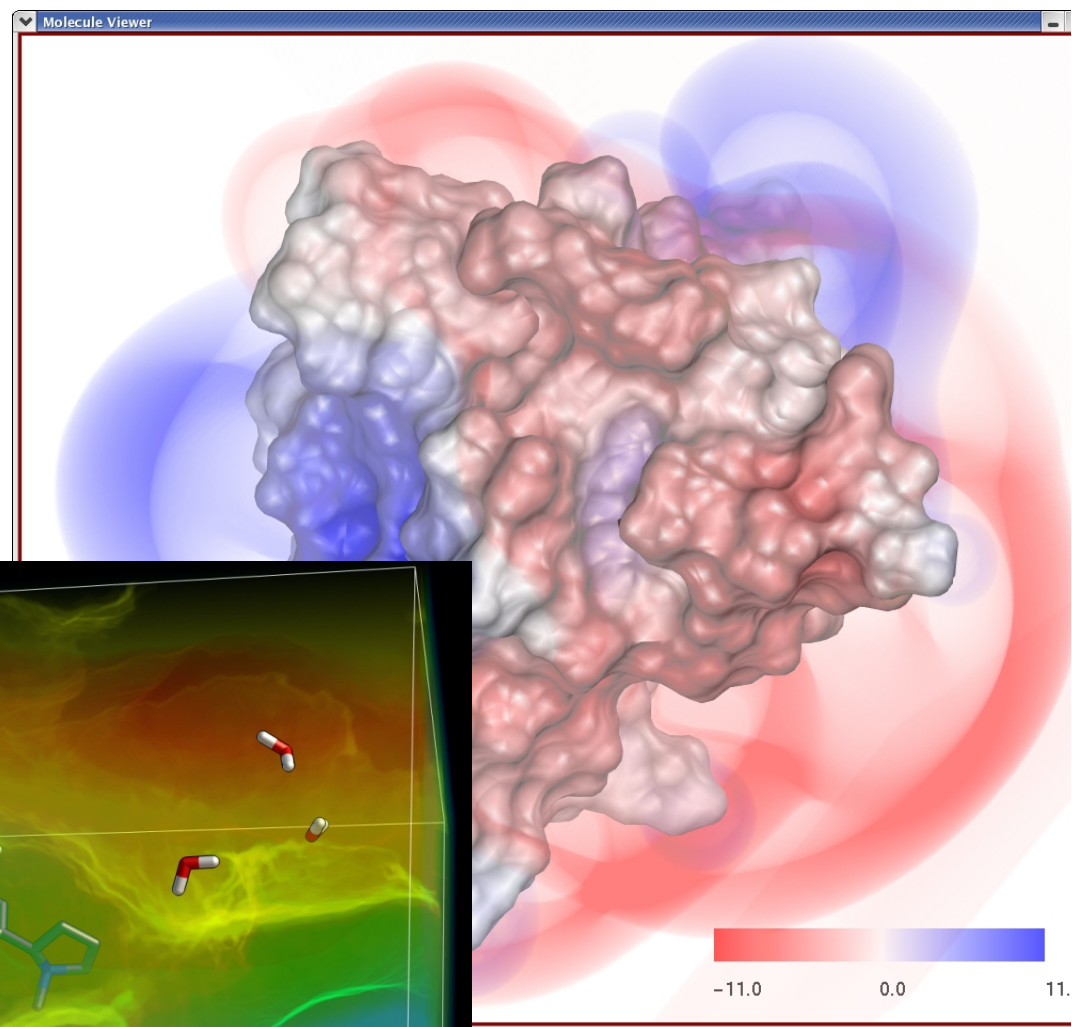
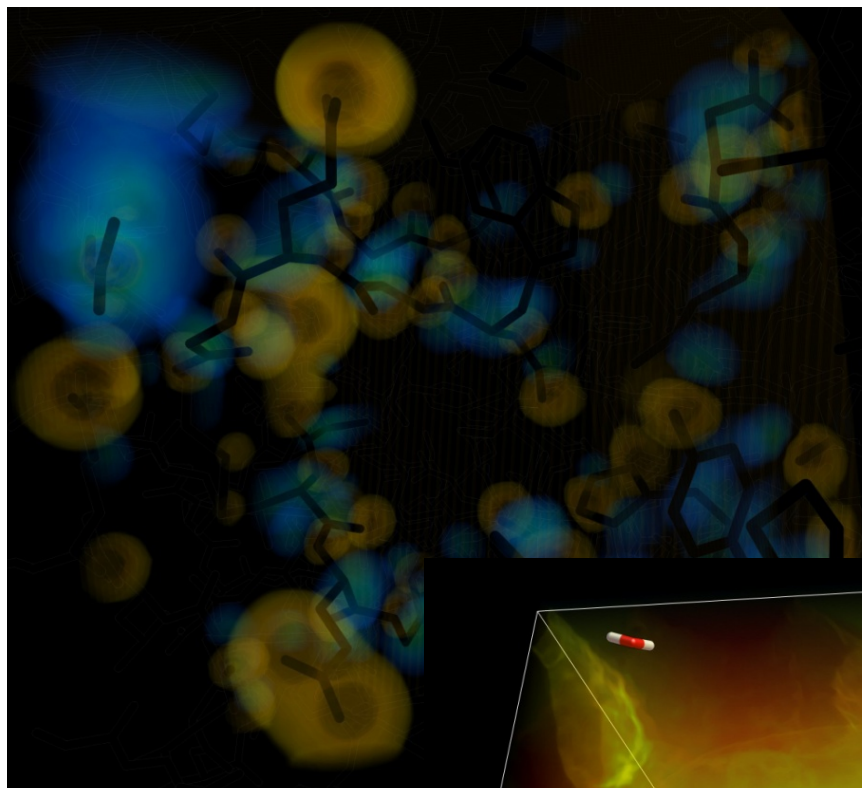
# Rendering: Volumetric data

- The Pmv interface to Volume

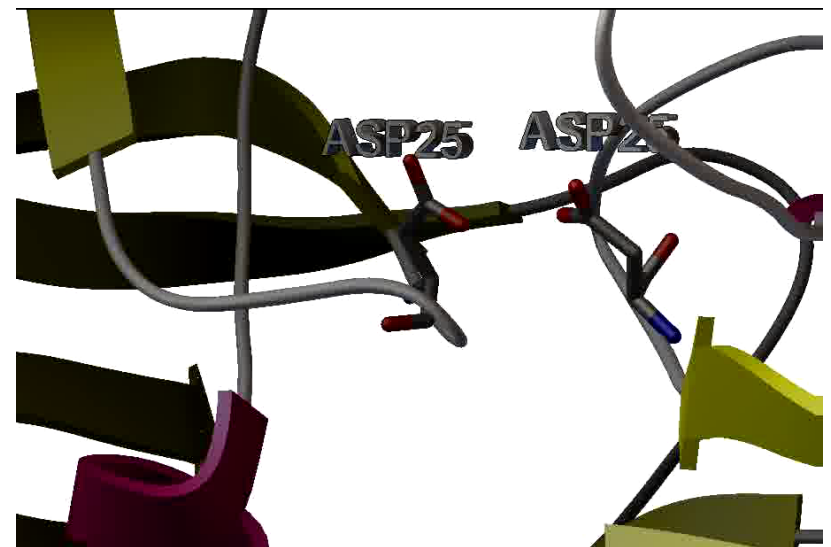
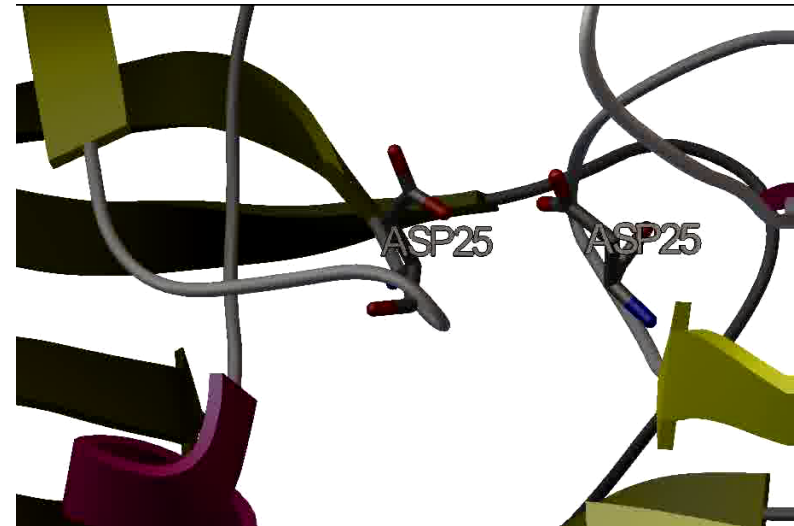
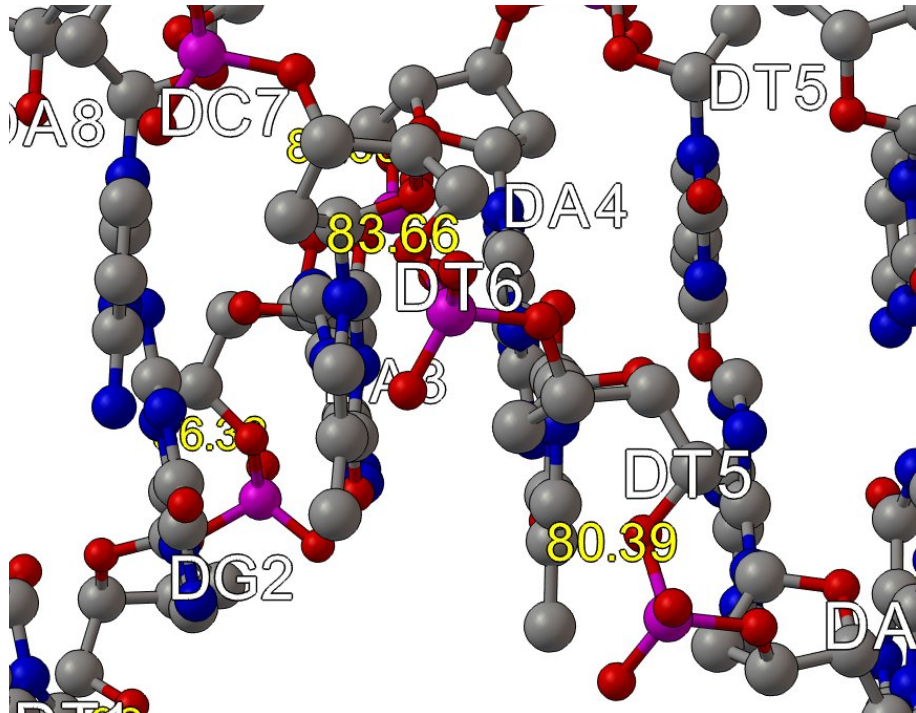




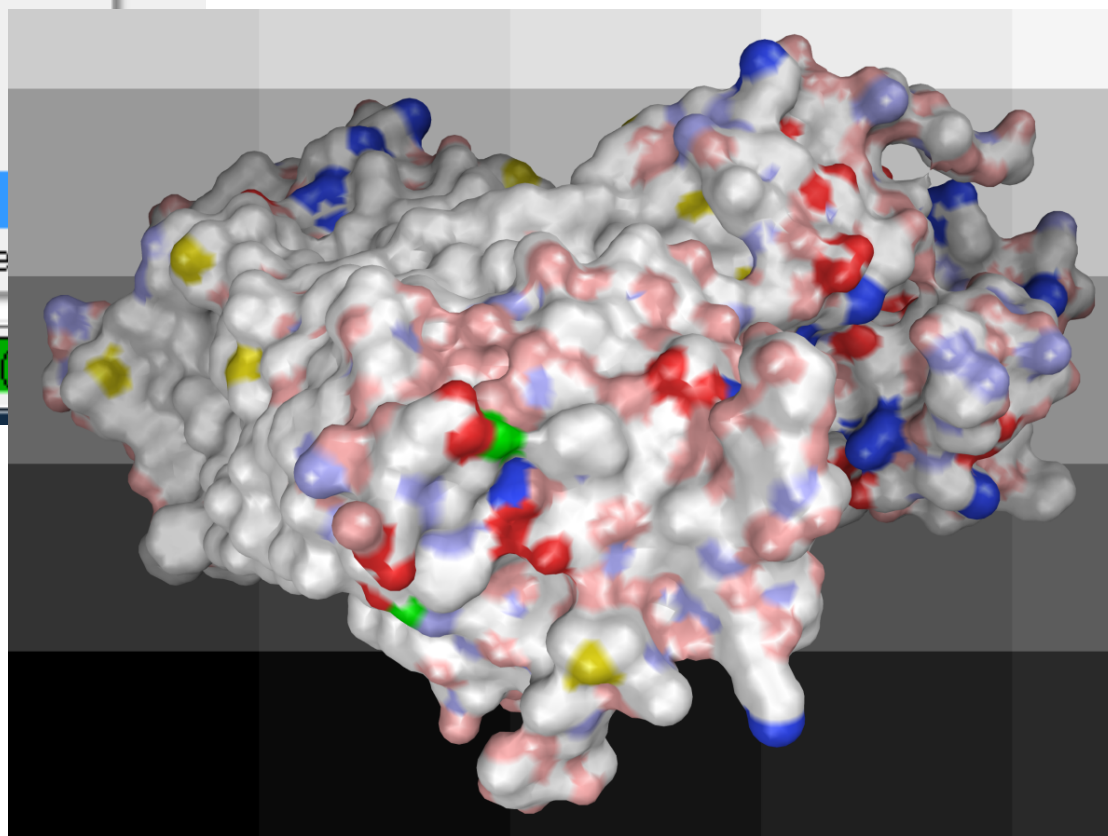
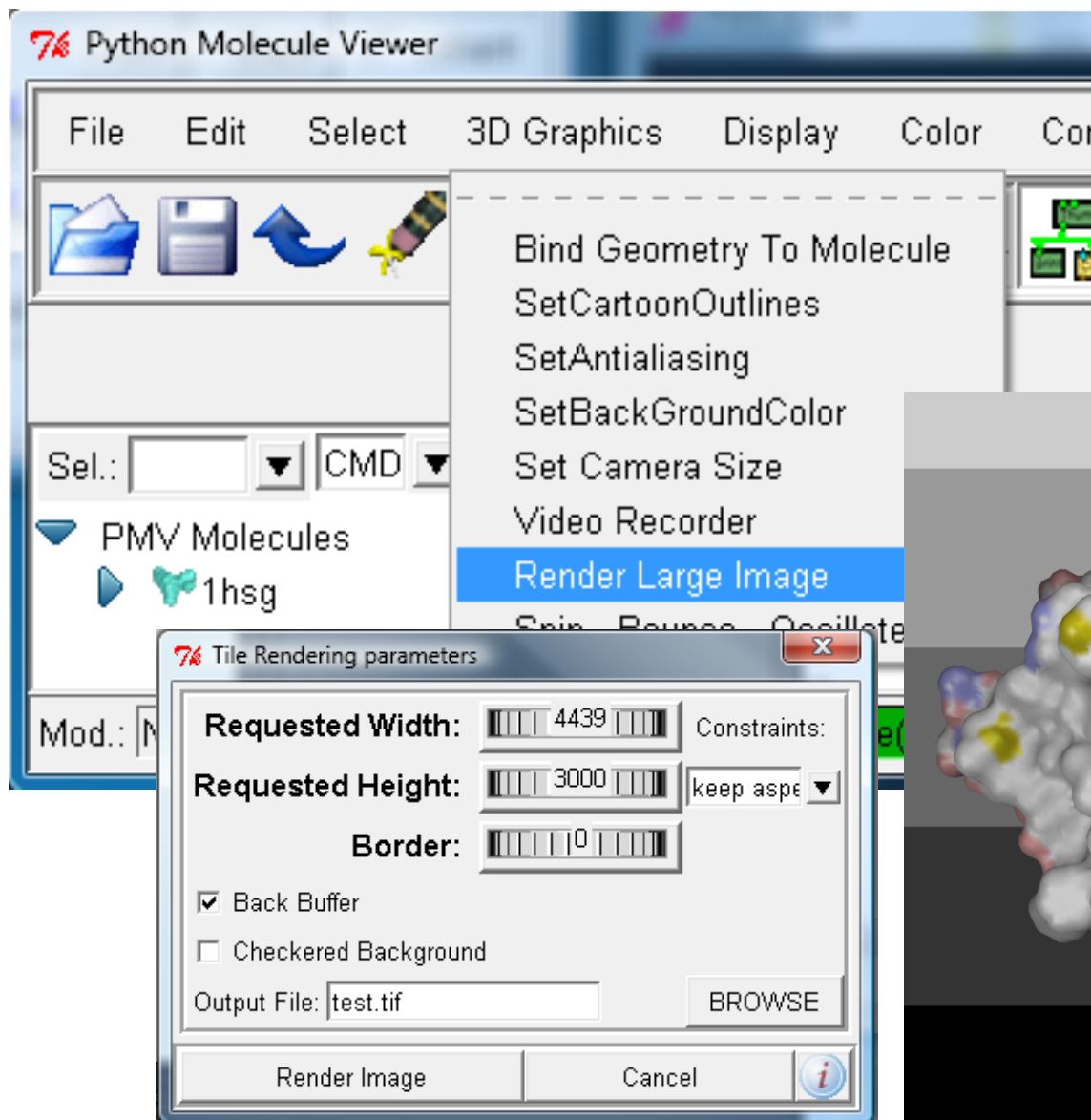
# Rendering Volumetric data



# Rendering: 3D Labels

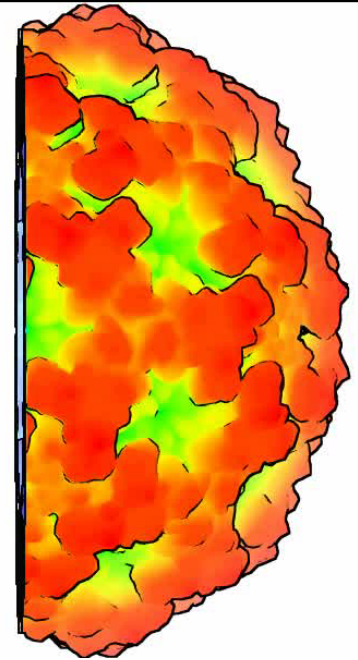
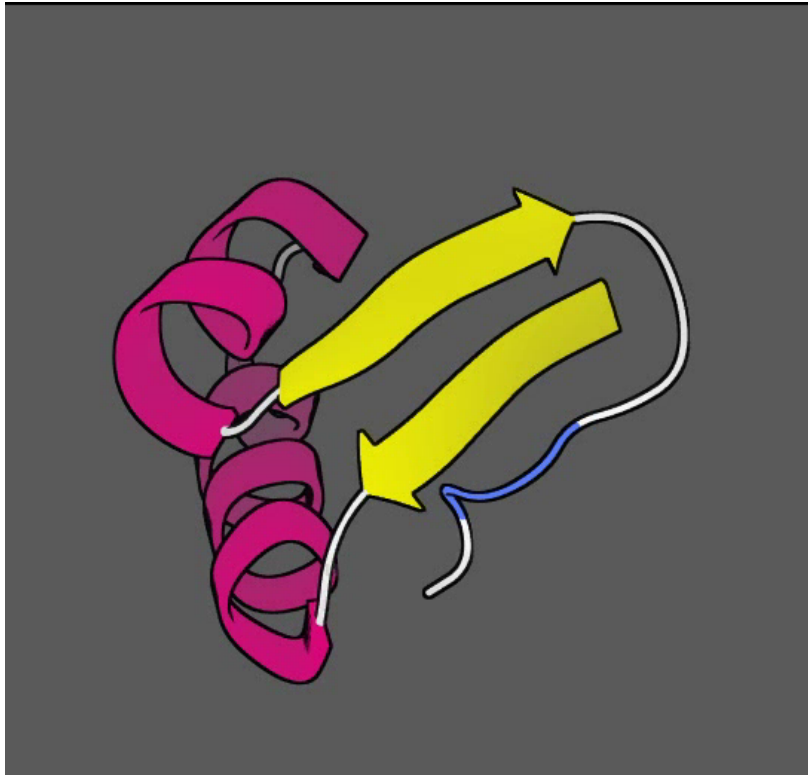


# Rendering Modes: Large Images



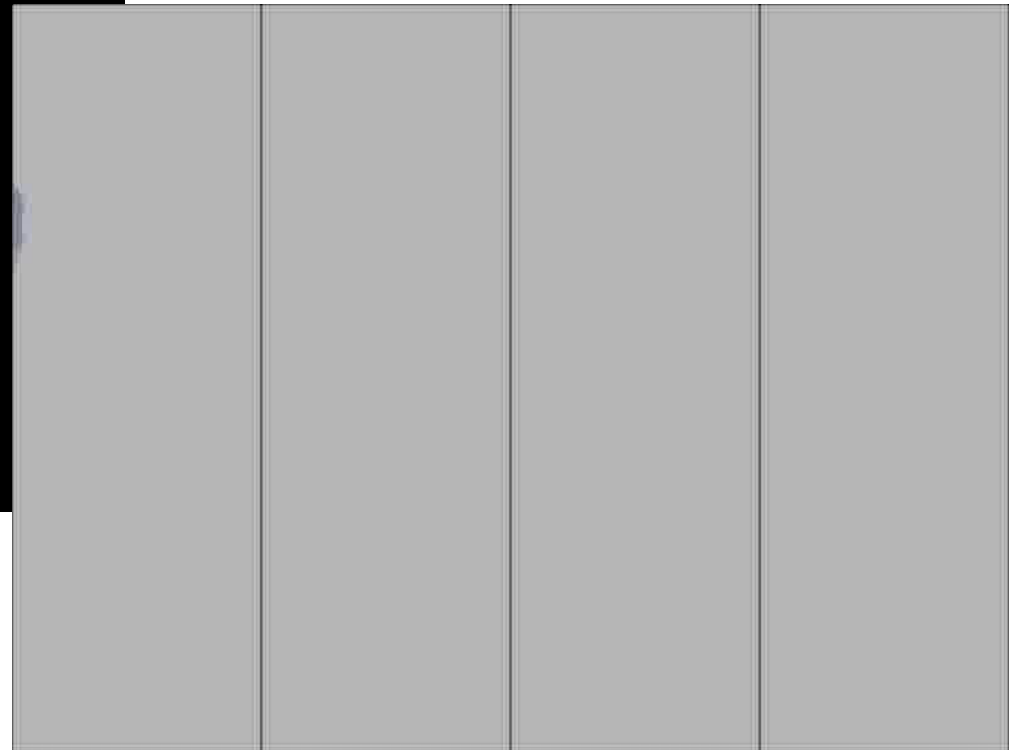


# Rendering Modes: NPR

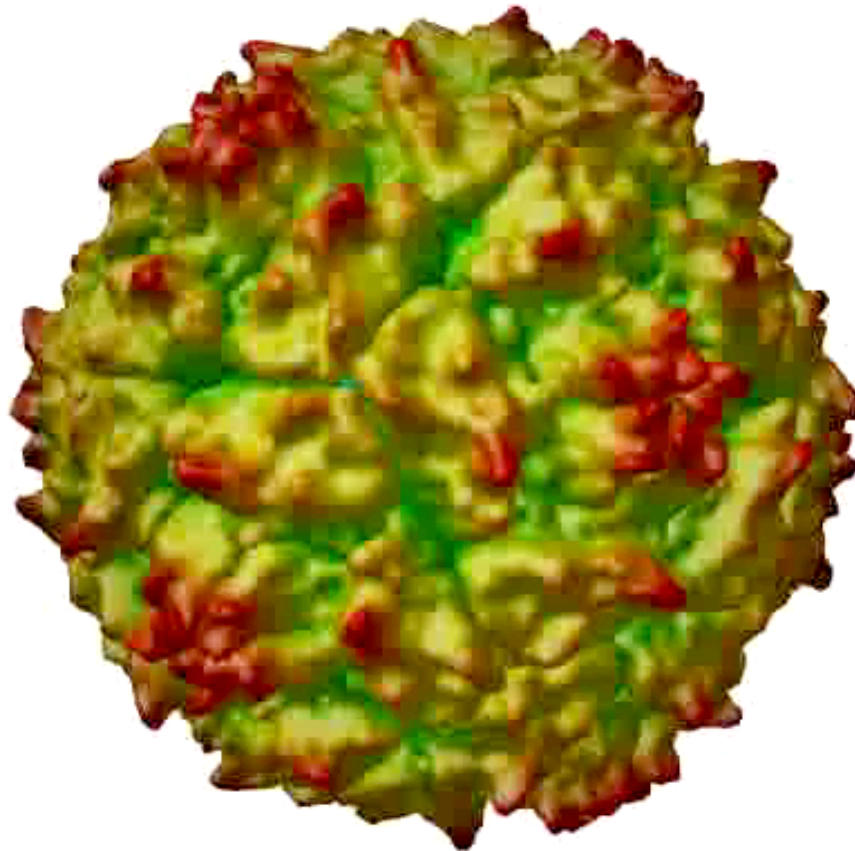




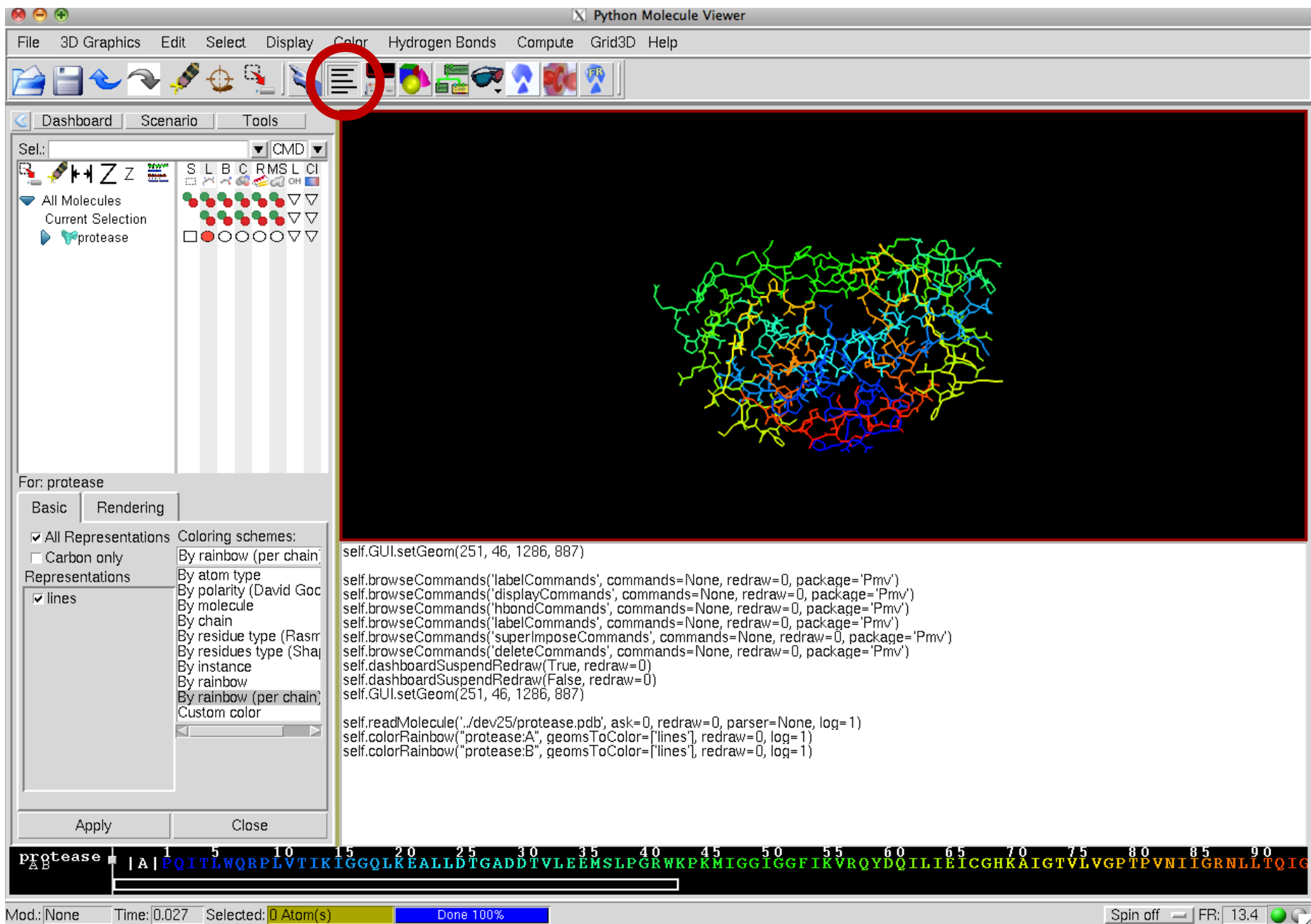
# OpenGL Scissors



# Support for point symmetry



# Vision: scripting Pmv



The screenshot displays the Python Molecule Viewer (Pmv) interface. The main window shows a 3D ribbon model of a protein structure, colored by chain. The interface includes a menu bar (File, 3D Graphics, Edit, Select, Display, Color, Hydrogen Bonds, Compute, Grid3D, Help) and a toolbar. A red circle highlights the 'Display' menu. The left sidebar contains a 'Sel.' dropdown, a 'CMD' dropdown, and a list of molecules (All Molecules, Current Selection, protease). Below this is a 'For: protease' section with 'Basic' and 'Rendering' tabs. The 'Rendering' tab is active, showing 'All Representations' checked and 'lines' selected. The 'Coloring schemes' list includes 'By rainbow (per chain)', 'By atom type', 'By polarity (David Goc)', 'By molecule', 'By chain', 'By residue type (Rasm)', 'By residues type (Shap)', 'By instance', 'By rainbow', 'By rainbow (per chain)', and 'Custom color'. The 'Apply' button is visible. The bottom status bar shows 'Mod.: None', 'Time: 0.027', 'Selected: 0 Atom(s)', and 'Done 100%'. The bottom right corner shows 'Spin off' and 'FR: 13.4'.

```
self.GUI.setGeom(251, 46, 1286, 887)

self.browseCommands('labelCommands', commands=None, redraw=0, package='Pmv')
self.browseCommands('displayCommands', commands=None, redraw=0, package='Pmv')
self.browseCommands('hbondCommands', commands=None, redraw=0, package='Pmv')
self.browseCommands('labelCommands', commands=None, redraw=0, package='Pmv')
self.browseCommands('superImposeCommands', commands=None, redraw=0, package='Pmv')
self.browseCommands('deleteCommands', commands=None, redraw=0, package='Pmv')
self.dashboardSuspendRedraw(True, redraw=0)
self.dashboardSuspendRedraw(False, redraw=0)
self.GUI.setGeom(251, 46, 1286, 887)

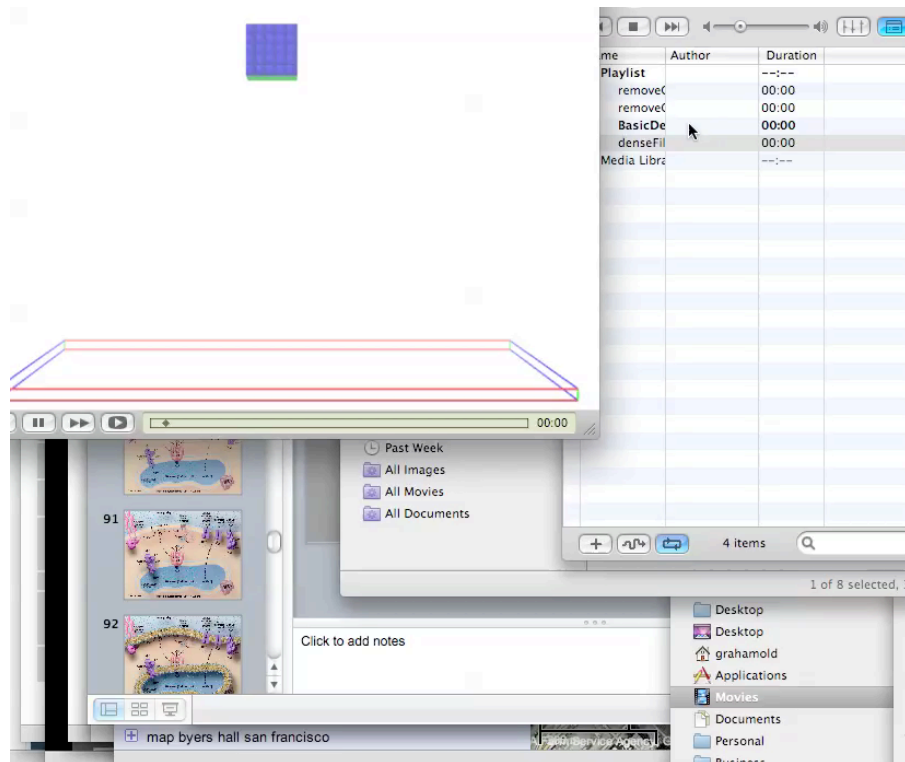
self.readMolecule('./dev25/protease.pdb', ask=0, redraw=0, parser=None, log=1)
self.colorRainbow("protease:A", geomsToColor=['lines'], redraw=0, log=1)
self.colorRainbow("protease:B", geomsToColor=['lines'], redraw=0, log=1)
```

protease | A | P Q I T L W Q R P L V T I K I G G Q L K E A L L D T G A D D T V L E E M S L P G R W K P K M I G G I G G F I K V R Q Y D Q I L I E I C G H K A I G T V L V G P T P V N I I G R N L L T Q I C

Mod.: None Time: 0.027 Selected: 0 Atom(s) Done 100% Spin off FR: 13.4

# 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

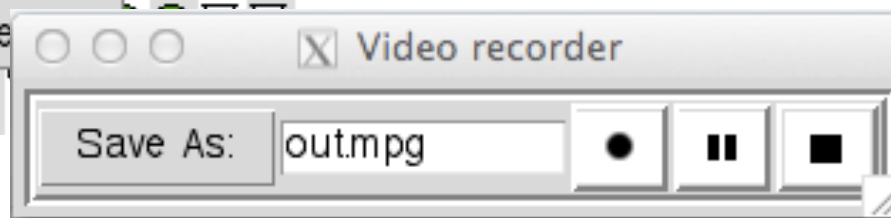
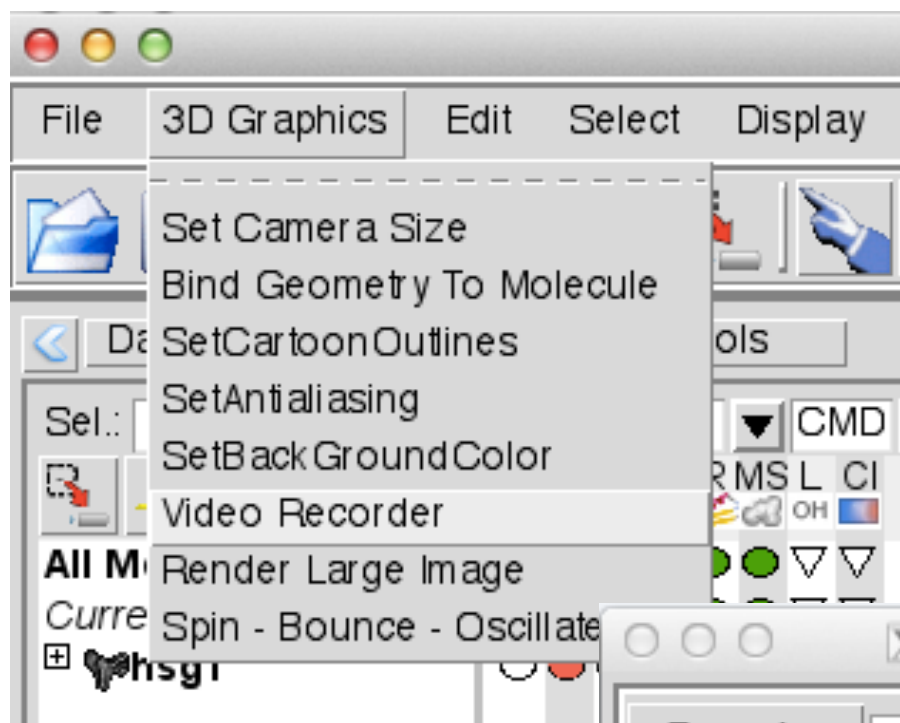
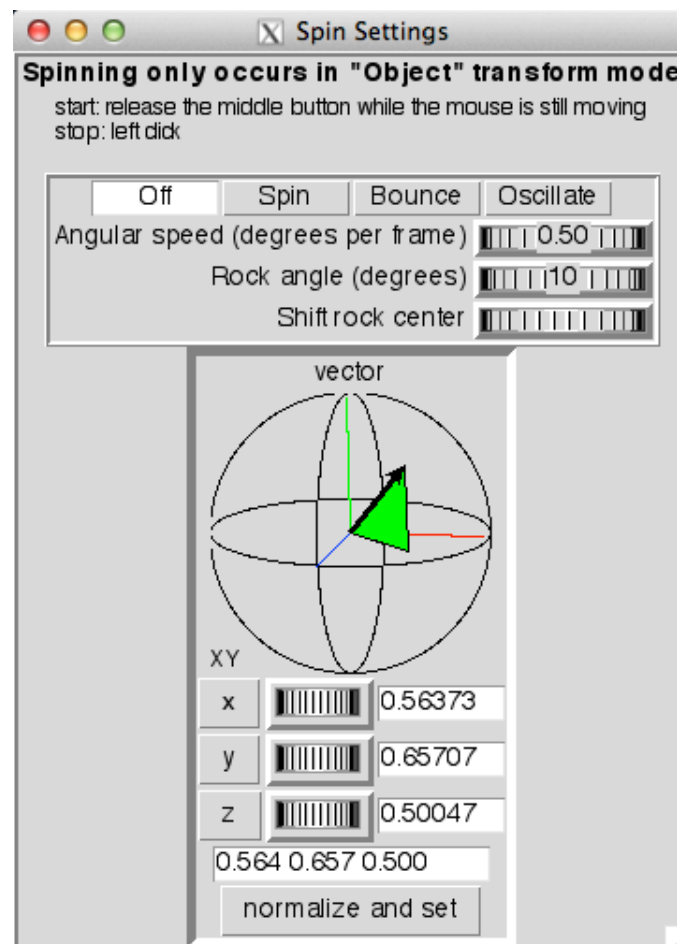
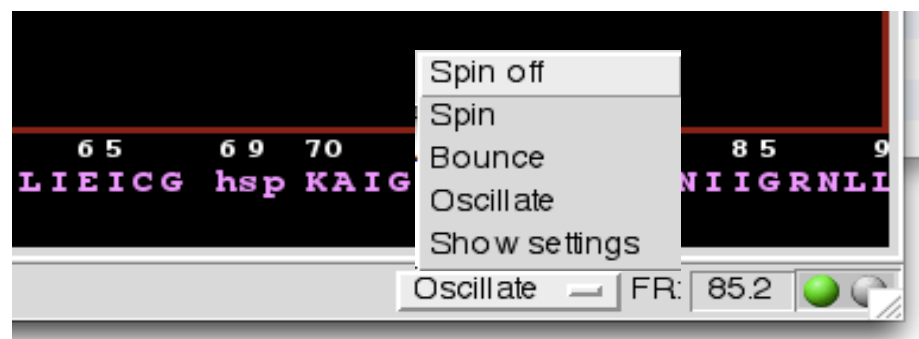
May 2005

375 lines of Python code

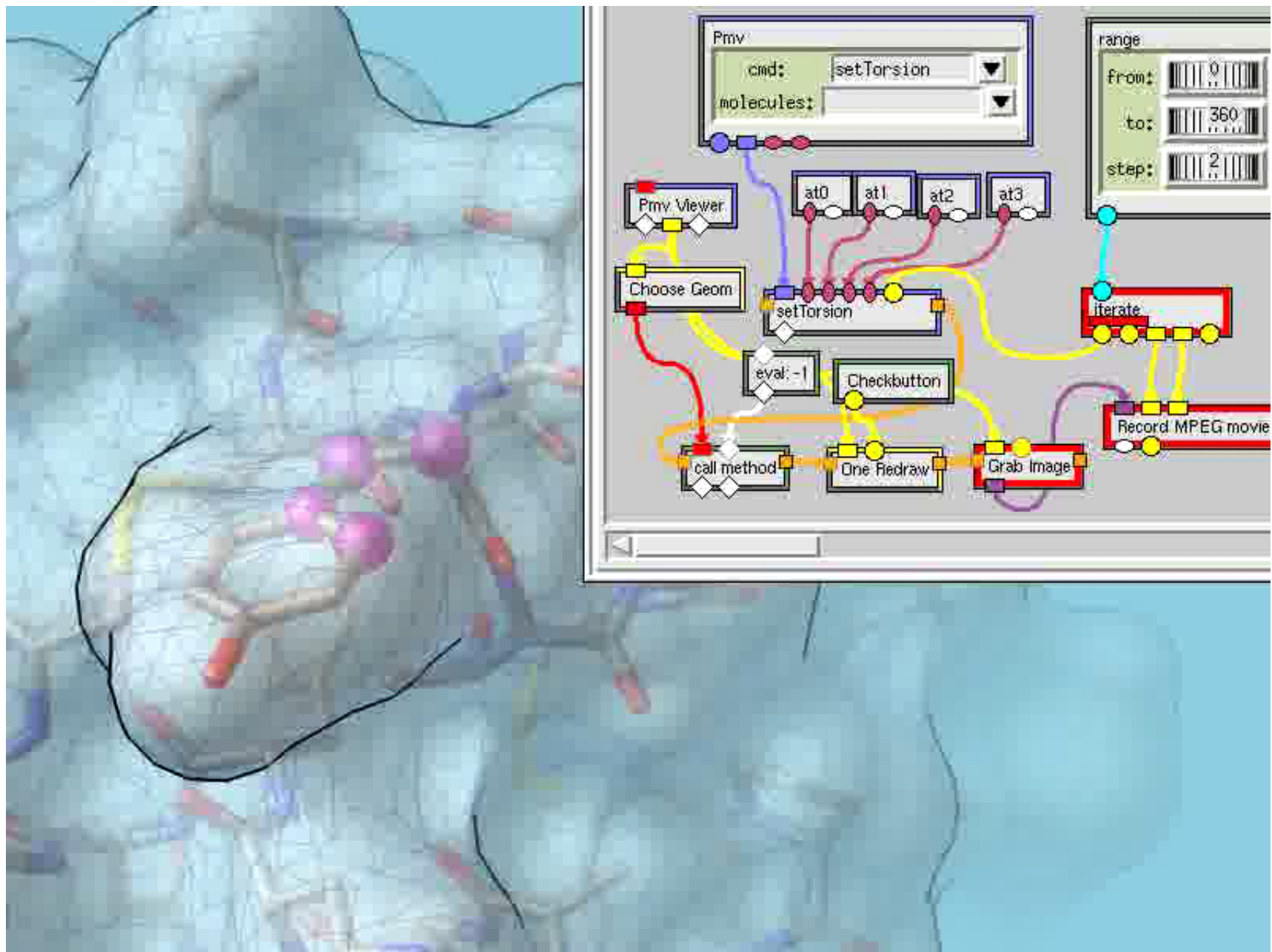
Interactive Frame grabbing



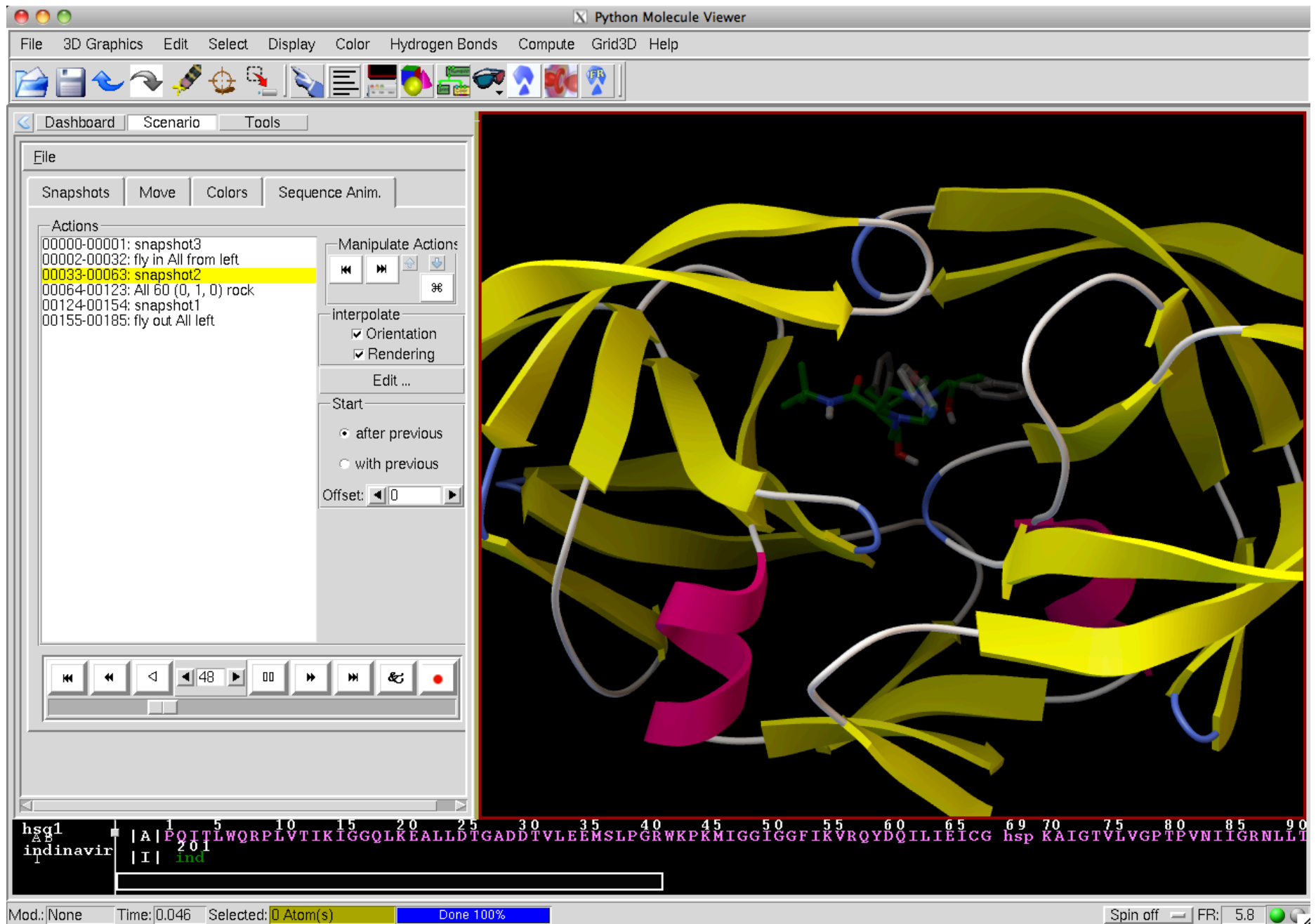
# Pmv: simple animations

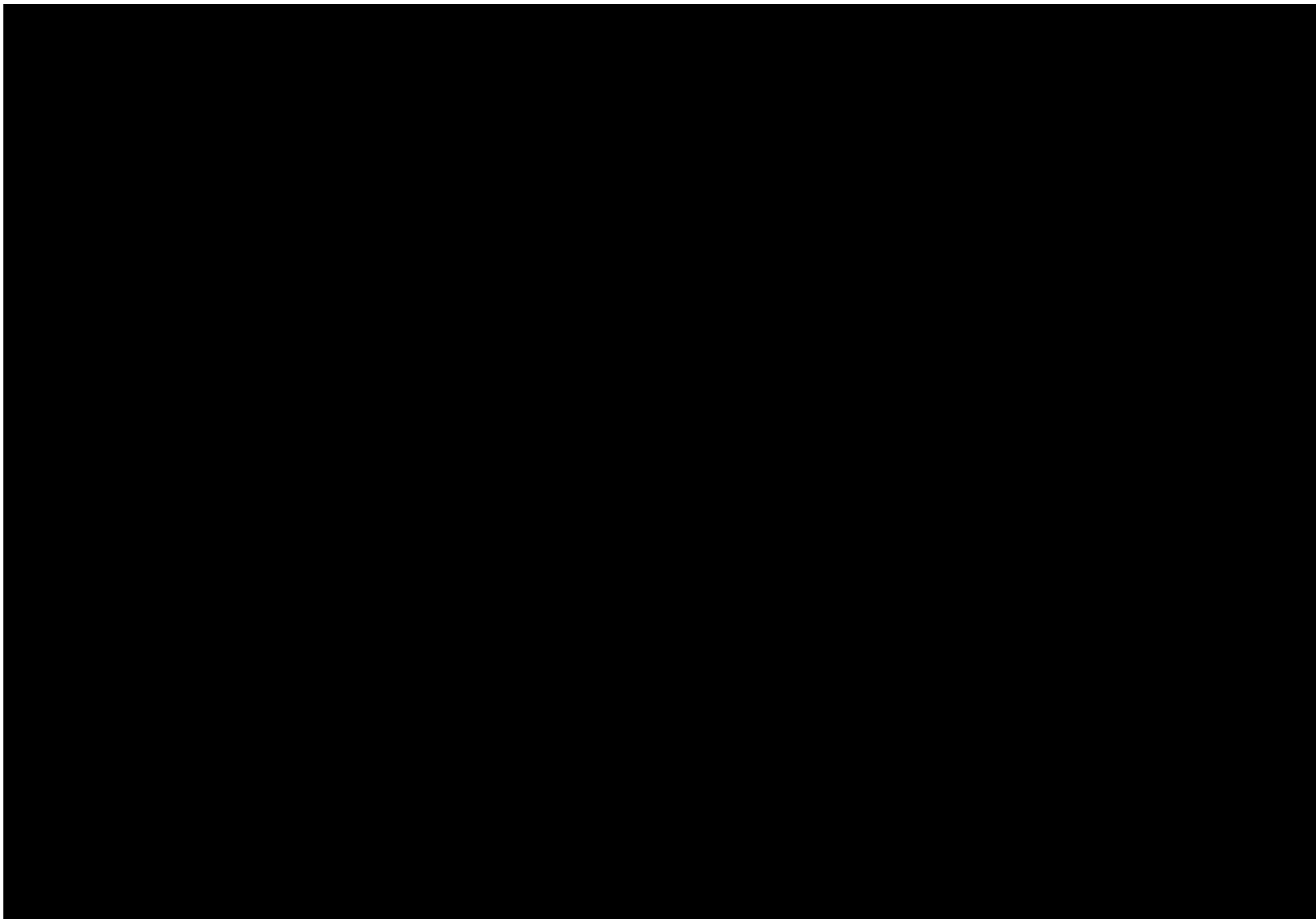


# Animation: Vision



# Amination: Scenario







# Installing Pmv

<http://mgltools.scripps.edu/downloads>

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

The screenshot shows a web browser window with the address bar displaying <http://mgltools.scripps.edu/downloads>. The page title is "Downloads — MGLTools". The website has a blue header with the "MGLTools" logo and navigation links: Home, Downloads, Screenshots, Documentation, Packages, ePMV, Blog, Support, and Forum. A "Log in" link is also present. The main content area is titled "Downloads" and includes a sub-header "by Sargis Dallakyan — last modified 2011-06-29 12:59" and "Contributors: Anna Omelchenko, Michel Sanner, Sowjanya Karnati". Below this is a "License Agreements" link and a "MGLTools 1.5.4 Release Notes" link. The main content is organized into a table with three columns: Operating System/Platform, Download Link, and File Size. The first column lists Windows, Linux, and Mac OS X. The second column lists the download links. The third column lists the file sizes. On the left side, there is a "Navigation" sidebar with links to Home, Downloads, Updates, Nightly Builds, Screenshots, Documentation, Packages, ePMV, and Blog. On the right side, there is a "News" sidebar with links to "MGLTools 1.5.6 RC2 Release Announcement" (2011-05-18), "Source Code Development in Progress" (2010-02-18), "New VISION Screencasts" (2009-05-12), "New Posts in Pmv Blog" (2009-05-08), and "New Splash-Screen".

**Downloads**

by [Sargis Dallakyan](#) — last modified 2011-06-29 12:59  
Contributors: Anna Omelchenko, Michel Sanner, Sowjanya Karnati

[License Agreements.](#)

[MGLTools 1.5.4 Release Notes](#)

Operating System/Platform	Download Link	File Size
Windows	<a href="#">MGLTools-1.5.4-Setup.exe (rc 30)</a> Fixes startup problems for most machines.	
Linux	<a href="#">MGLTools-1.5.4-Linux-x86-Install (41MB)</a> GUI installer (GLIBC_2.3, libstdc++.5.X).	<a href="#">mgltools_i86Linux2_1.5.4.tar.gz (39MB)</a> Tarball installer (GLIBC_2.3, libstdc++.5.X).
Linux	<a href="#">MGLTools-1.5.4-Linux-x86-64-Install (41MB)</a> GUI installer (GLIBC_2.4, libstdc++.6.X).	<a href="#">mgltools_x86_64Linux2_1.5.4.tar.gz (40MB)</a> Tarball installer (GLIBC_2.4, libstdc++.6.X).
Mac OS X	<a href="#">(Snow) Leopard – Mac OS X 10.5 and 10.6 – Intel</a>	<a href="#">mgltools_i86Darwin9_1.5.4.tar.gz (31MB)</a>
Mac OS X	<a href="#">(Snow) Leopard – Mac OS X 10.5 and 10.6 –</a>	<a href="#">mgltools_ppcDarwin9_1.5.4.tar.gz (31MB)</a>

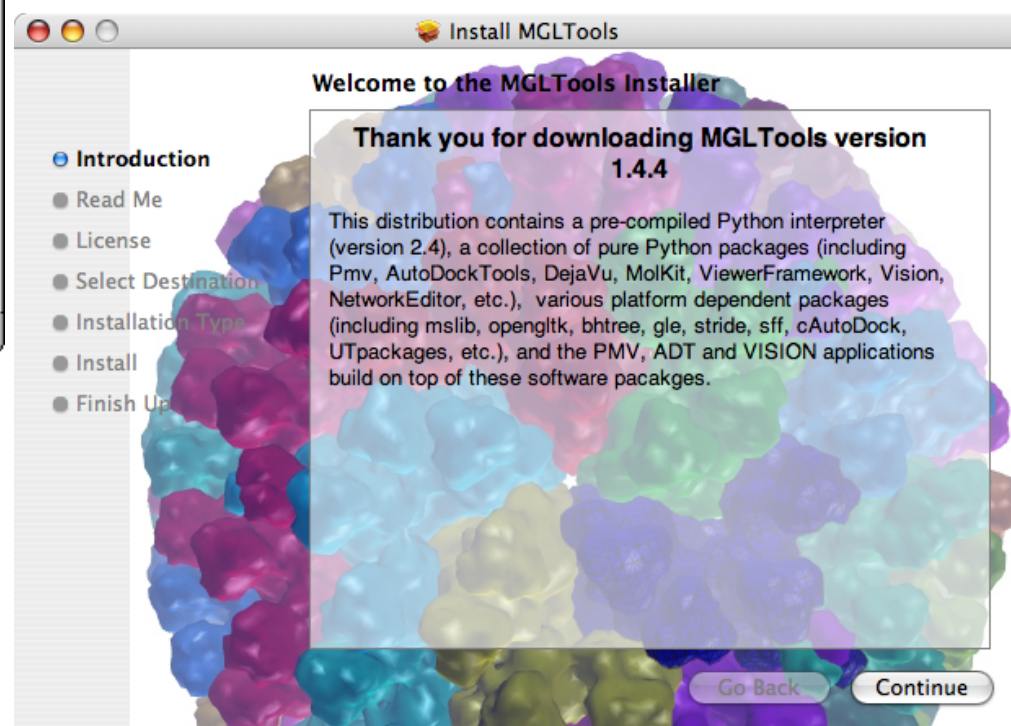
**Navigation**

- Home
- Downloads
- Updates
- Nightly Builds
- Screenshots
- Documentation
- Packages
- ePMV
- Blog

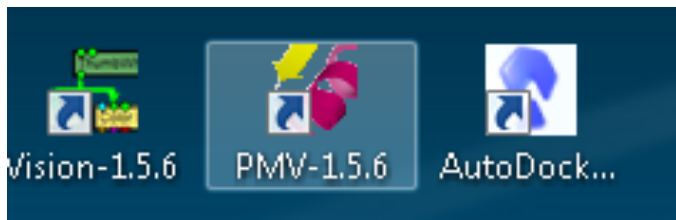
**News**

- [MGLTools 1.5.6 RC2 Release Announcement](#)  
2011-05-18
- [Source Code Development in Progress](#)  
2010-02-18
- [New VISION Screencasts](#)  
2009-05-12
- [New Posts in Pmv Blog](#)  
2009-05-08
- [New Splash-Screen](#)

# Installing Pmv



# Starting Pmv



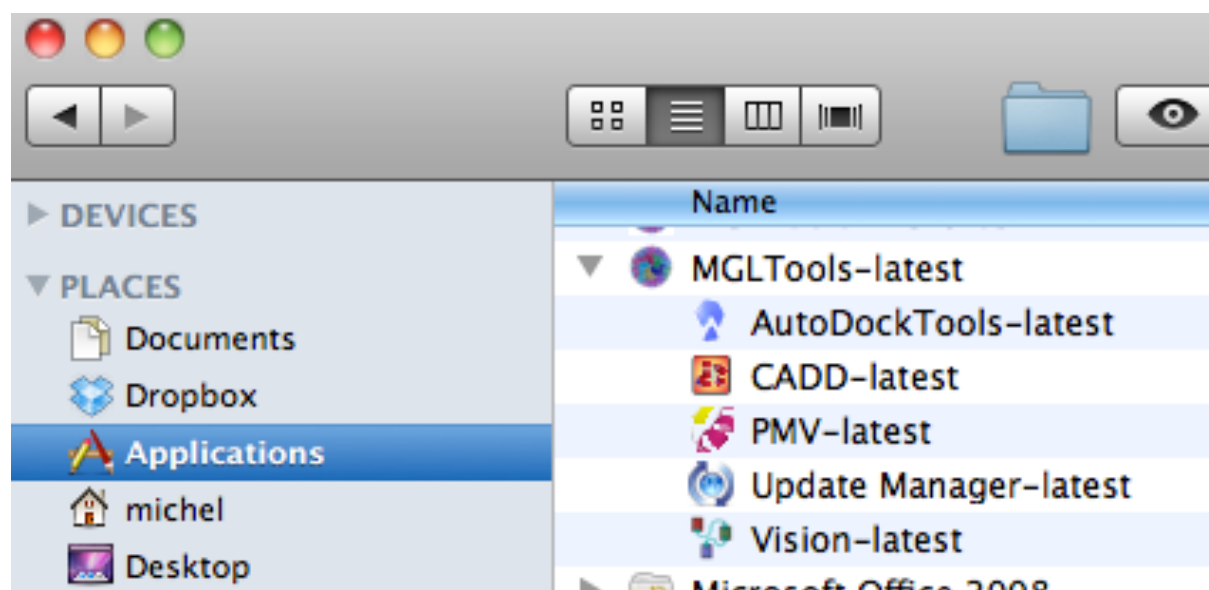
The installer placed 3 icons on the desktop. To start Vision double click on the Vision icon.



The installer created the pmv shell script

`$MGLROOT/bin/pmv.`

Where MGLROOT is the folder you chose to install the software



# Starting Pmv

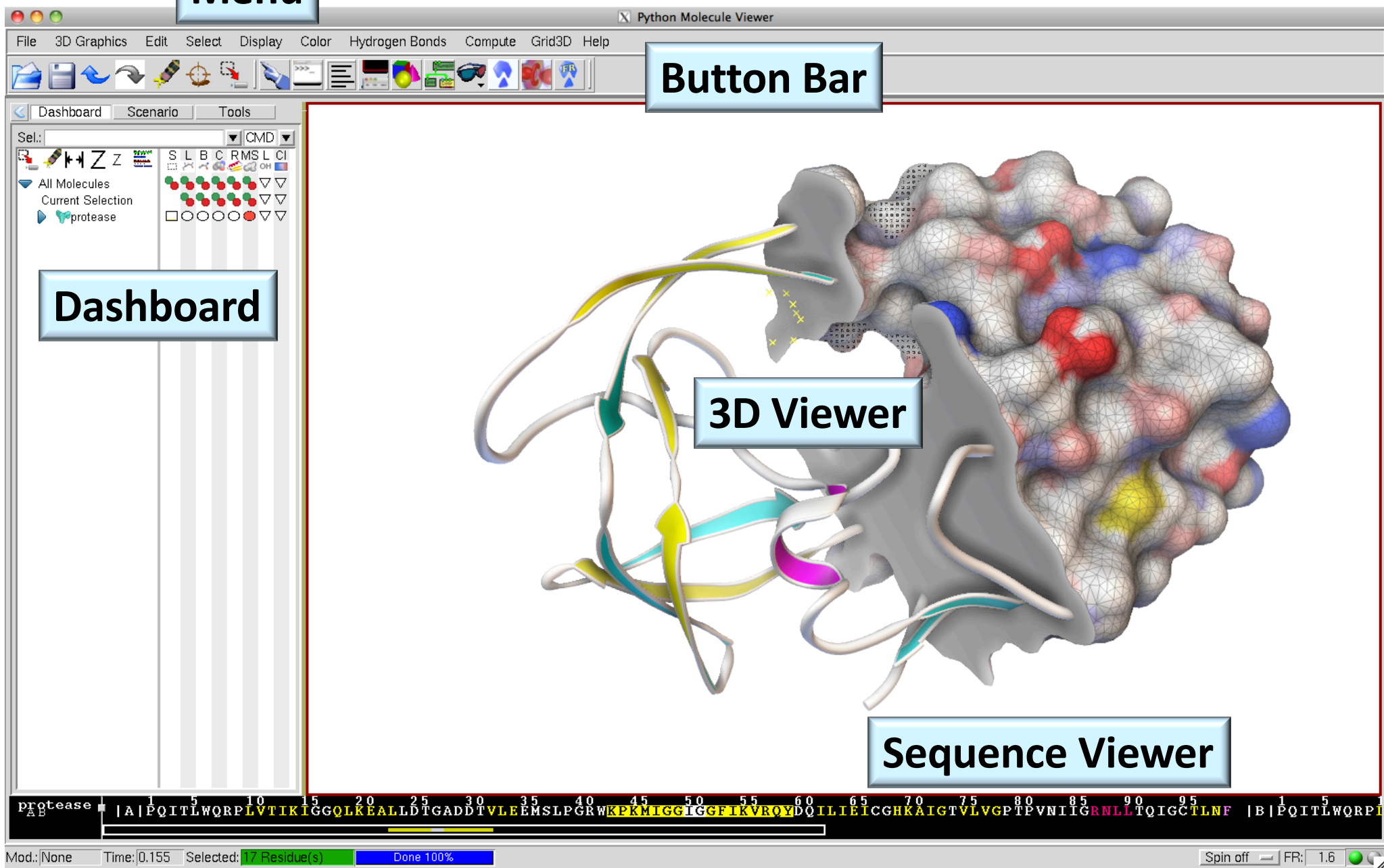
Menu

Button Bar

Dashboard

3D Viewer

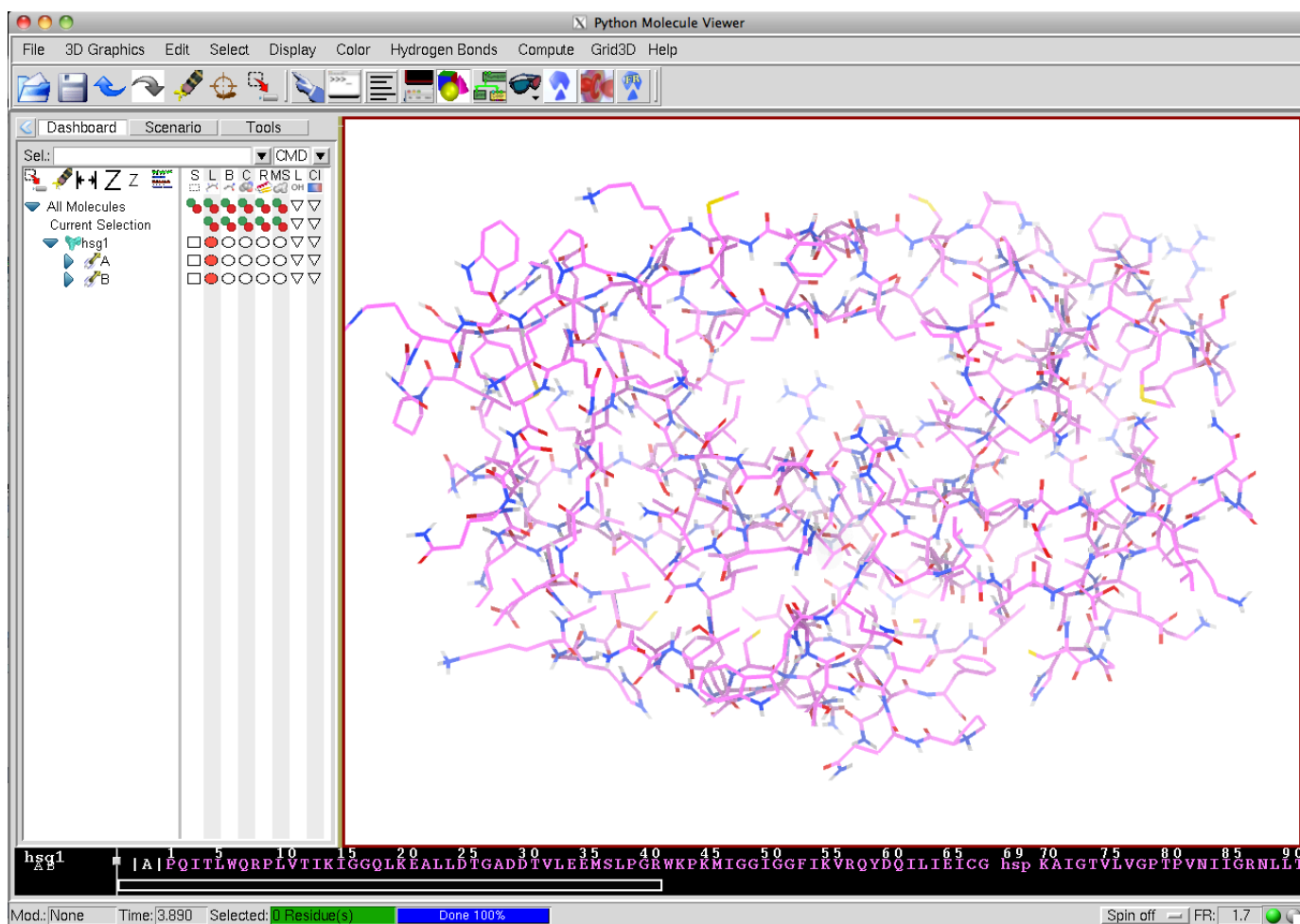
Sequence Viewer



# 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:

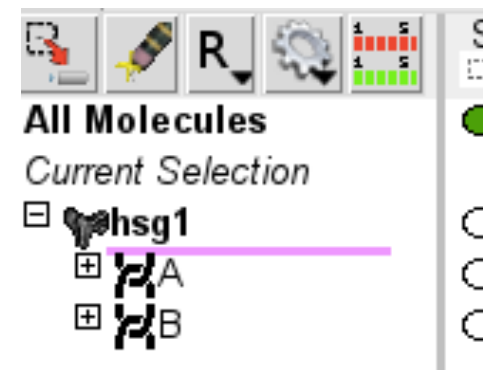
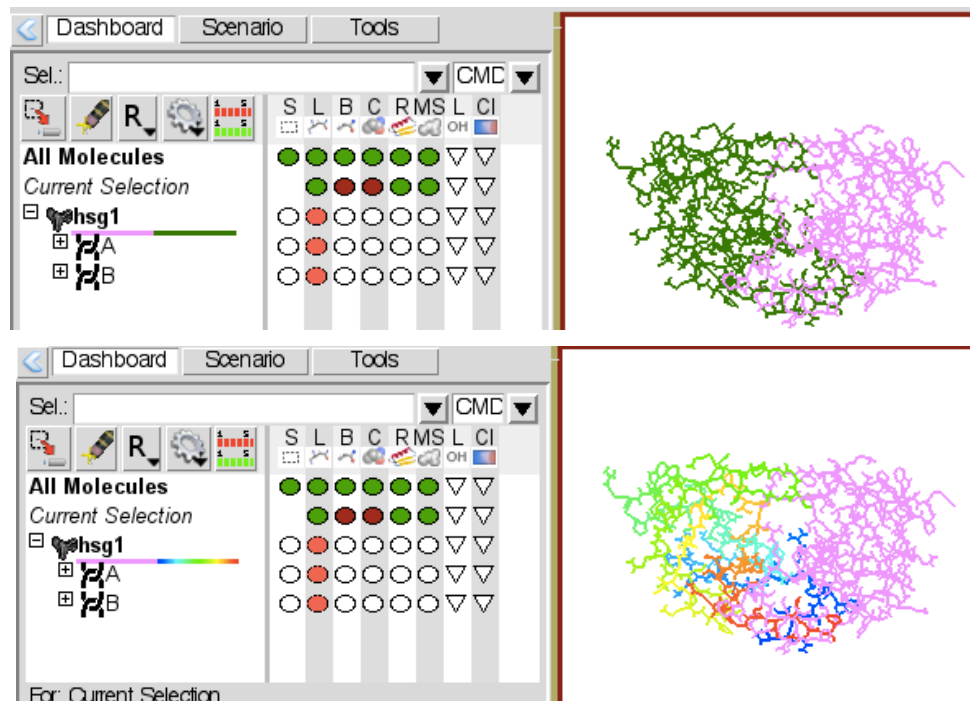
- 1 – multiple molecules can be selected in the file browser
- 2 – wildcards can be used on the command line (e.g. `pmv -i test*.pdb`)
- 3 – using a pdb id on the command line will fetch the protein from web unless it is in the cache

# 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

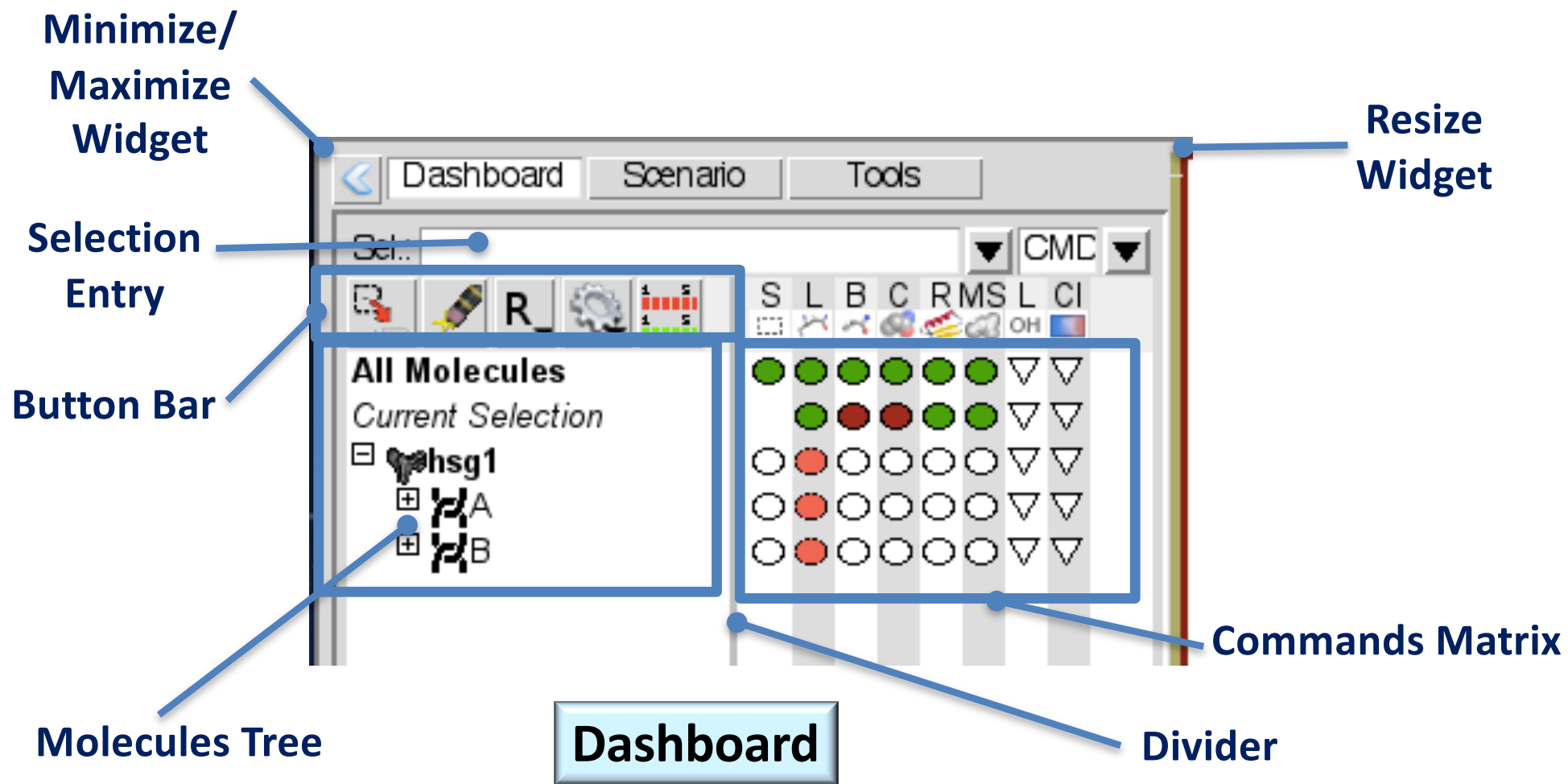
<b>Button</b> <b>Mod</b>	<b>Left</b>	<b>Middle</b>	<b>Right</b>	<b>Wheel</b>
<b>None</b>	<i>Rotate</i>		<i>Translate left/right (X) and up/down (Y)</i>	<i>Zoom</i>
<b>Shift</b>	<i>Add to Selection</i>		<i>Translate in/out (Z)</i>	
<b>Ctrl</b>	<i>Remove from Selection</i>		<i>Center on Pixel</i>	

# Exercise: Pmv key bindings

**Task: learn PMV viewer keystrokes**

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

# Pmv dashboard



# Exercise: Pmv dashboard

## Task: dashboard

- 1 – hover 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

Select   Lines   Balls & Sticks   CPK   Ribbon   Surface   Label   Color

	S	L	B	C	RMS	L	CI
All Molecules	●	●	●	●	●	▽	▽
Current Selection	●	●	●	●	●	▽	▽
hsg1	○	○	○	○	○	▽	▽
hsg1:A	○	○	○	○	○	▽	▽
hsg1:B	○	○	○	○	○	▽	▽

display/undisplay atomic spheres for hsg1:A

## Notes:

- Tool tips on all command buttons



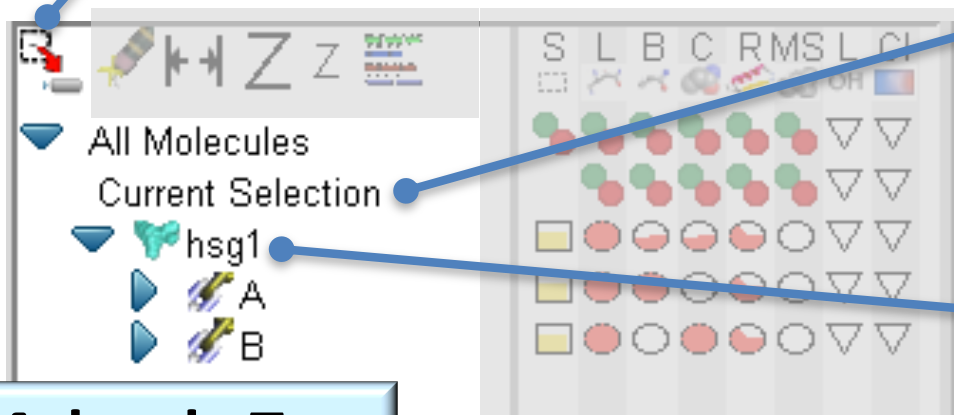
# Dashboard Molecule Tree

Create a set using  
the current selection

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

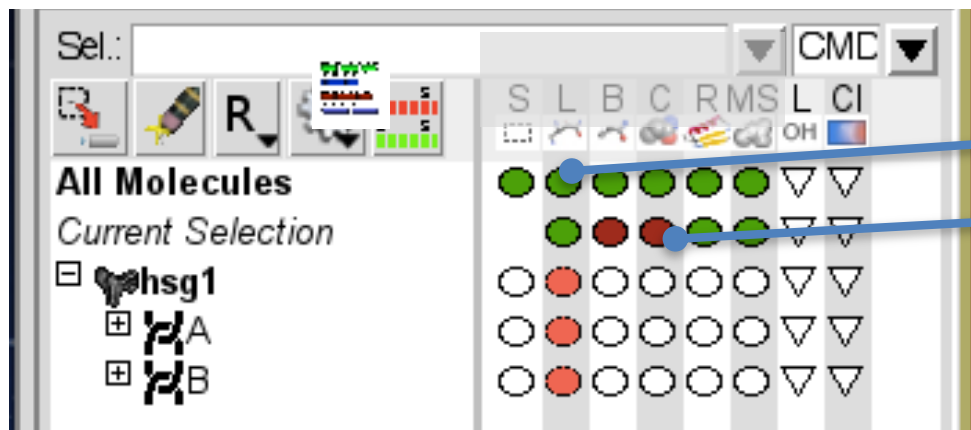
**Molecules:** can be expanded  
to show chains, residues, atoms

Molecule Tree



# Dashboard Command Buttons

## On/Off Buttons



Left click to:

Display lines for all molecules

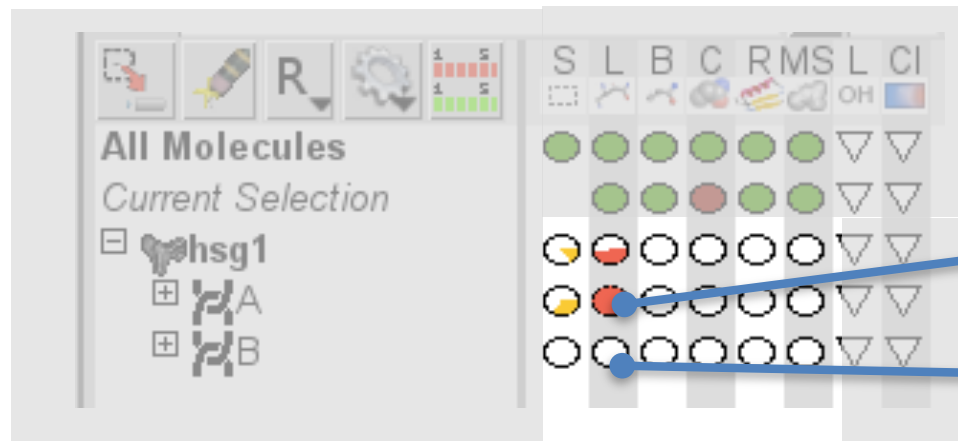
Undisplay CPK for the current selection

### 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

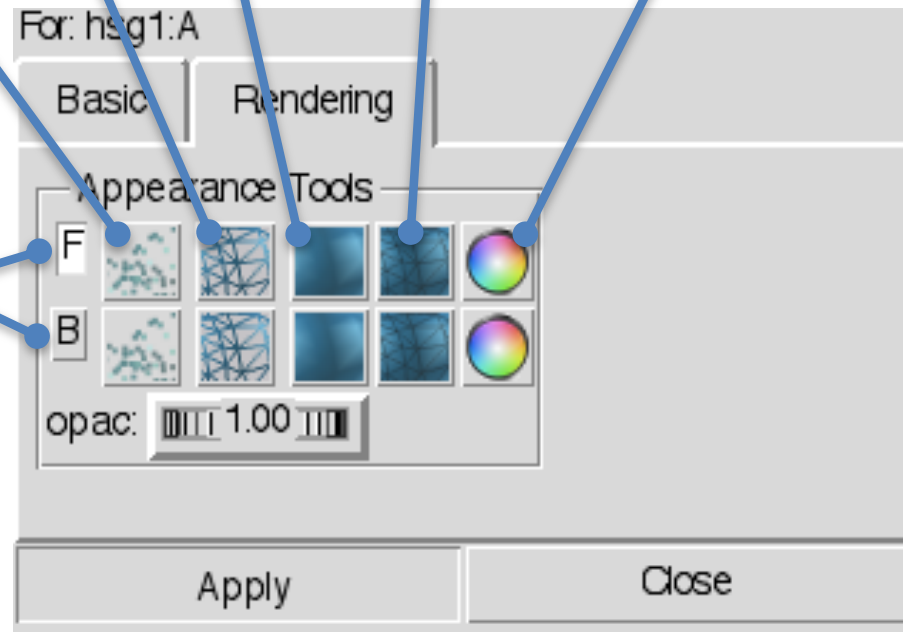
# Exercise: Display Balls and Sticks

**Task: geometry quality and rendering options**

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

Points Lines Shaded Outlined Color

Toggle Front and Back  
Faces rendering on/off



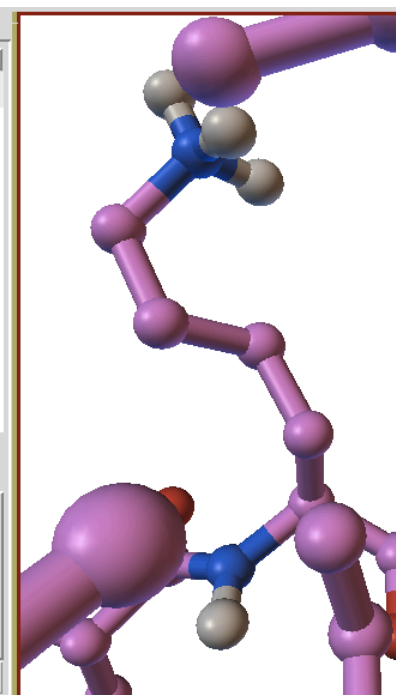
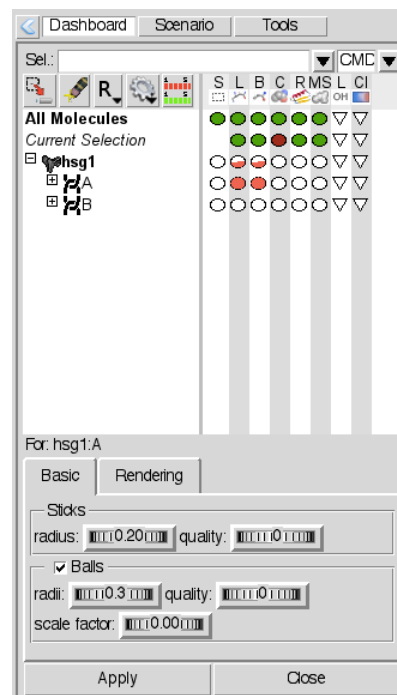
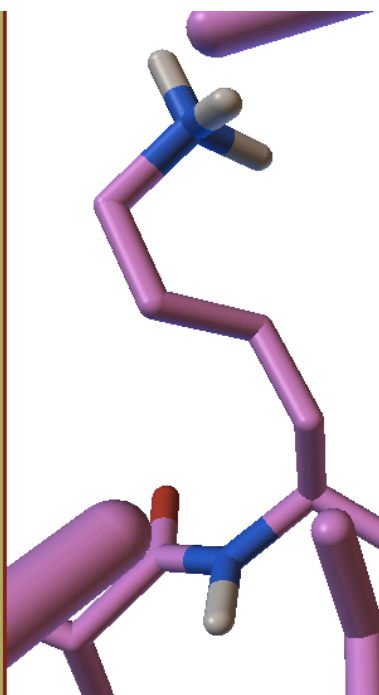
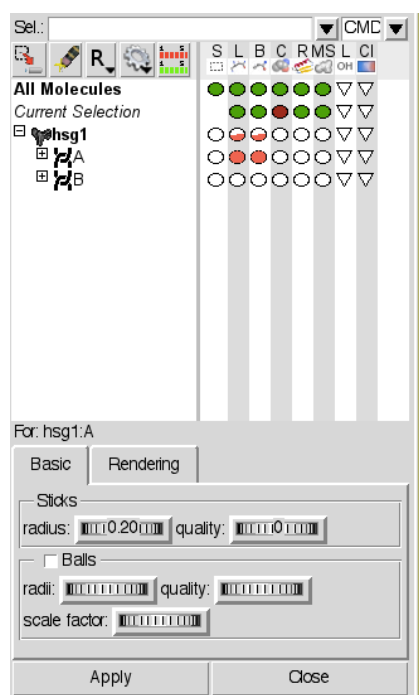


# Exercise: Display Balls and Sticks

## 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

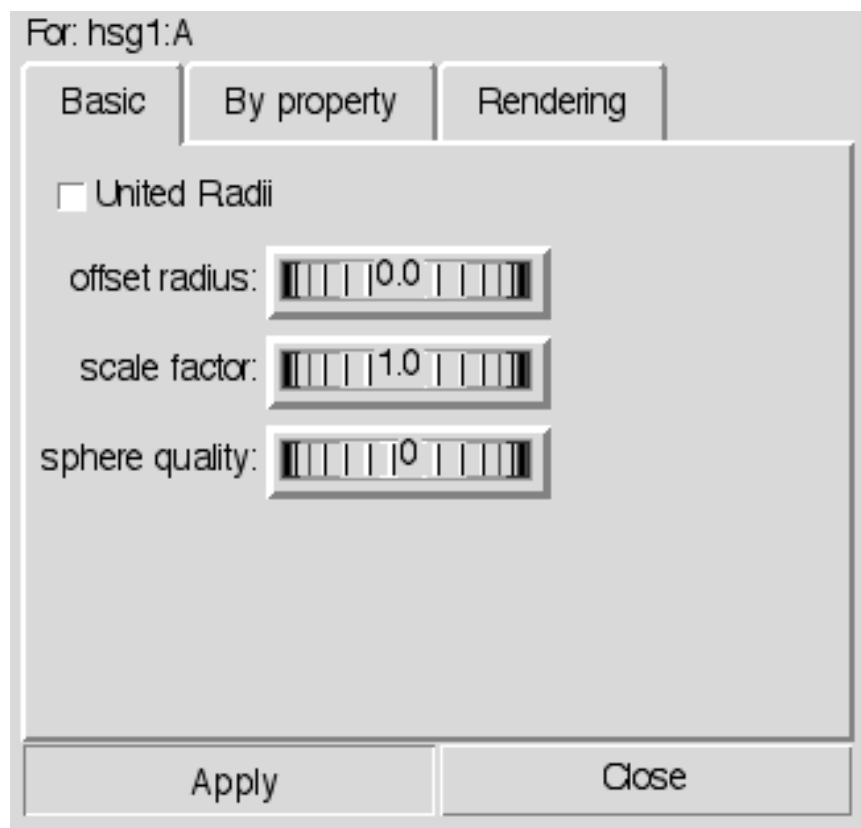


Quality changes the number of polygons used  
0 automatically selects the tessellation

# 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

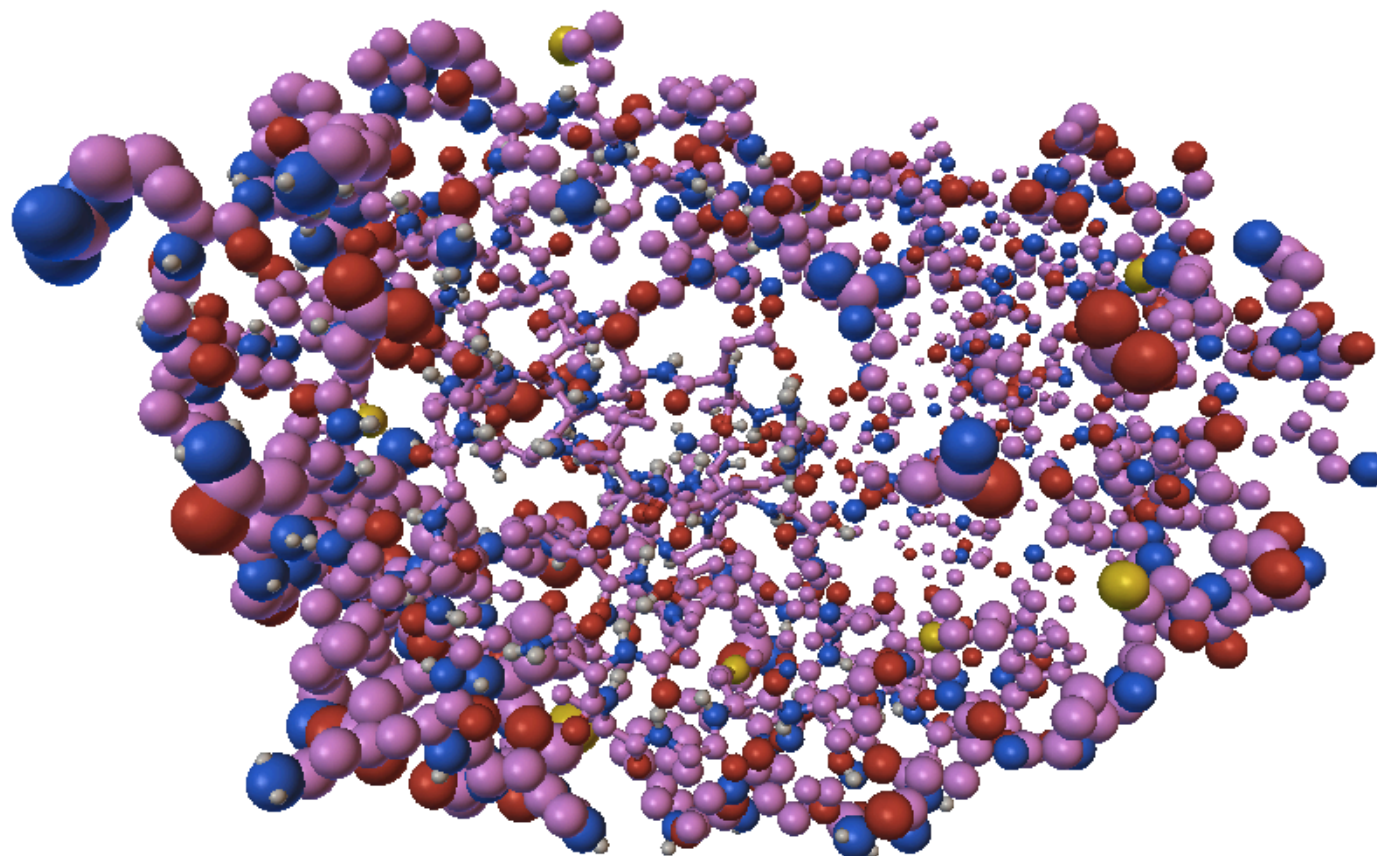


Radius = offset + atom radius\*scale

# Exercise: Display CPK

## Task: display CPK

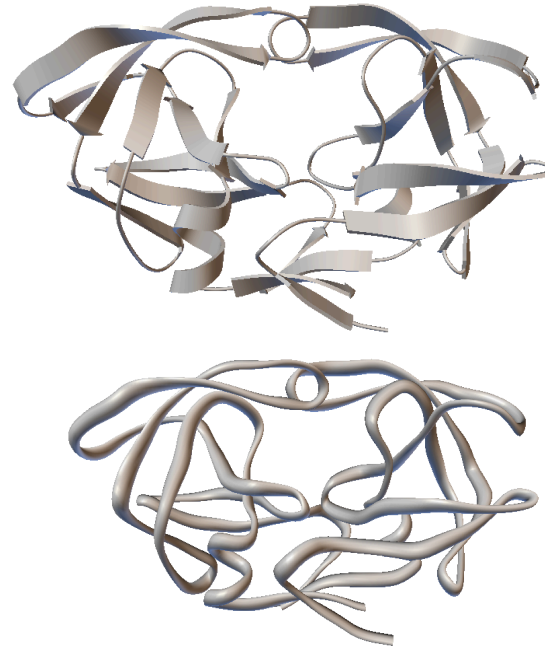
- 1 – Right click on CPK for hsg1
- 2 – check “By Property” button
- 3 – select atomic property temperature Factor
- 4 – set scaling to 0.02



# Exercise: Display Ribbon

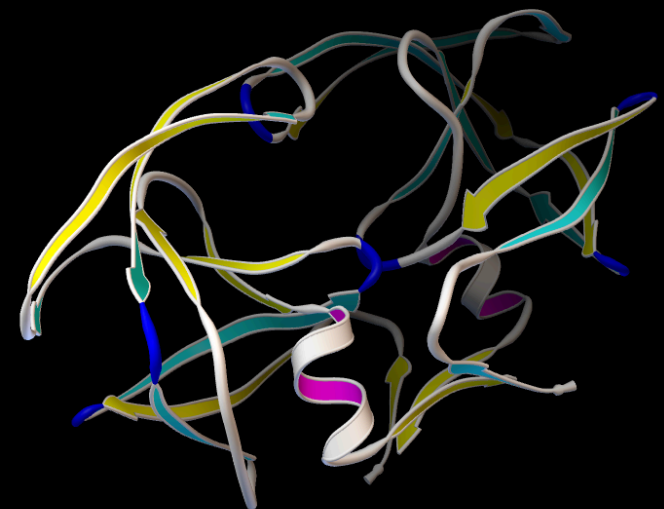
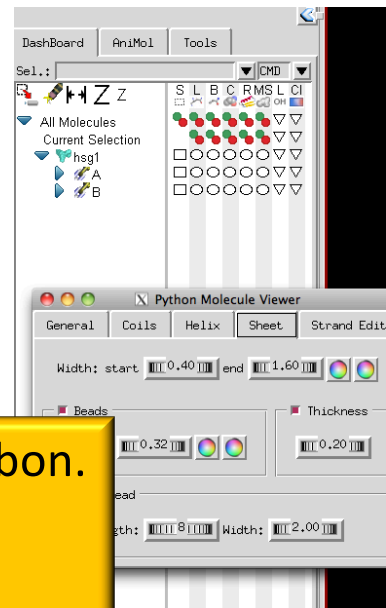
## Task: display Ribbons

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



## Task: Beaded Ribbons

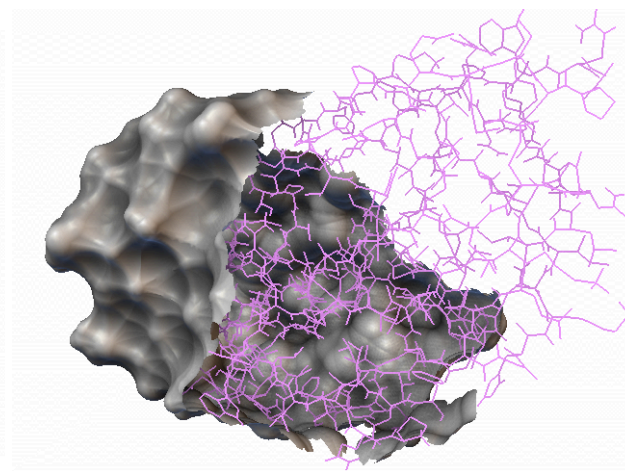
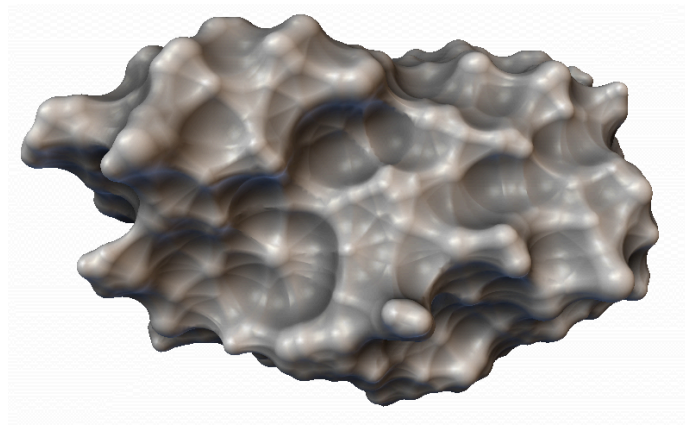
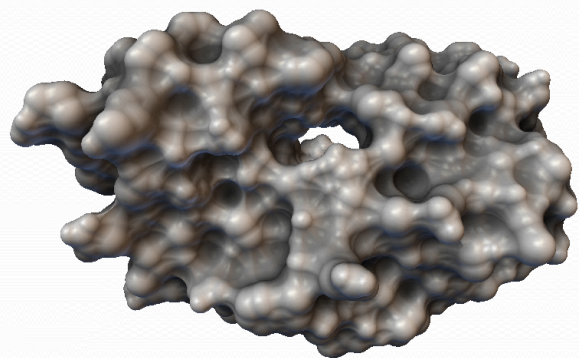
- 1 – use menu entry Compute -> beaded ribbon.
- 2 – un-display all lines
- 3 – un-display all ribbons



# 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



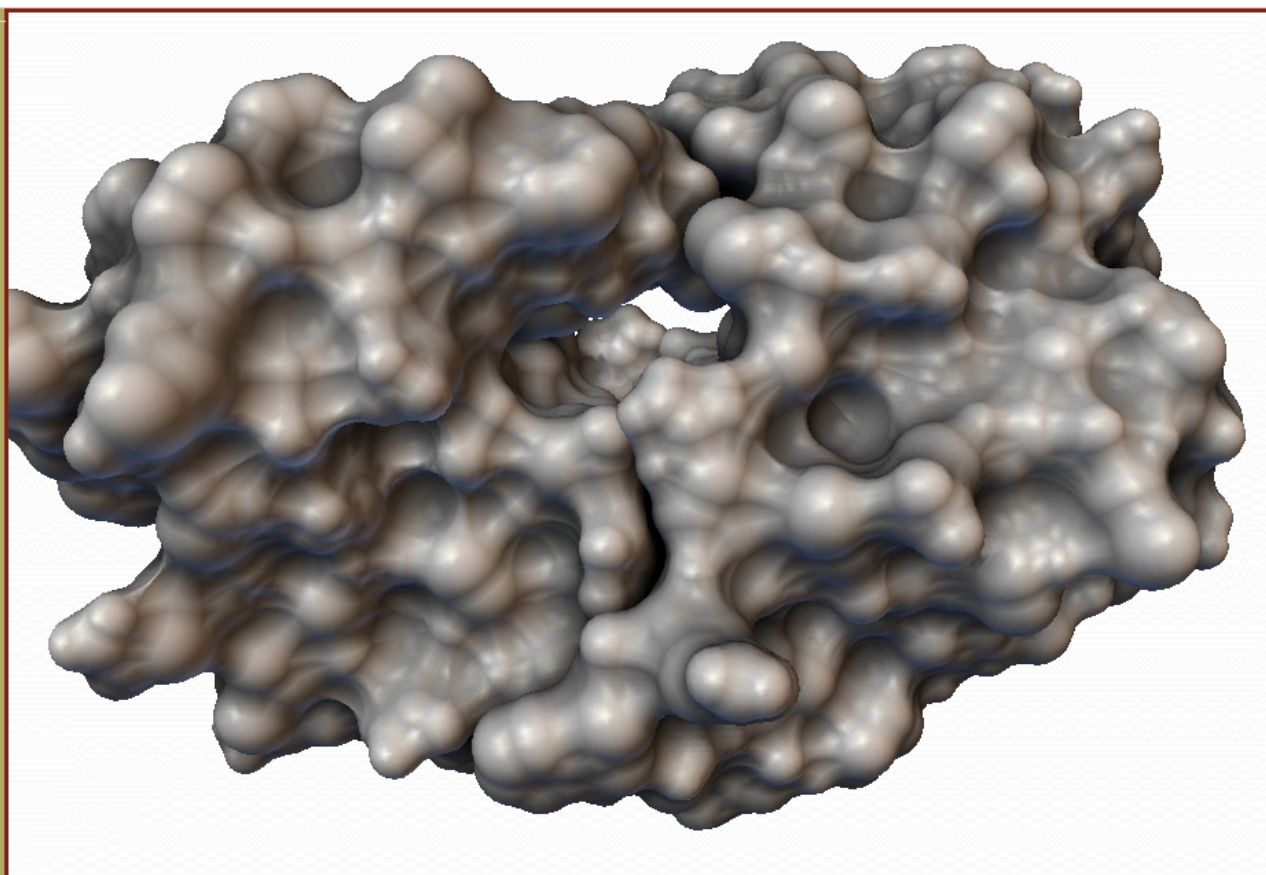
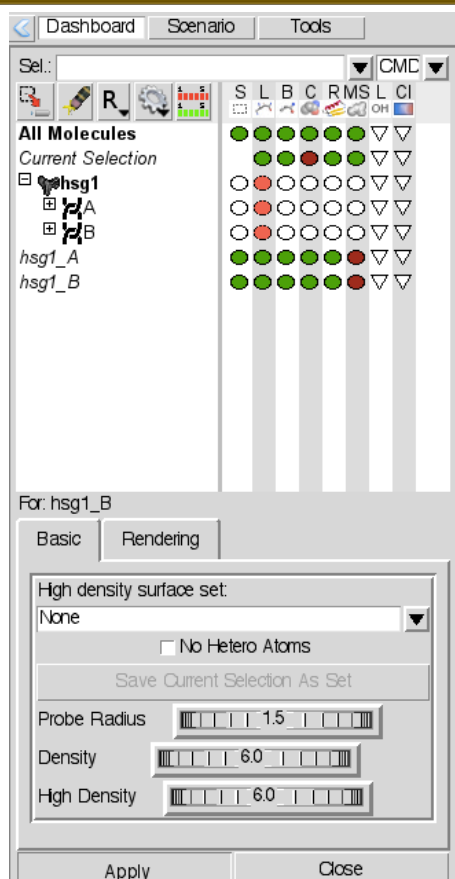


# Exercise: Closed surfaces for chains

## Task: display closed surfaces

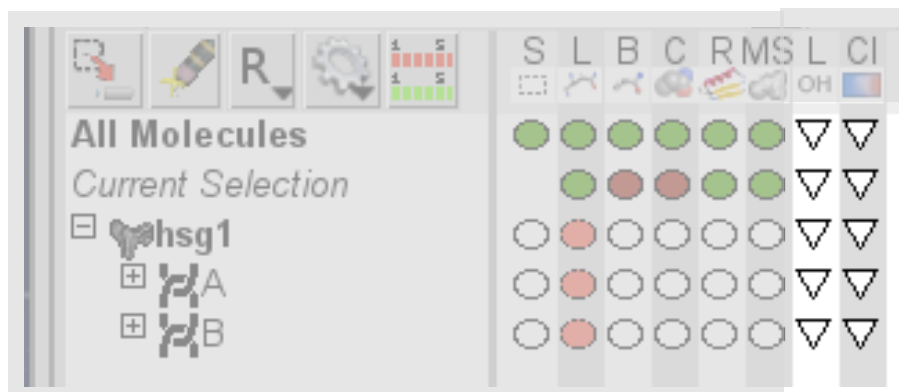
To close the surface:

- 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**

1 – select ARG8 (type ::ARG8 <Return> in Sel.: box)  
2 – display S&B for current selection  
3 – click in Label triangle icon for current selection  
4 – Select “Residue” in Level  
5 – select “name” in properties

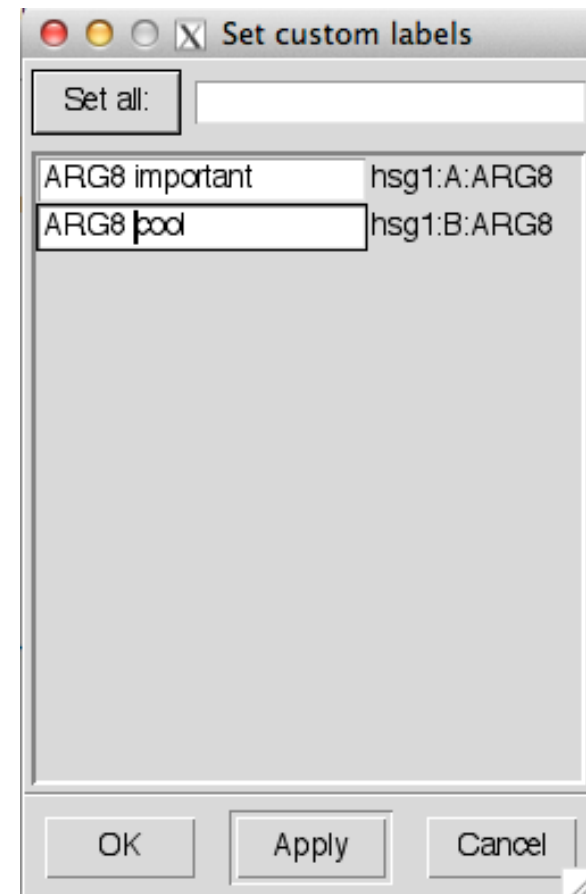
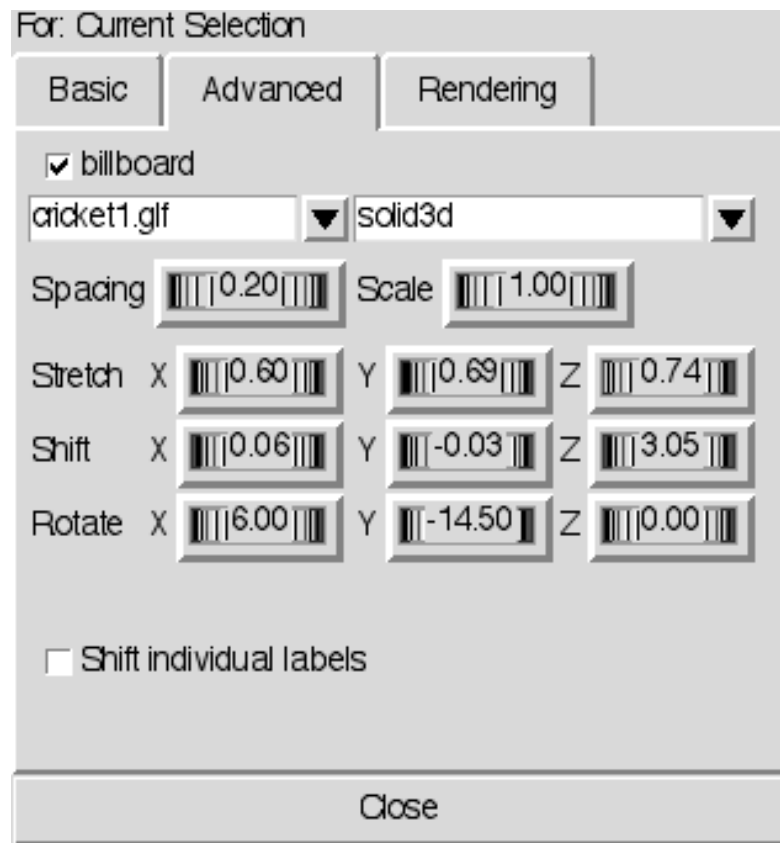
hsg1 A B 1 5 10 15 20 25 30 35 40 45 50 55 60 65 69 70 75 80 85 9  
| A | P Q I T L W Q P L V T I K I G G Q L K E A L L D T G A D D T V L E E M S L P G R W K P K M I G G I G G F I K V R Q Y D Q I L I E I C G h s p K A I G T V L V G P T P V N I I G R N L I

Mod.: None Time: 0.021 Selected: 2 Residue(s) Done 100% Spin off FR: 35.4

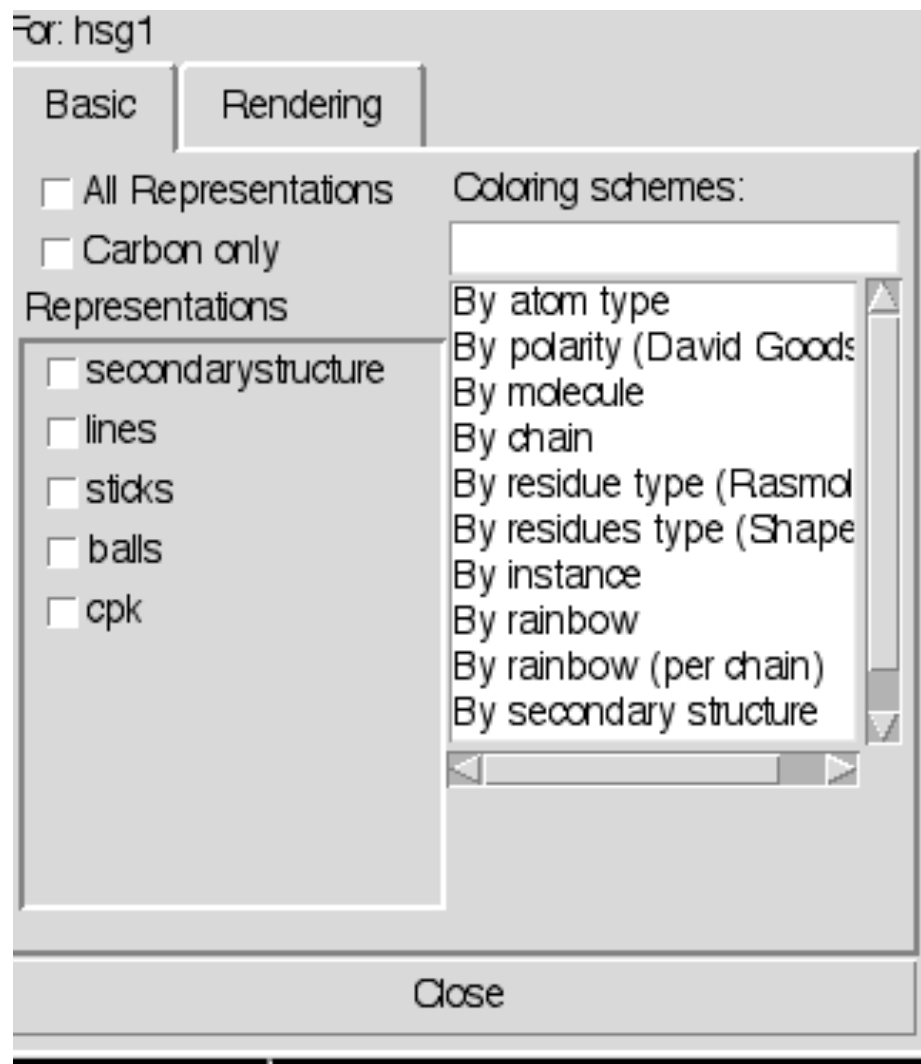
# Exercise: Labeling options

## 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



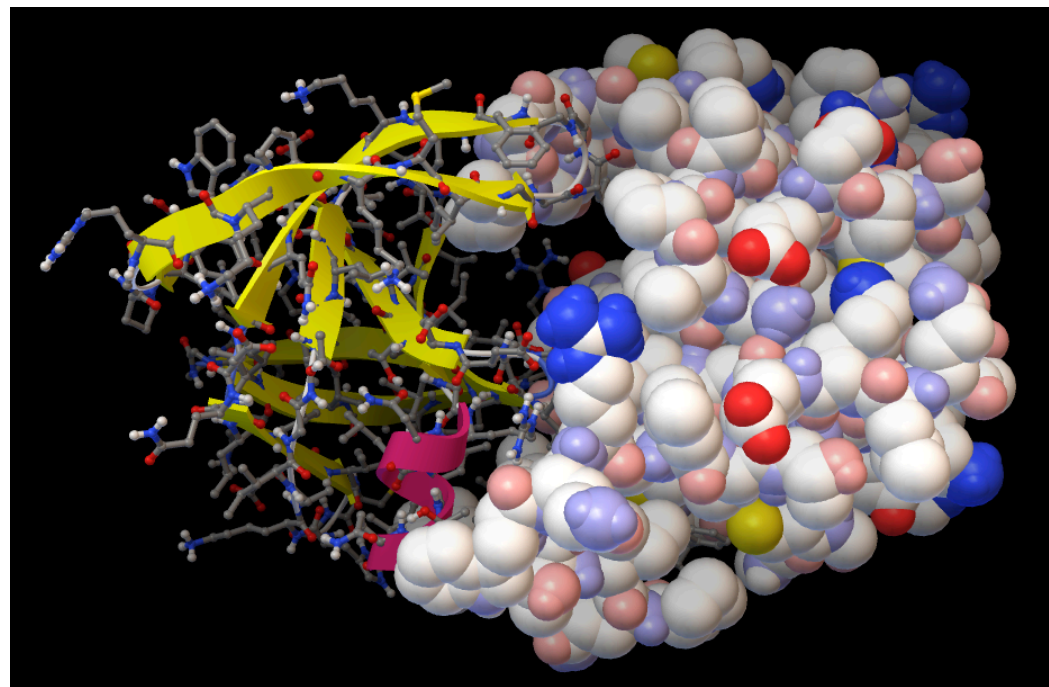
## Notes:

- 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.

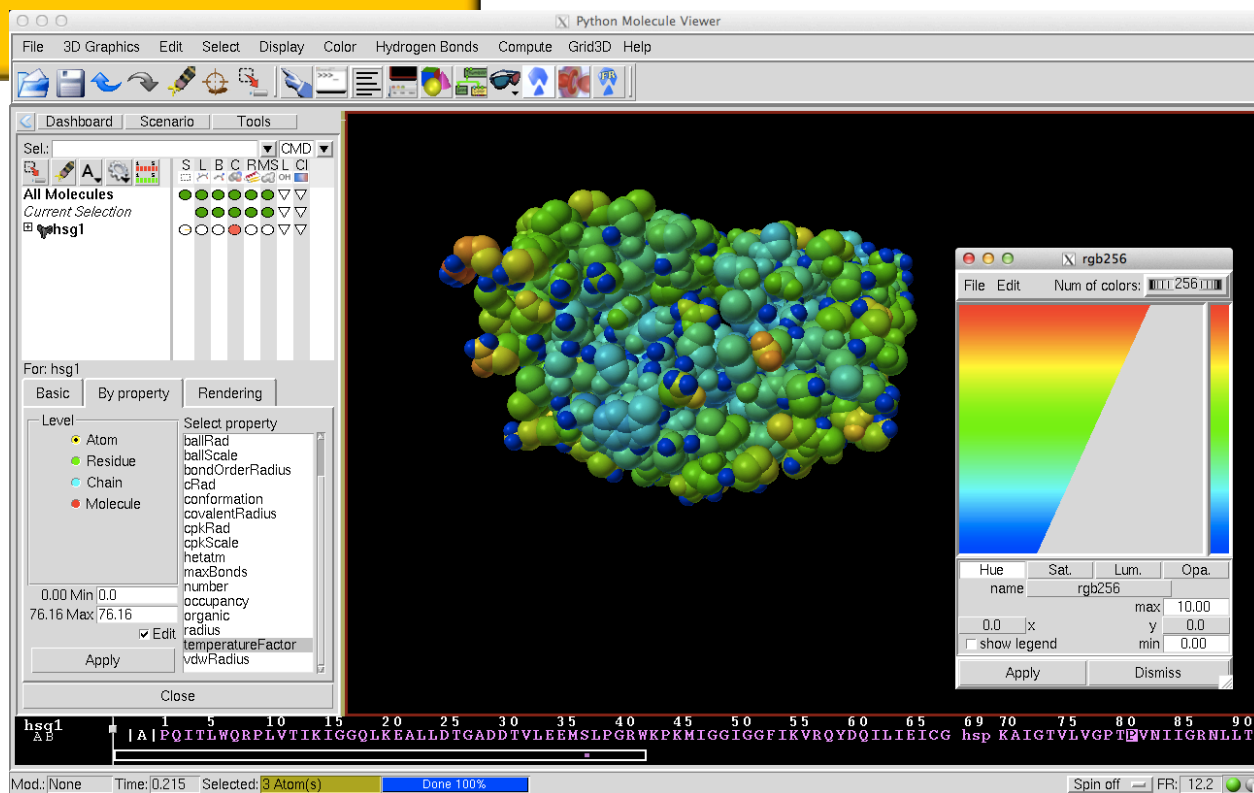




# Exercise: Color By Property

## 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

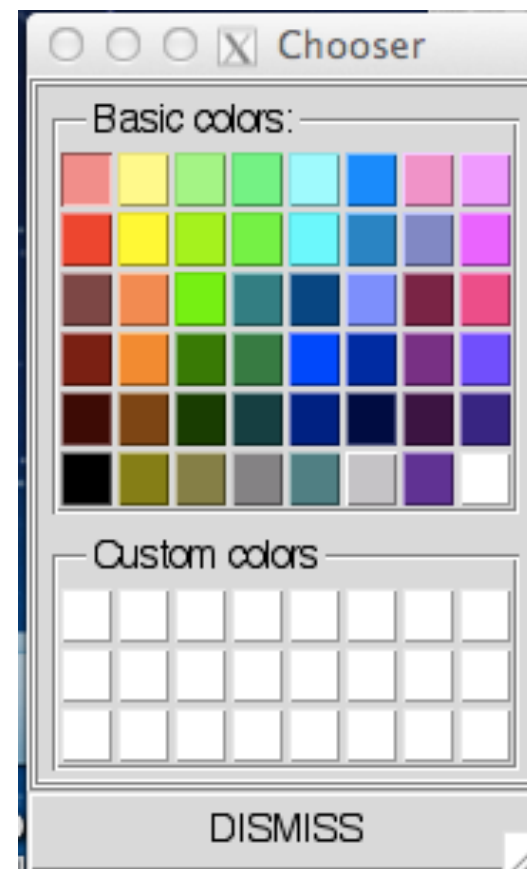


# Exercise: Color Palettes

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

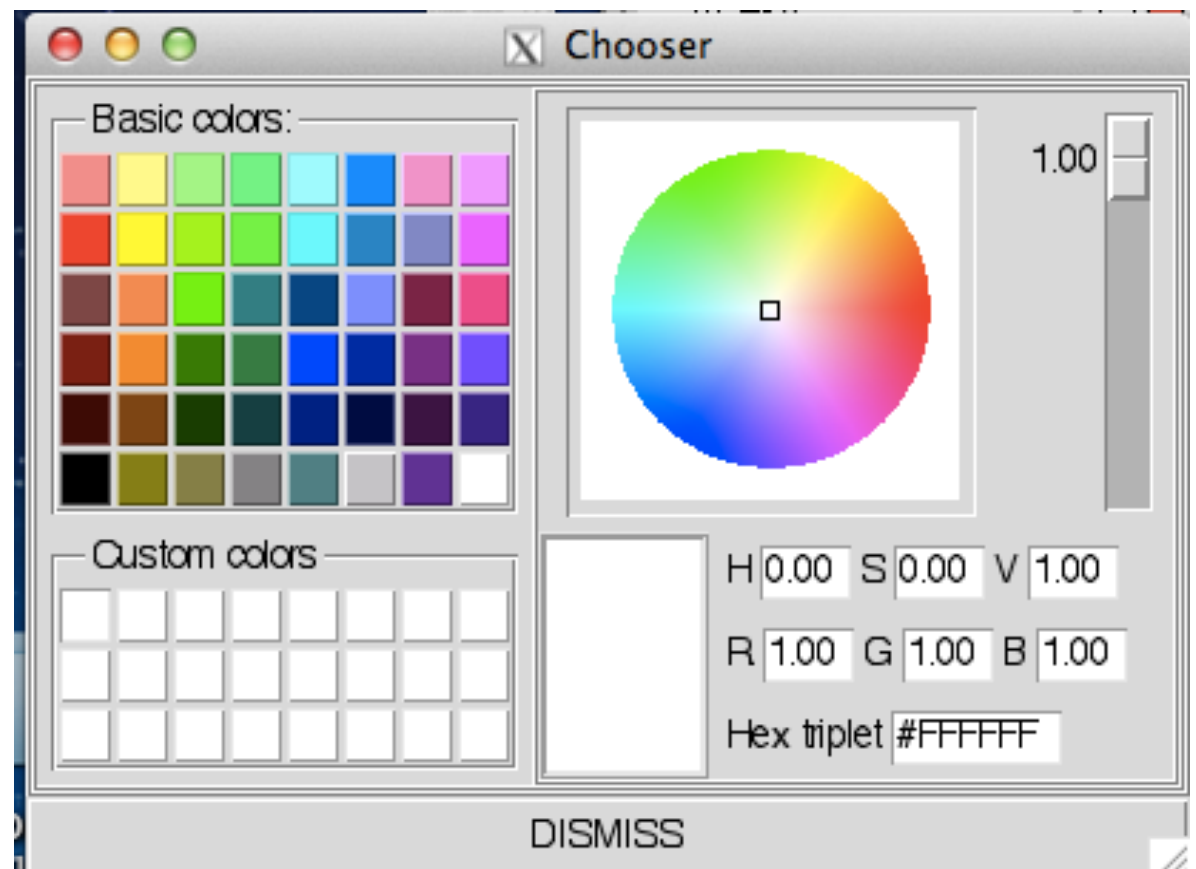
- 1 – Edit -> Color Palettes -> Edit Color by Molecule
- 2 – click on color 0
- 3 – select new color in color chooser
- 4 - Restore default

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



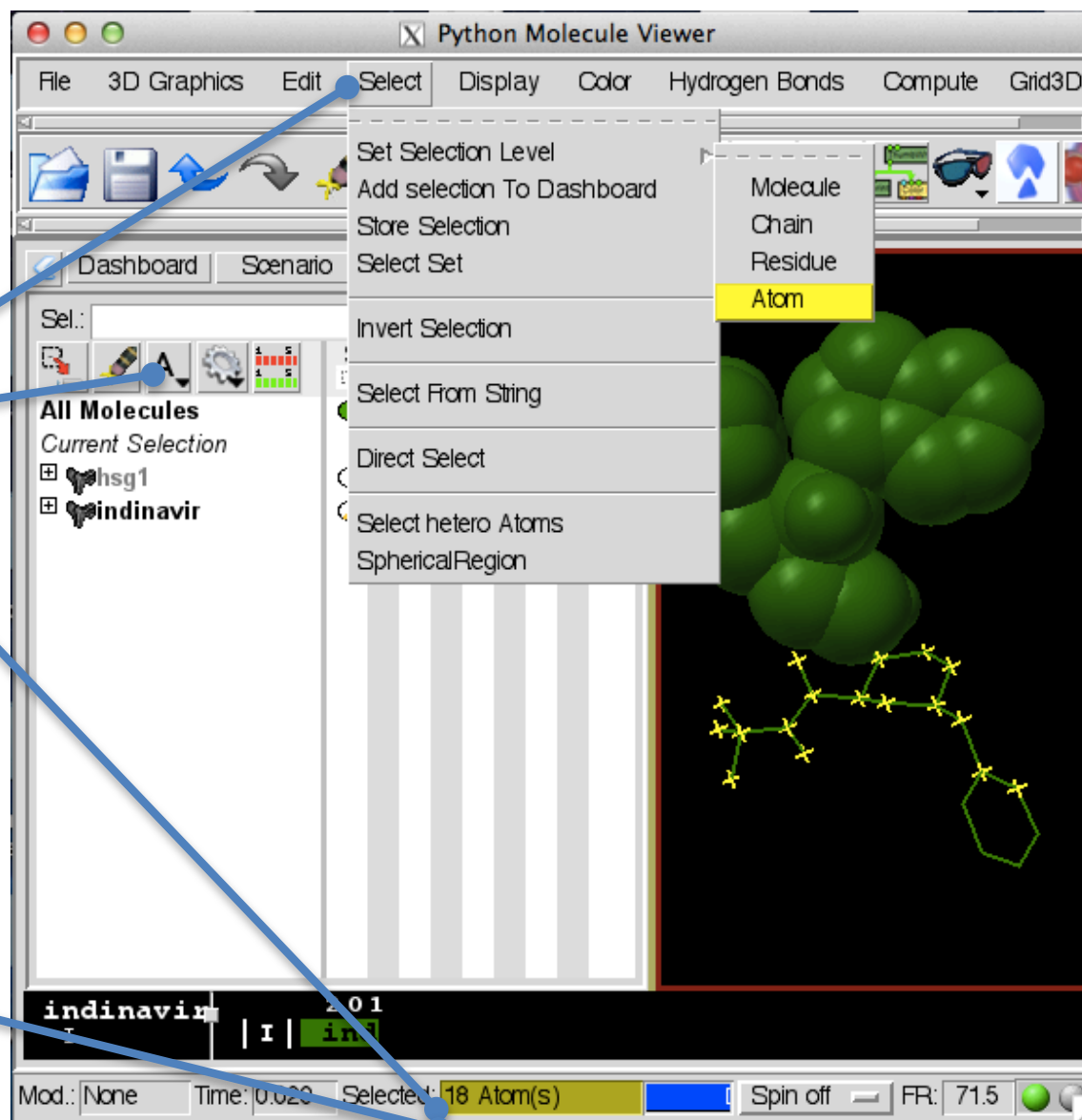
# Pmv selection



Clear selection

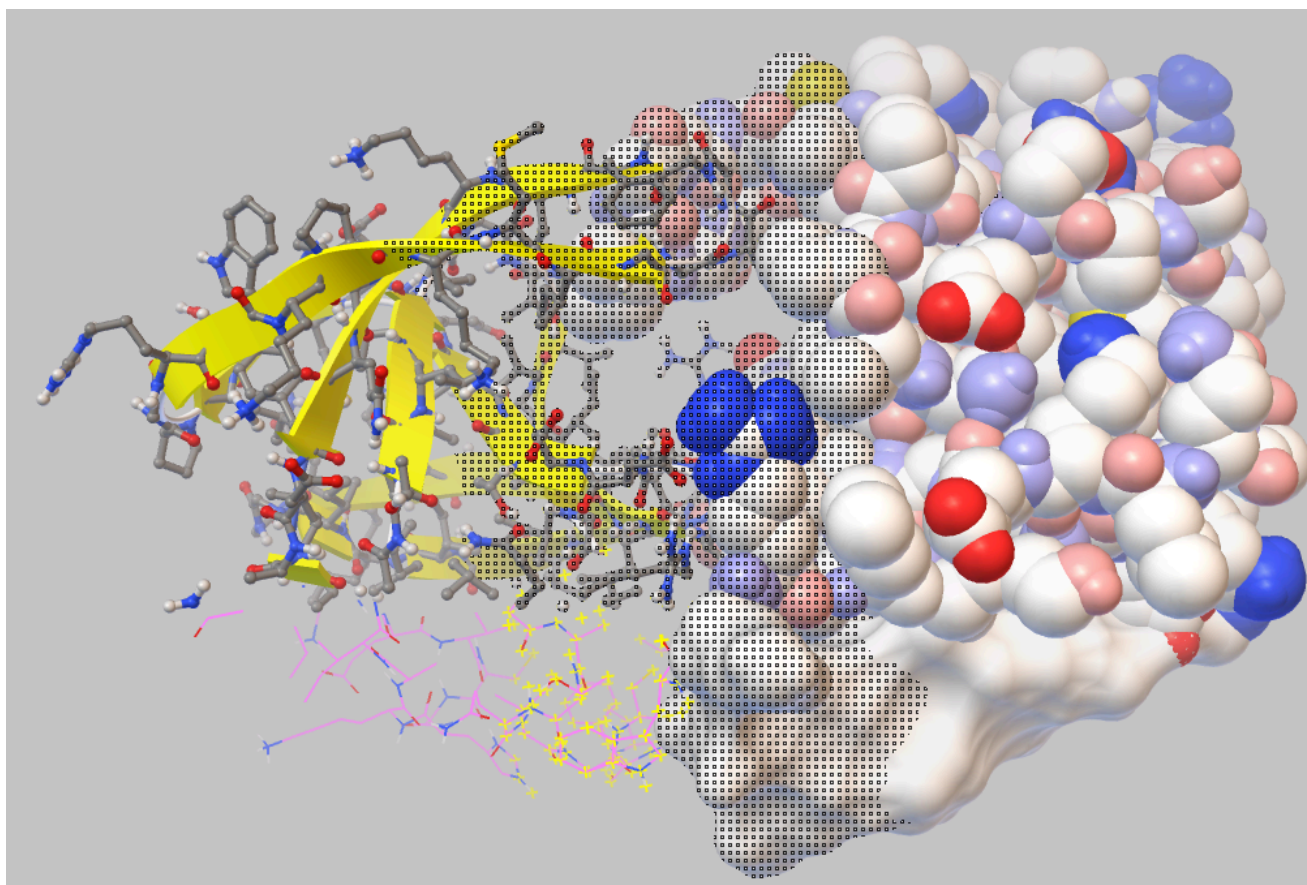
Set selection level

Current selection  
description



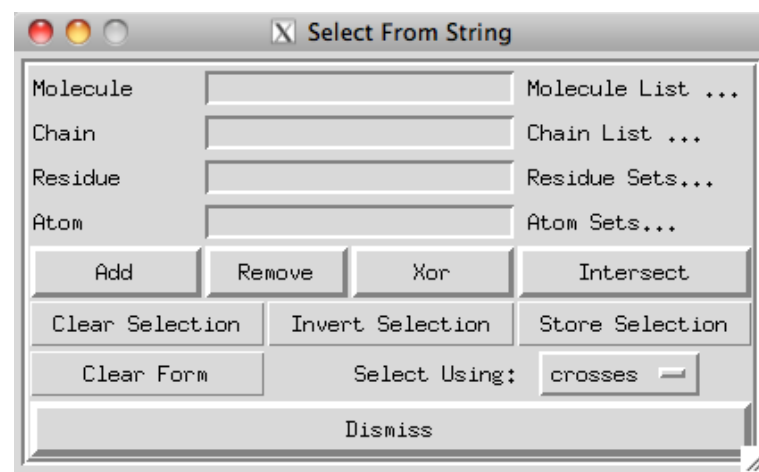
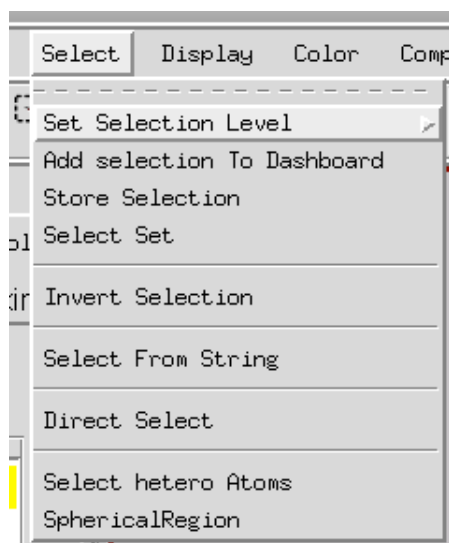
# Pmv selections

- Visual feed back of selected atoms on all representations



# Creating selections

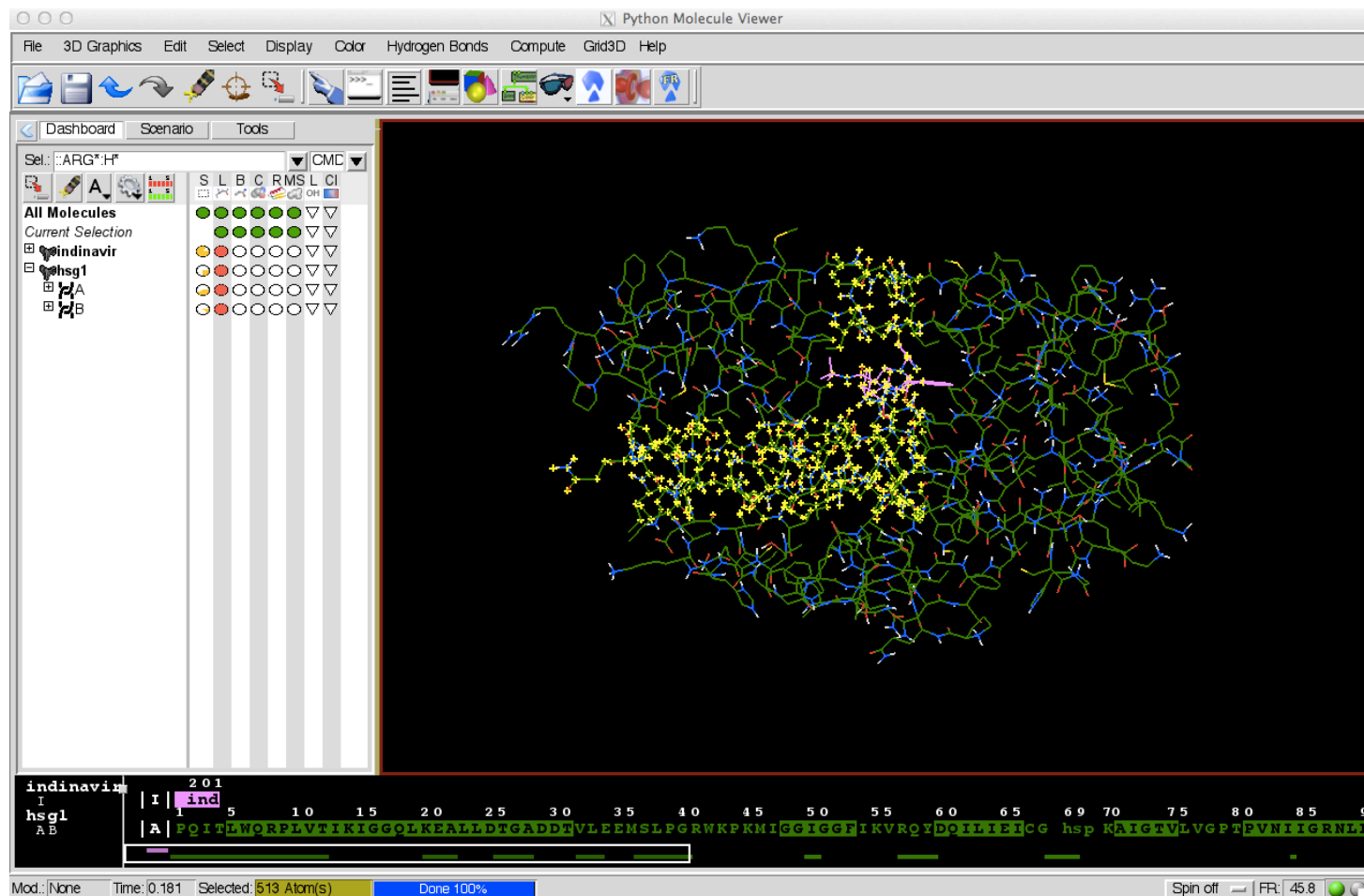
- Pmv menu commands and dashboard entry “current selection” operate on selection
- Pmv has various way to build complex selections
  - Shift left click and drag in 3D Viewer
  - Dashboard selection column and sel.: entry
  - Selecting residues in sequence viewer
  - Menu Select ->





# Creating selections

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



# Creating selections

## Notes:

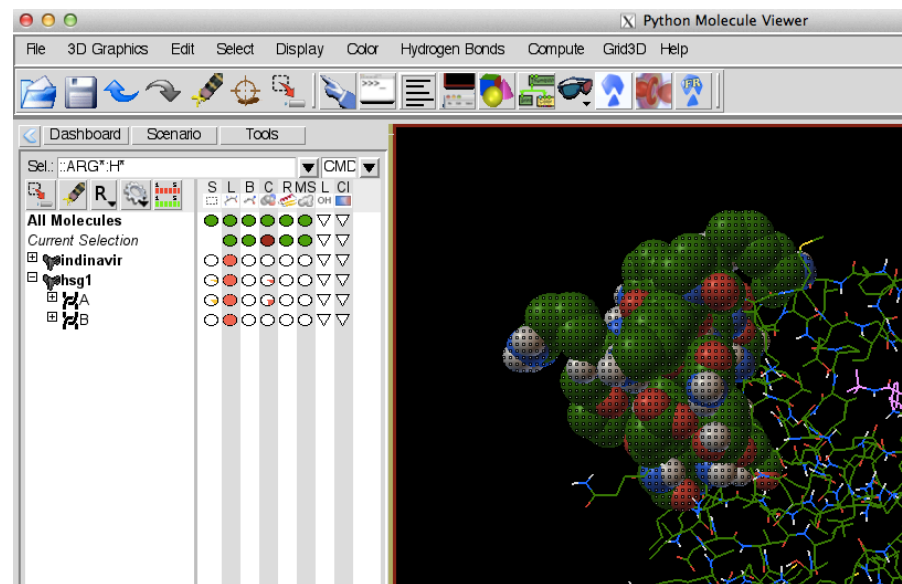
- clicking without dragging will only select the one atom closest to the viewer. Dragging will draw a rectangle and select all atoms falling inside the rectangle.
- Selection is performed at the current selection level. If the level is residue, selecting a single atom will select the whole residue

# Creating selections

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

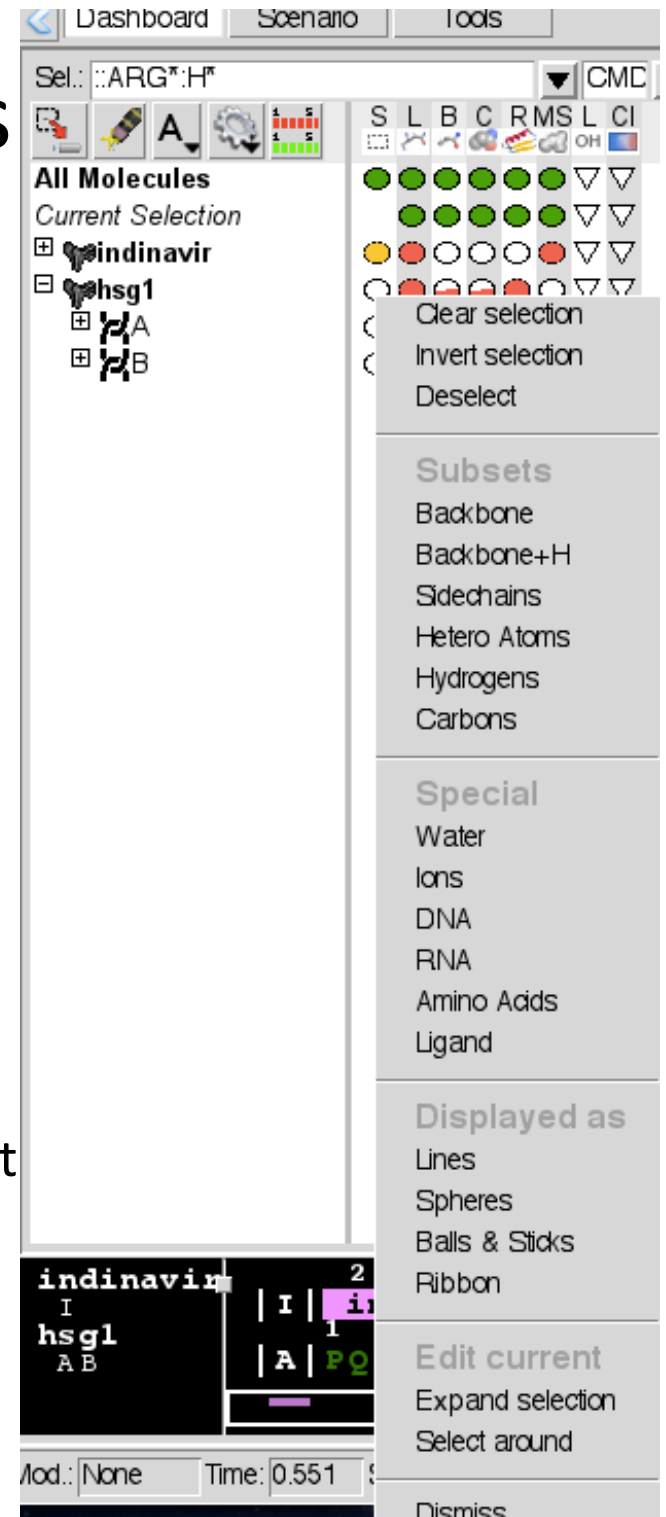
**Task: create selections using the dashboard at various levels**

- 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

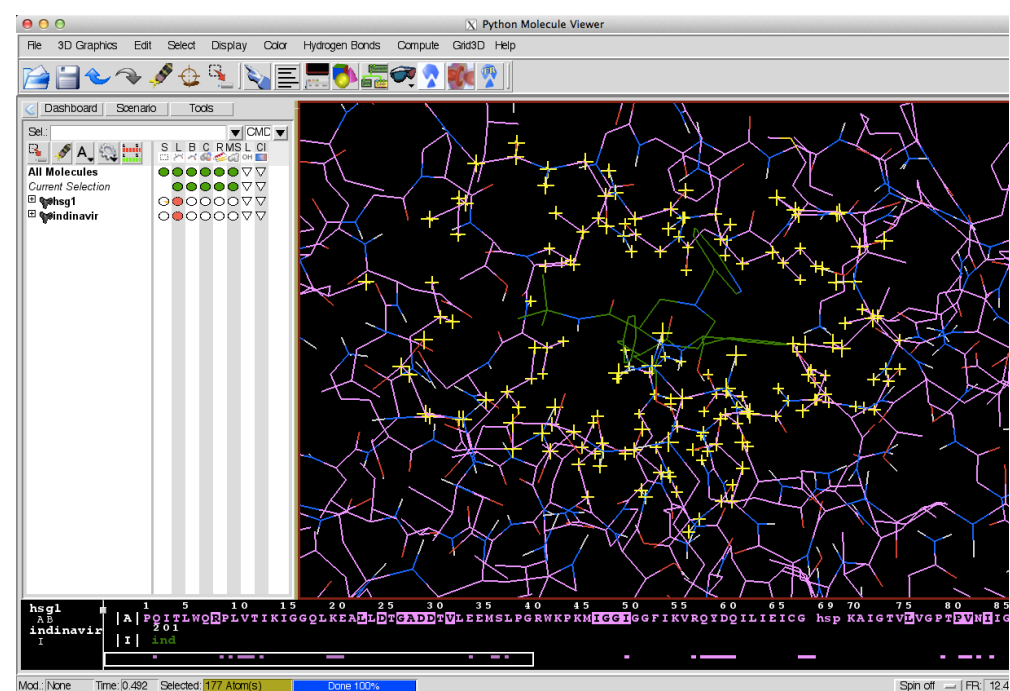
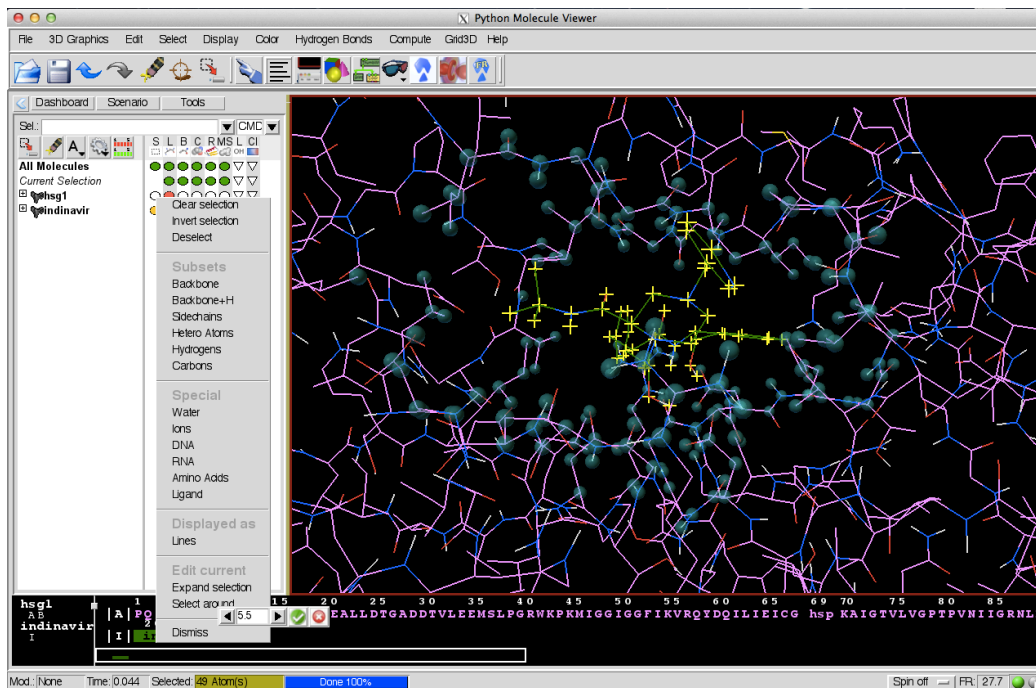
- Dashboard selection menu
  - **Clear** selection
  - **Invert** selection within fragment
  - **Deselect** fragment
  - Select **subsets** of atoms
  - Select **special** residues
  - Select atoms **Displayed as**
  - Edit selection:
    - Expand selection within fragment
    - Select around selection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

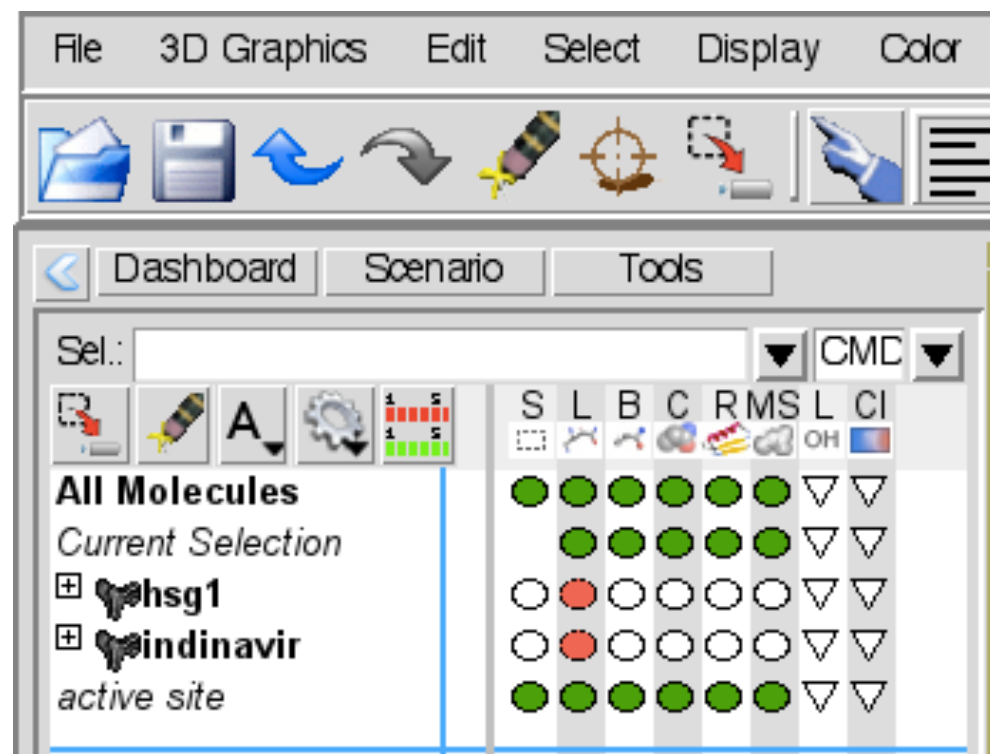
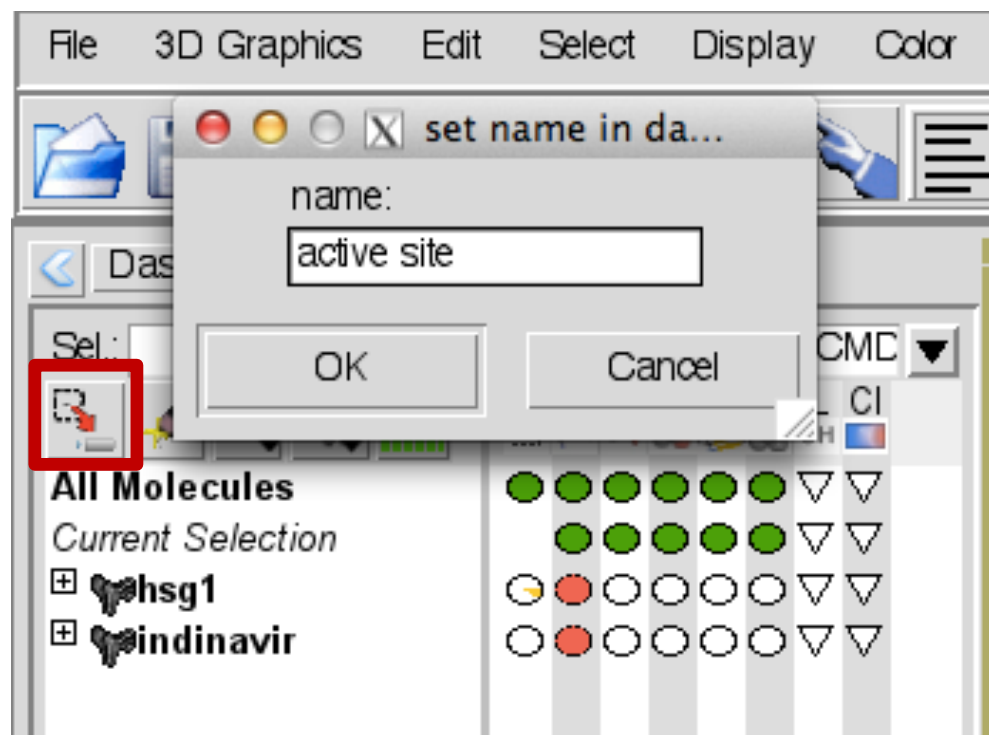
- Powerful selection mechanism using regular expressions:
  - moleculeRE:ChainRE:ResiduesRE:AtomsRE
  - wildcards such as (e.g. \*) and ranges (e.g. PRO1-ARG8)
- Available in the Python shell and dashboard
  - Examples:
    - “::” will select all Atoms in all Residues in all Chains in all Molecules in 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://mglddev.scripps.edu/docs/mgltools/1.5.6/Selection%20Strings.htm>



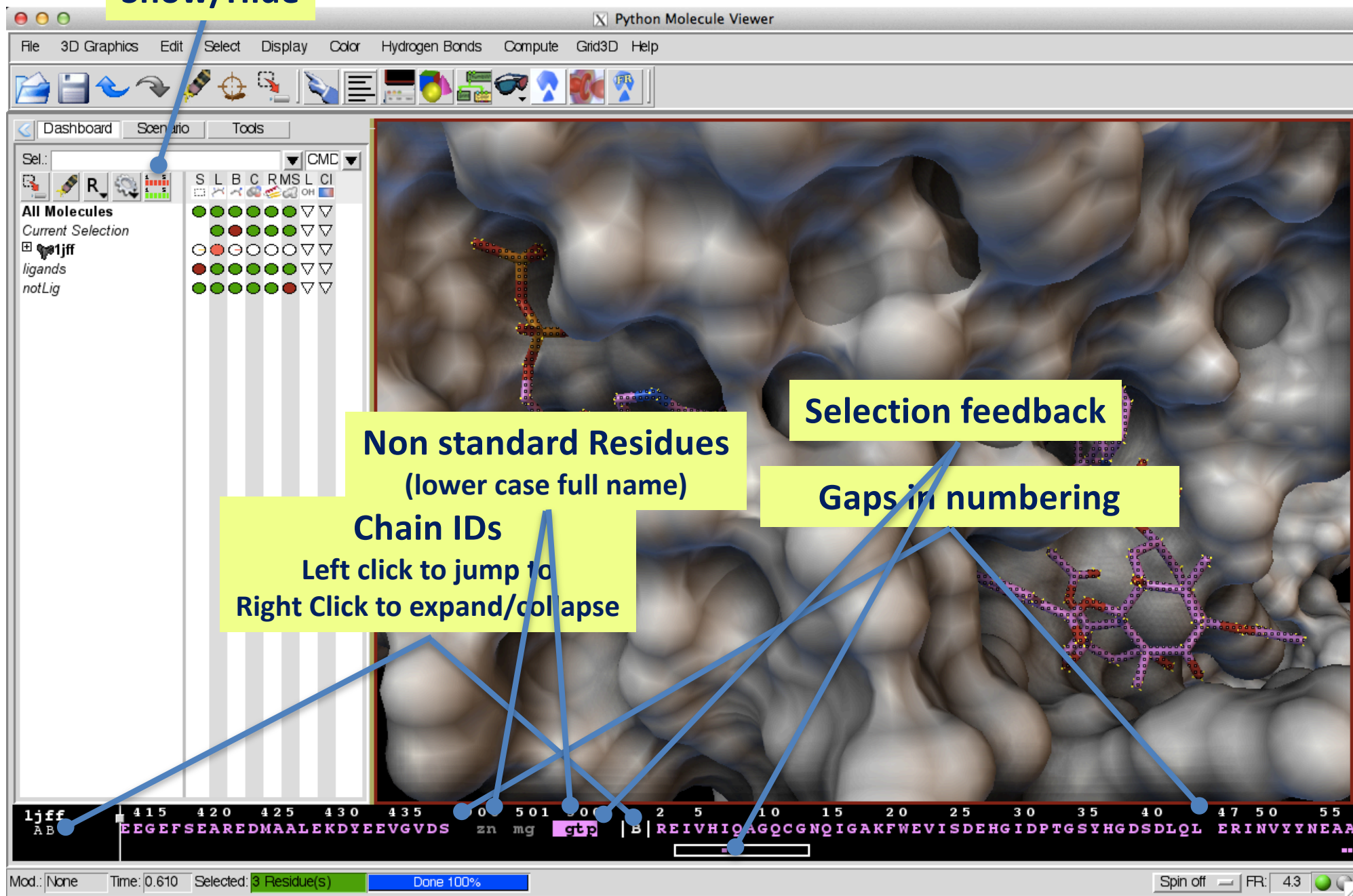
# Dashboard User Sets

- Shortcut for operating on selections



# Sequence Viewer

Show/Hide



# 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

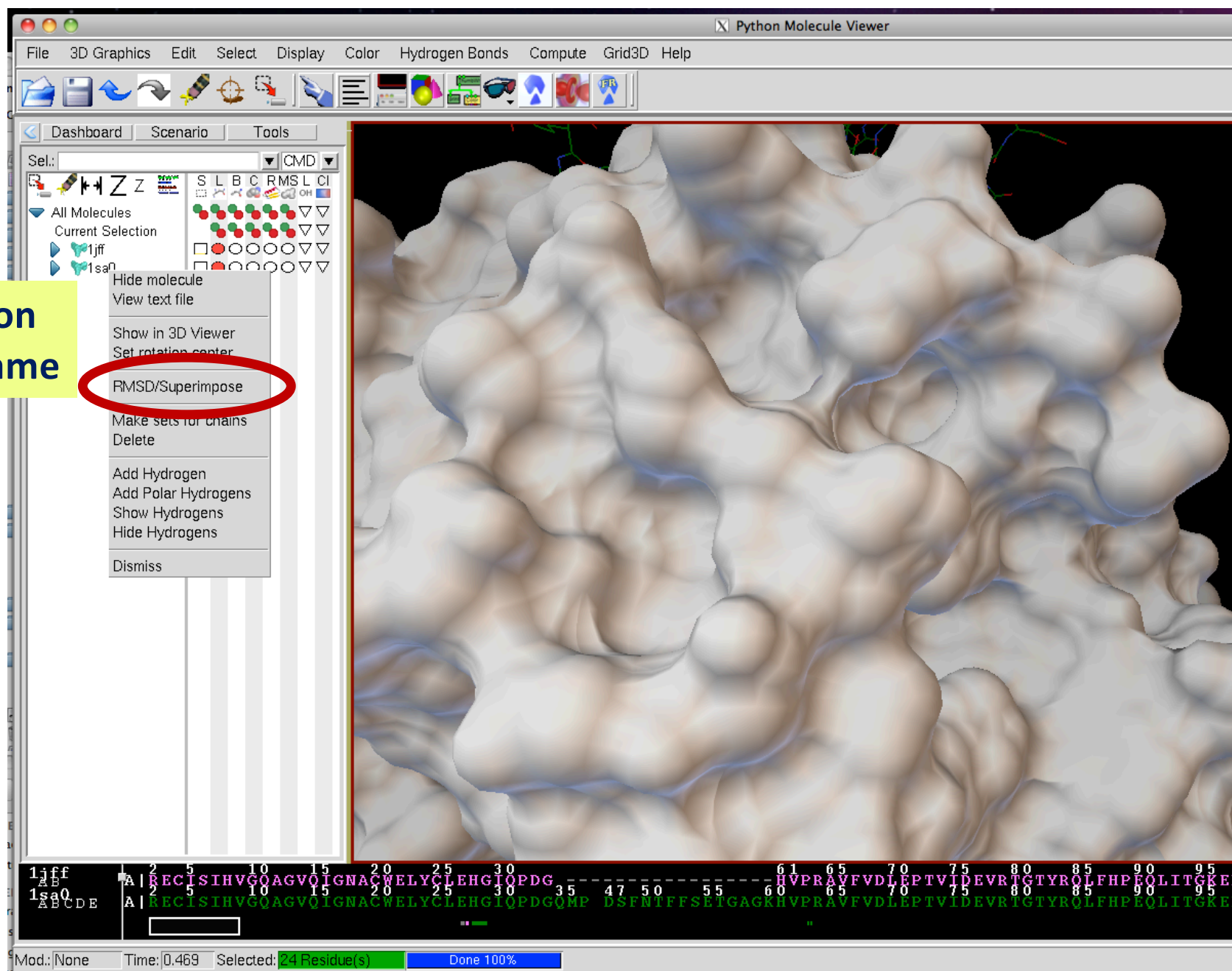
## Task: manual alignments

- 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



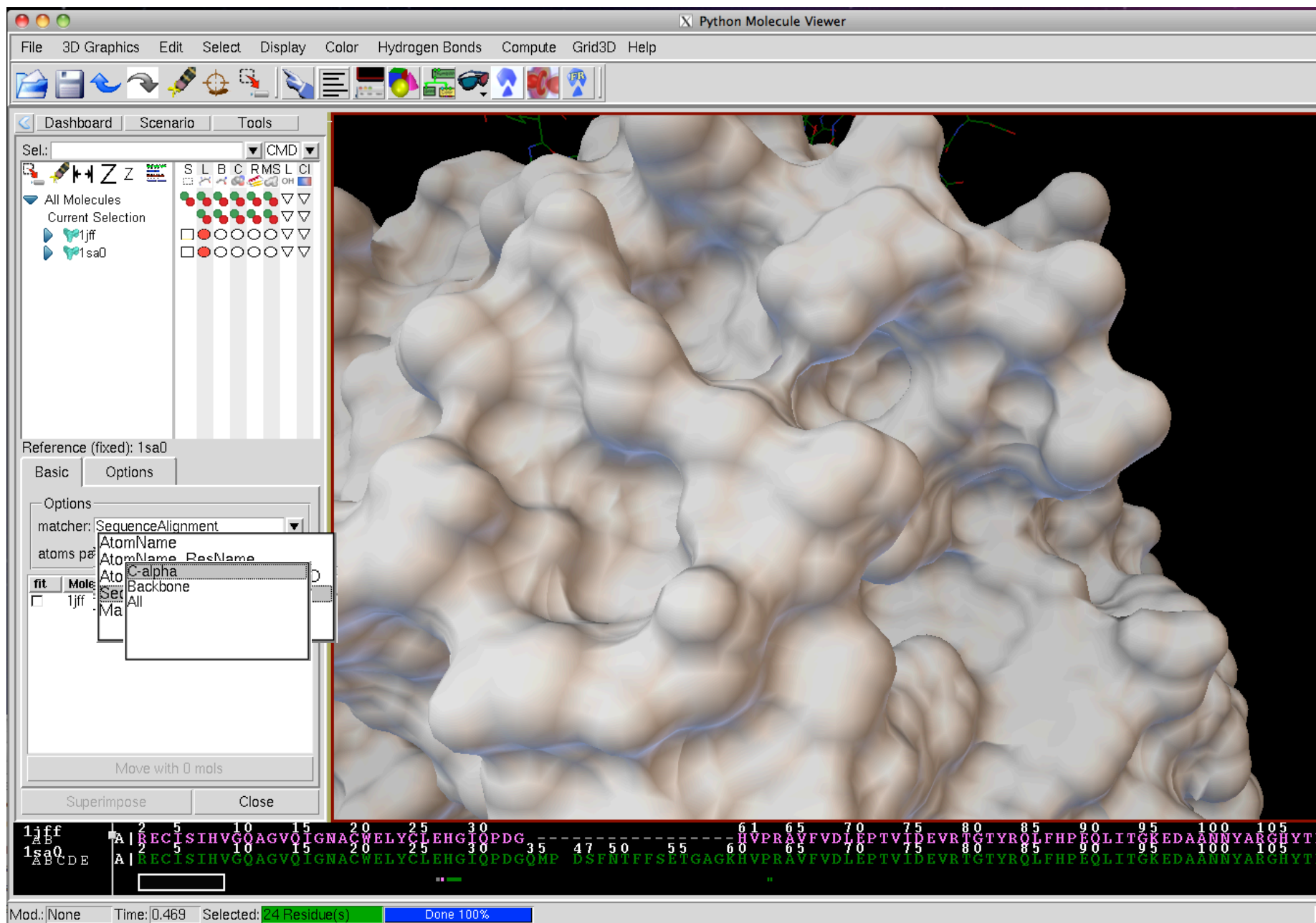
# RMDS/Superimpose

Right click on  
molecule name

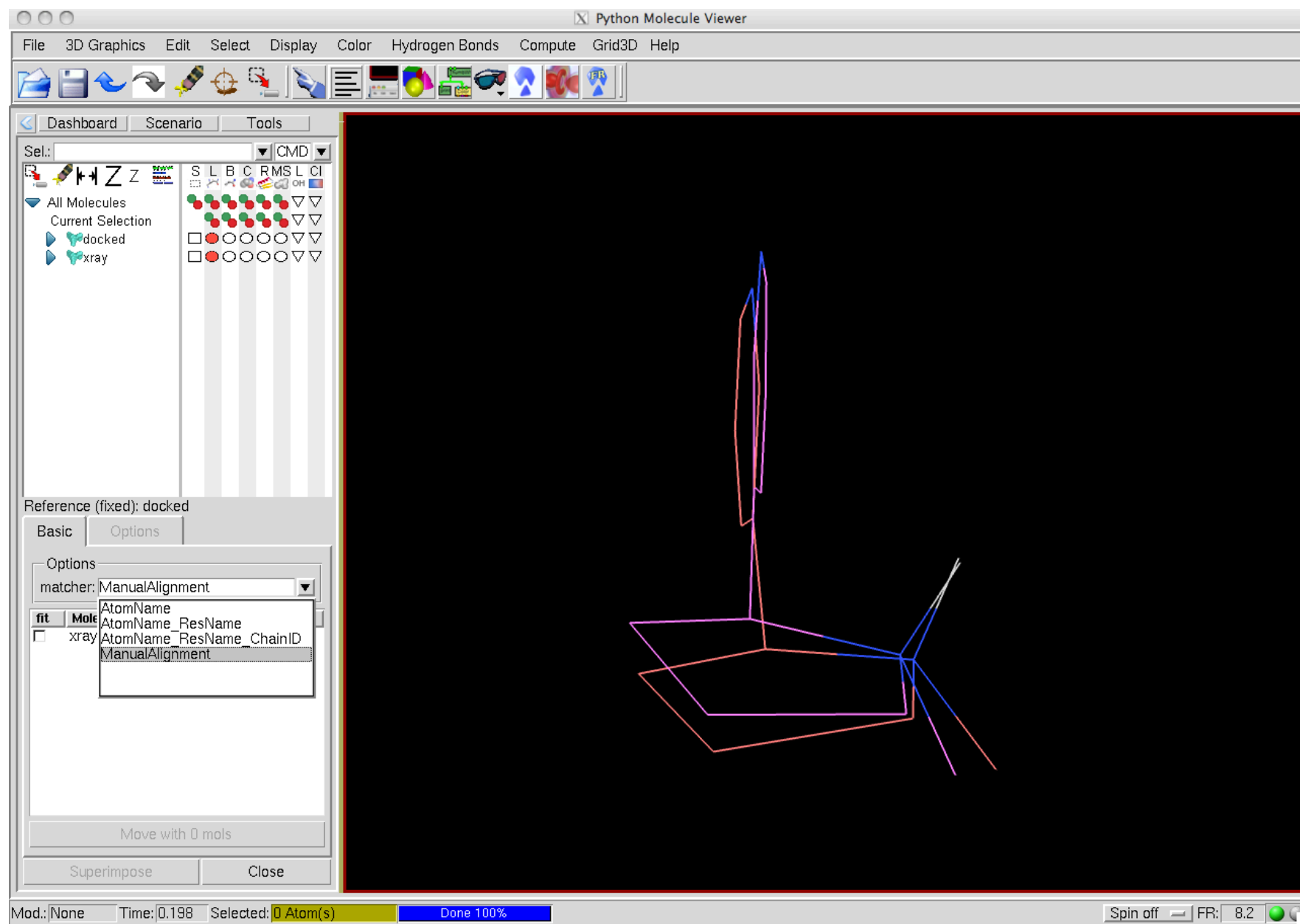




# RMDS/Superimpose

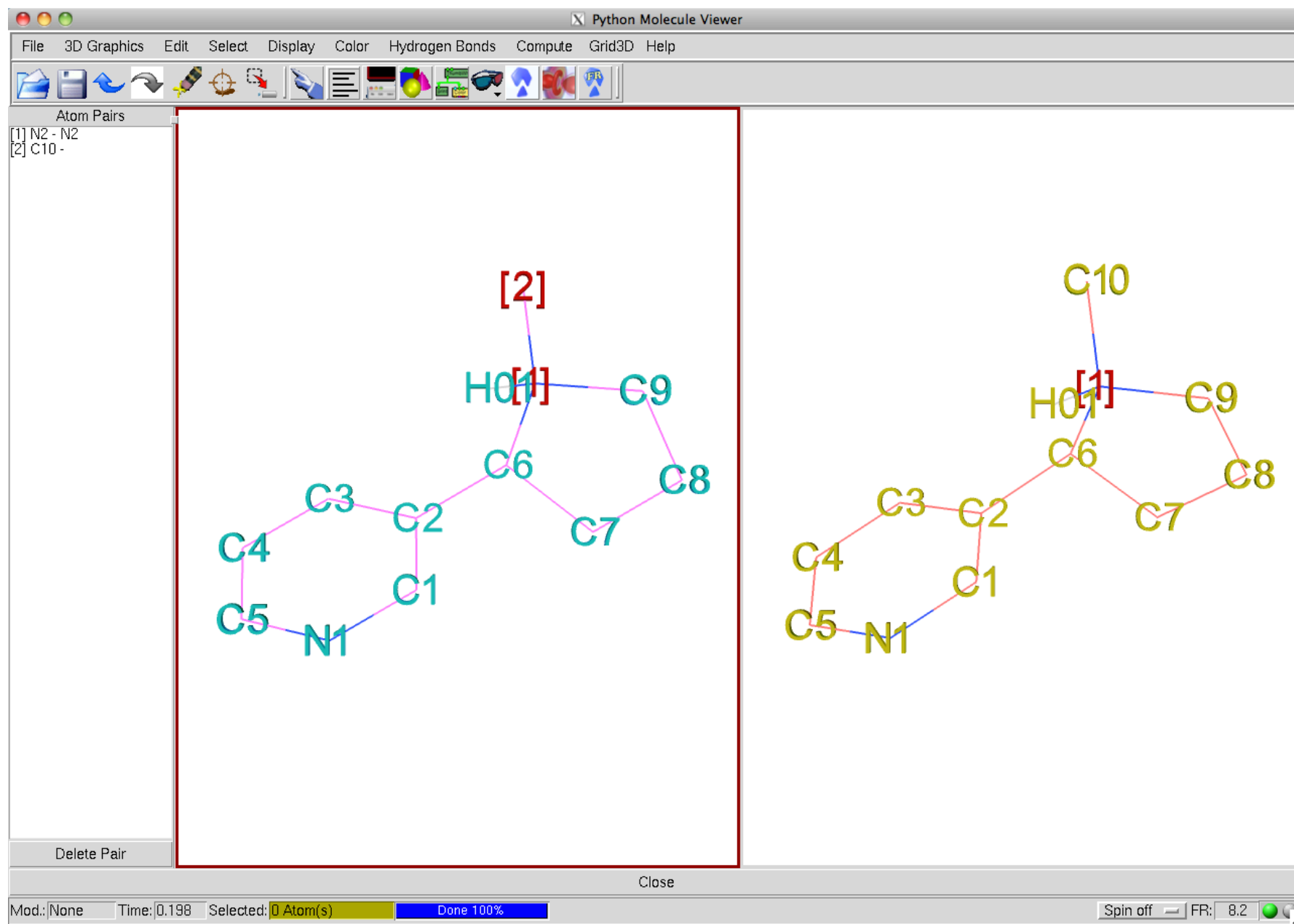


# RMDS/Superimpose





# RMDS/Superimpose



# Scenario Animations: snapshots

The image shows the Python Molecule Viewer software interface. The main window displays a 3D ribbon diagram of a protein structure, primarily yellow, with a grey surface representation of a binding site. A snapshot editor dialog box is open in the foreground, allowing users to record snapshots for animation. The dialog includes options for interpolating orientation and rendering, setting speed (slow, medium, fast, custom), and Z-sorting polygons. The bottom status bar shows the current model is 'None', time is 0.003, and 0 residues are selected.

**Python Molecule Viewer**

File 3D Graphics Edit Select Display Color Hydrogen Bonds Compute Grid3D Help

Dashboard Scenario Tools

File

Snapshots Move Colors Sequence Anim.

Record Snapshot

Add to animation  
Edit  
Rename  
Delete

**Snapshot Editor**

Interpolate  
☒ Orientation ☒ Rendering

Record:  
Orientation Rendering

speed (in frames)  
☐ slow ☒ medium ☐ fast ☐ custom

Zsort Polygons  
☐ +Zsort ☒ -Zsort ☐ Never ☒ Once ☐ Always

OK Preview Cancel

hsgl  
AB  
indinavir  
I

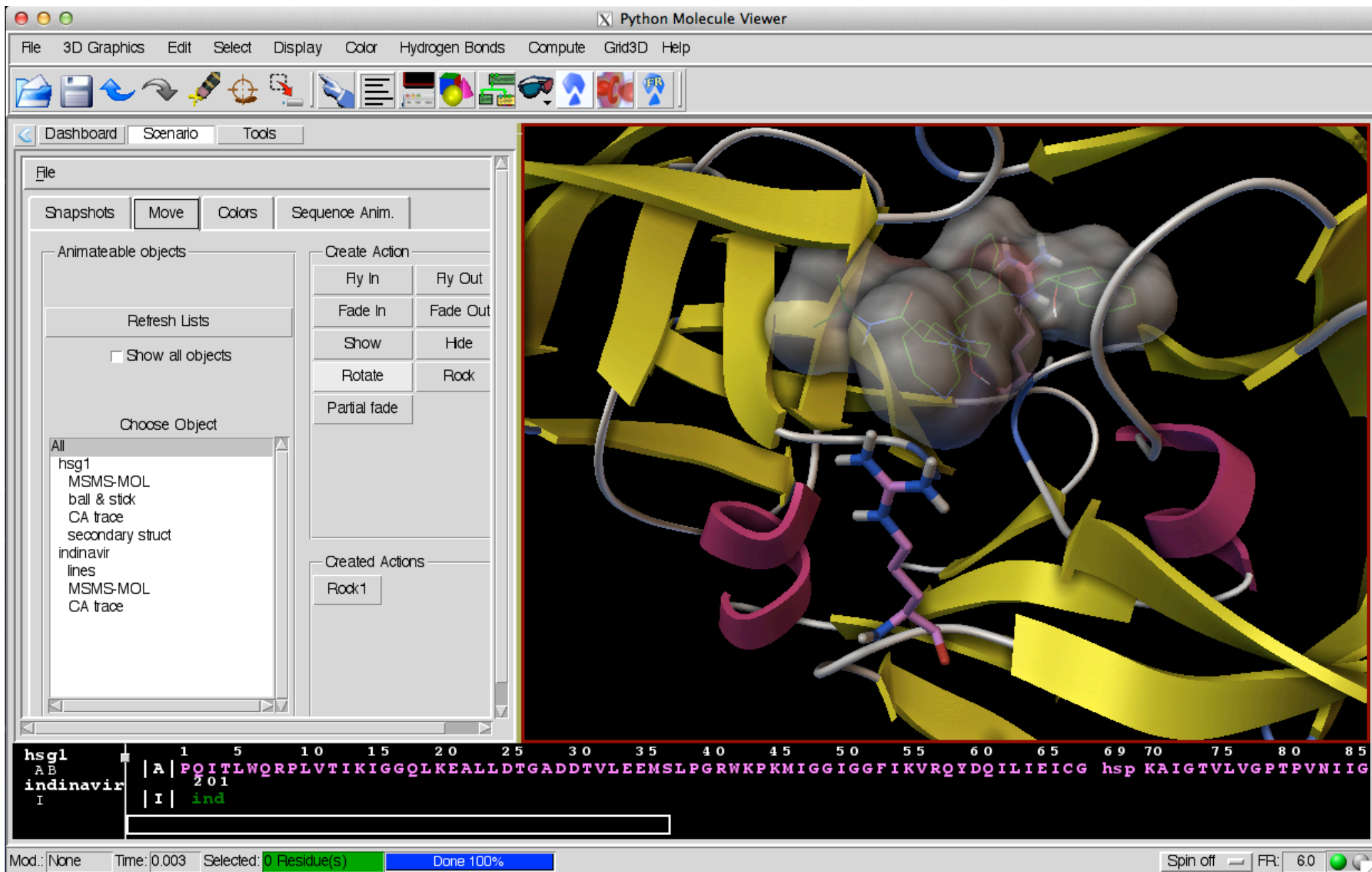
1 5 10 15 20 25 30 35 40 45 50 55 60 65 69 70 75 80 85

| A | P O I T L W Q R P L V T I K I G G Q L K E A L L D T G A D D T V L E E M S L P G R W K P K M I G G I G G F I K V R Q Y D Q I L I E I C G h s p K A I G T V L V G P T P V N I I G  
2 0 1  
| I | i n d

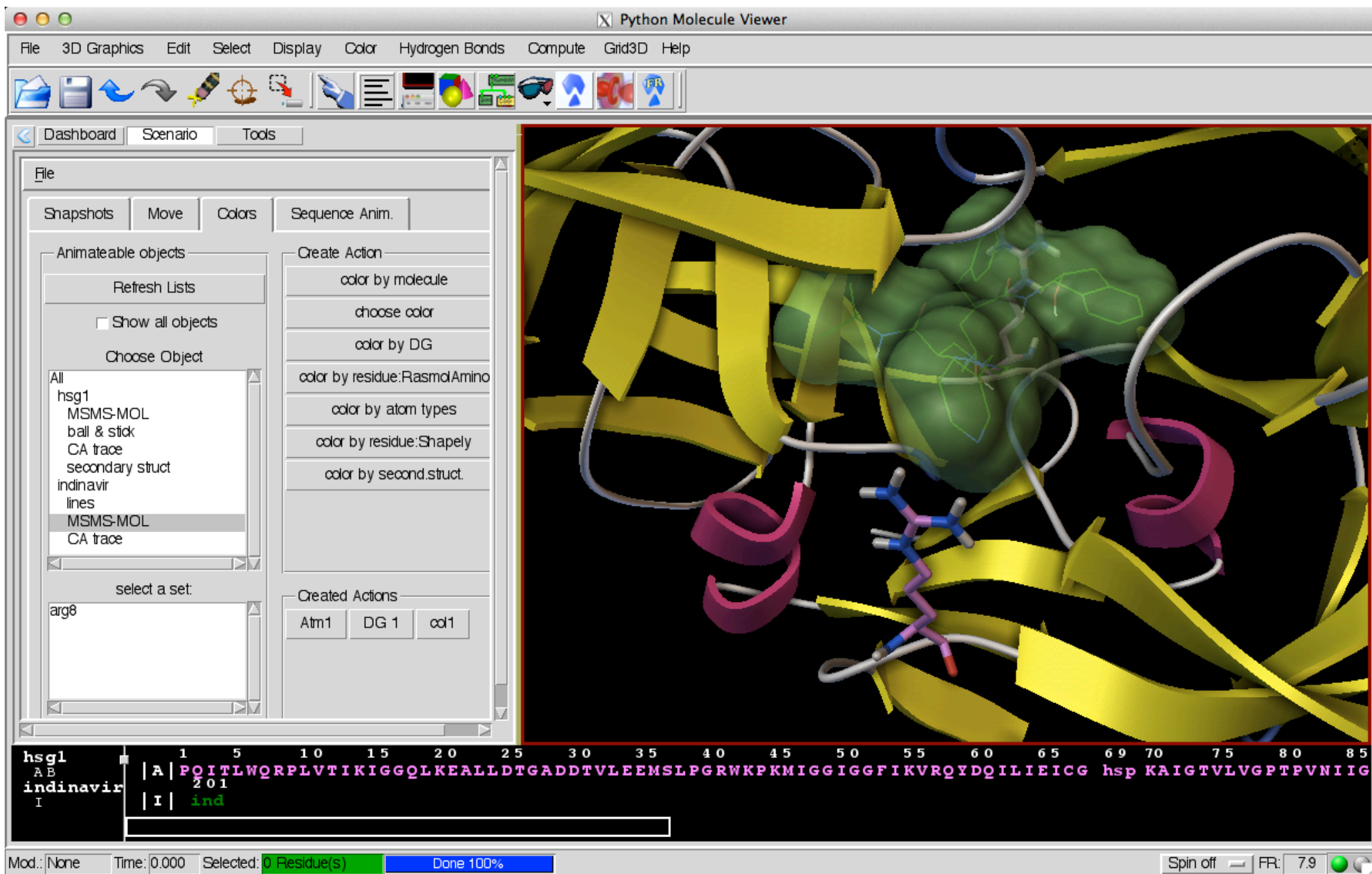
Mod.: None Time: 0.003 Selected: 0 Residue(s) Done 100%

Spin off FR: 8.5

# Scenario Animations: moves



# Scenario Animations: color



# Scenario Animations: sequence

Python Molecule Viewer

File 3D Graphics Edit Select Display Color Hydrogen Bonds Compute Grid3D Help

Dashboard Scenario Tools

File

Snapshots Move Colors Sequence Anim.

Actions

- 00000-00030: fly in All from left
- 00031-00100: snapshot1
- 00101-00160: All 60 (0, 1, 0) rock
- 00101-00131: snapshot2
- 00132-00162: snapshot4
- 00163-00222: All 60 (0, 1, 0) rock
- 00223-00253: fly out All right
- 00254-00284: fly out All right

Manipulate Actions

delete

force

- ☒ Orientation
- ☒ Rendering

Edit ...

Start

- ☒ after previous
- ☐ with previous

Offset: 0

Video(mpg) duration(sec): 12

hsg1  
AB  
indinavir  
I

1 5 10 15 20 25 30 35 40 45 50 55 60 65 69 70 75 80 85 90

| A | P O I T L W R P L V T I K I G G Q L K E A L L D T G A D D T V L E E M S L P G R W K P K M I G G I G G F I K V R Q Y D Q I L I E I C G h s p K A I G T V L V G P T P V N I I G R N L I

| I | i n d

Mod.: None Time: 0.031 Selected: 0 Atom(s) Done 100%

Spin off FR: 8.0



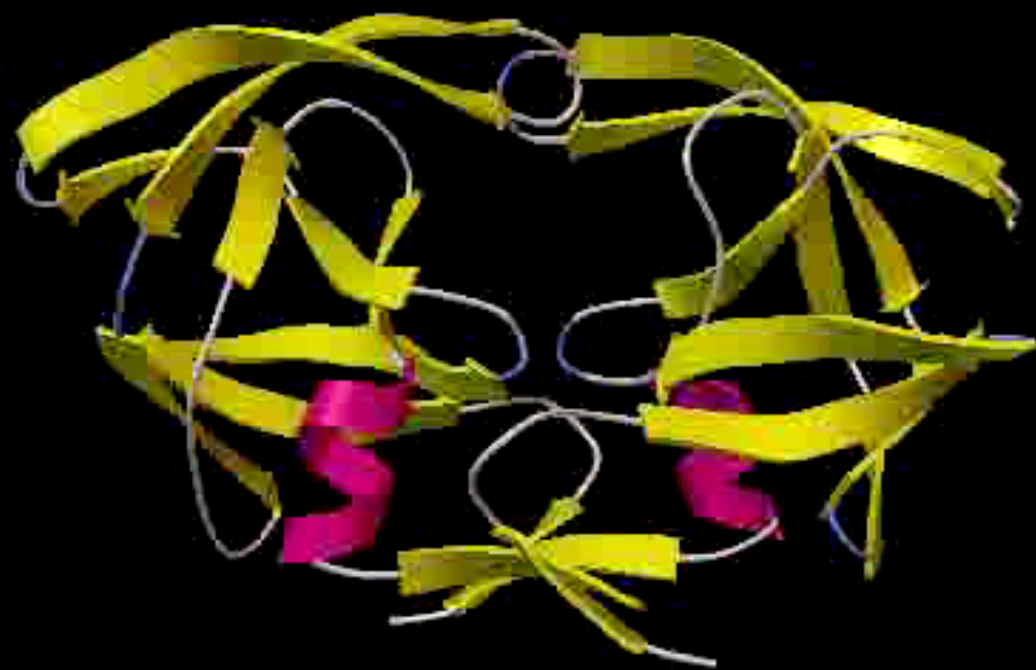
# Scenario Animations: sequence

## 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 snippets get saved in the session file**





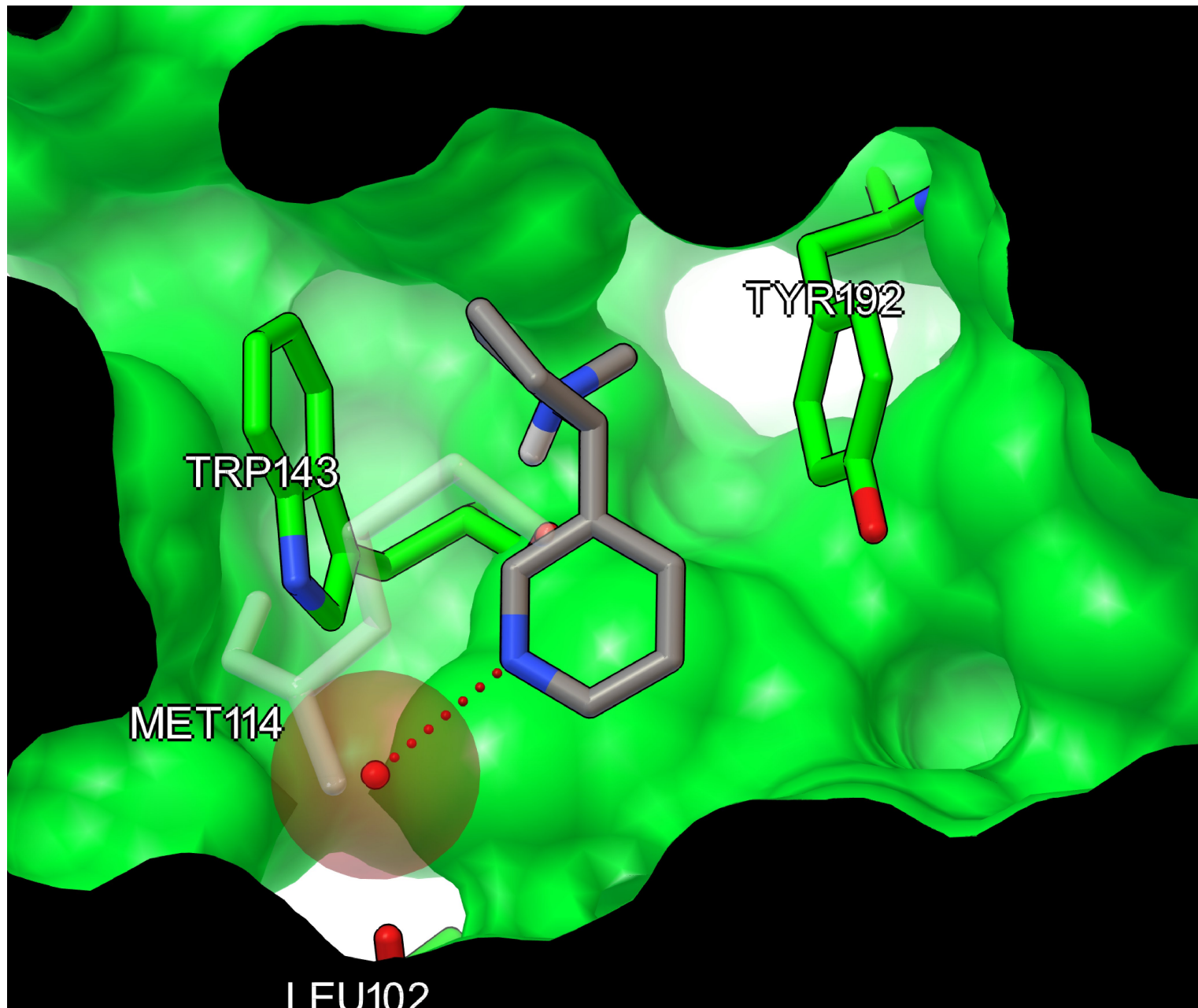
# Scenario Animations

**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



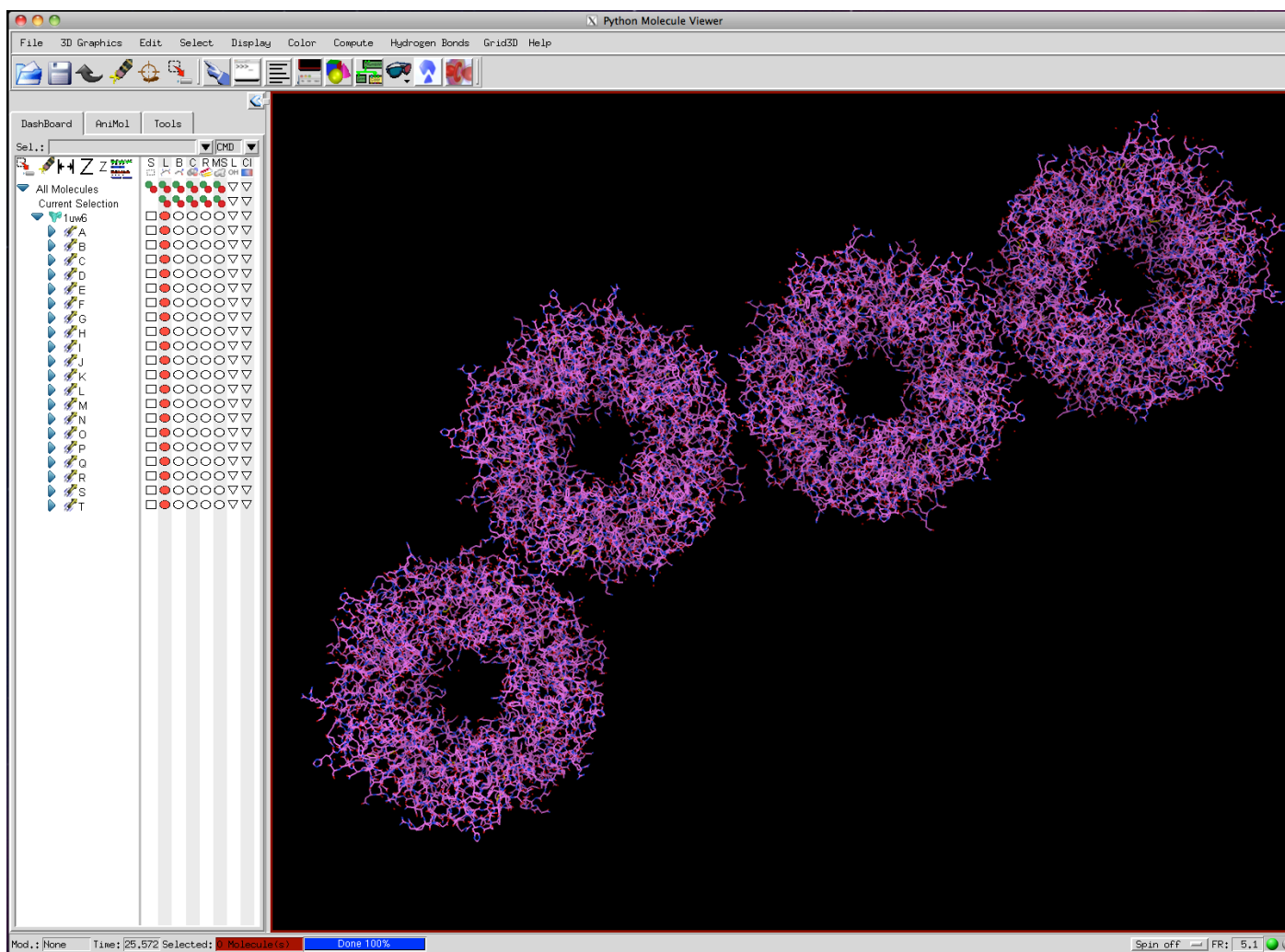
# Example: 1uw6



# Exercise: selections

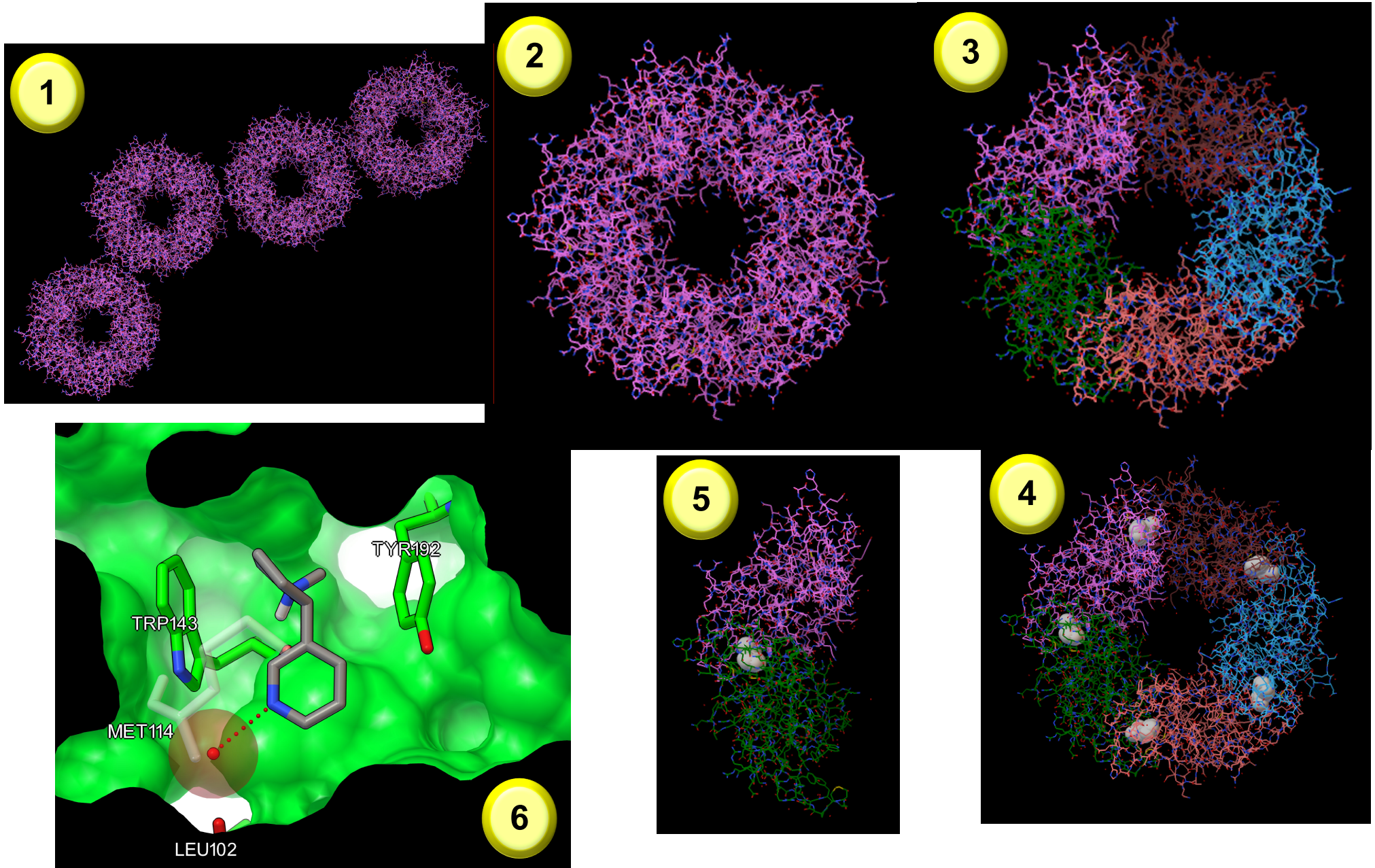
**Task: get structure and get familiar with it**

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**

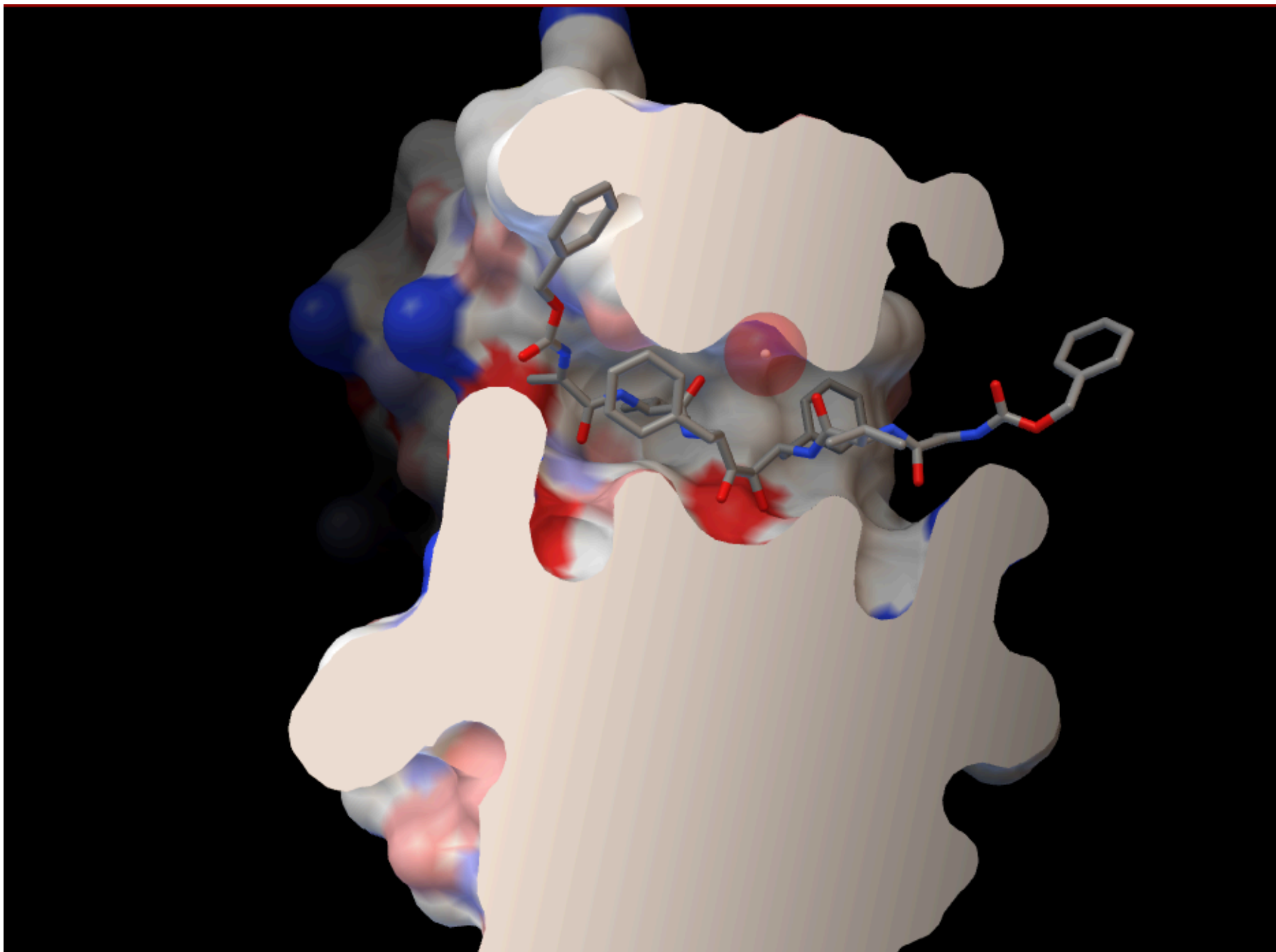
- 1 – select ligand set
- 2 – “select around” in protein with cutoff 4.0
- 3 – create “binding with water” set
  
- 4 – select “binding with water” set
- 5 – de-select water
- 6 – create “binding” set
  
- 7 – select “binding with water”
- 8 – de-select “binding” set
- 9 – create “water” set

# Exercise: selections

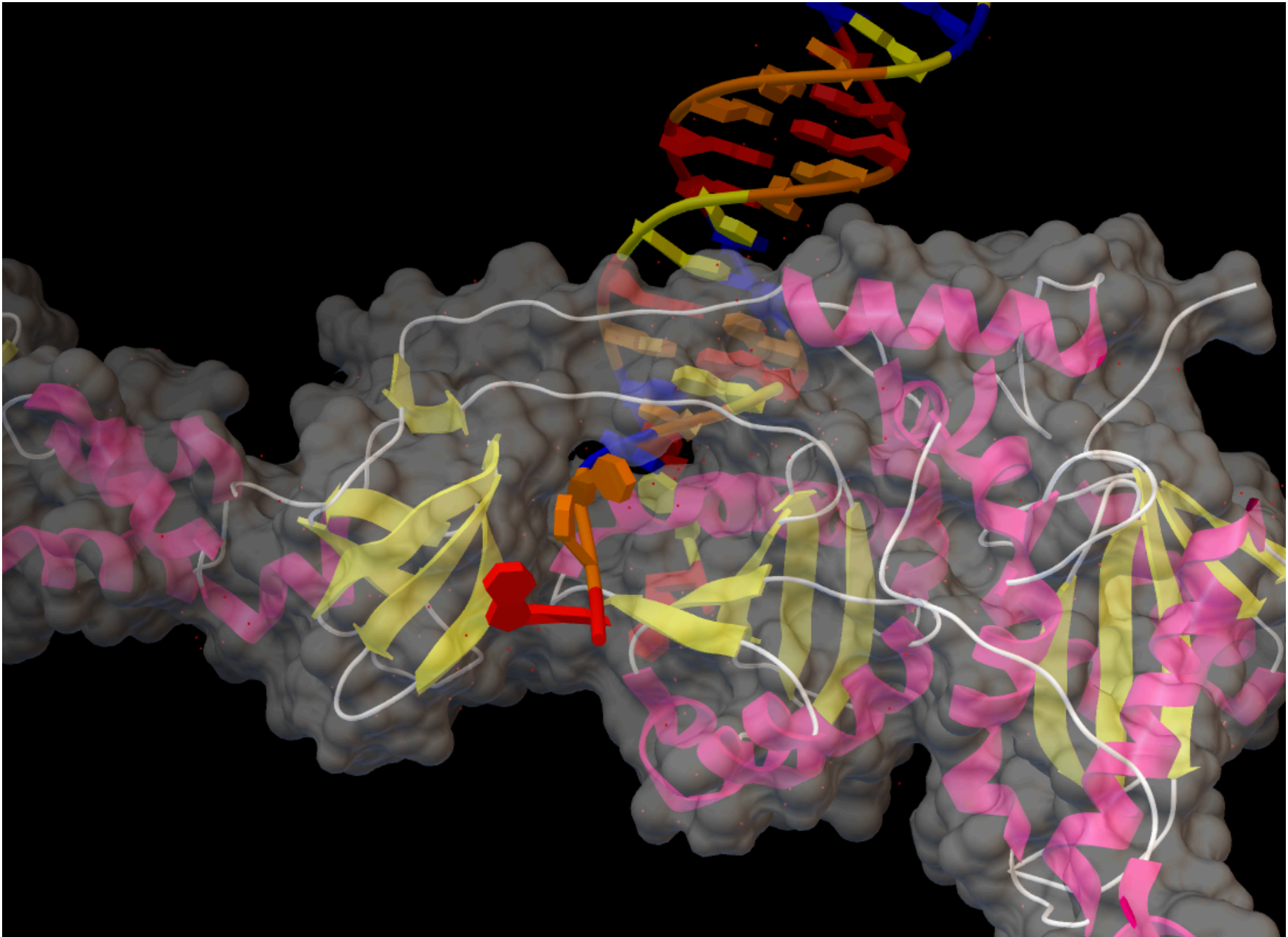
## Task: compute surface

- 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

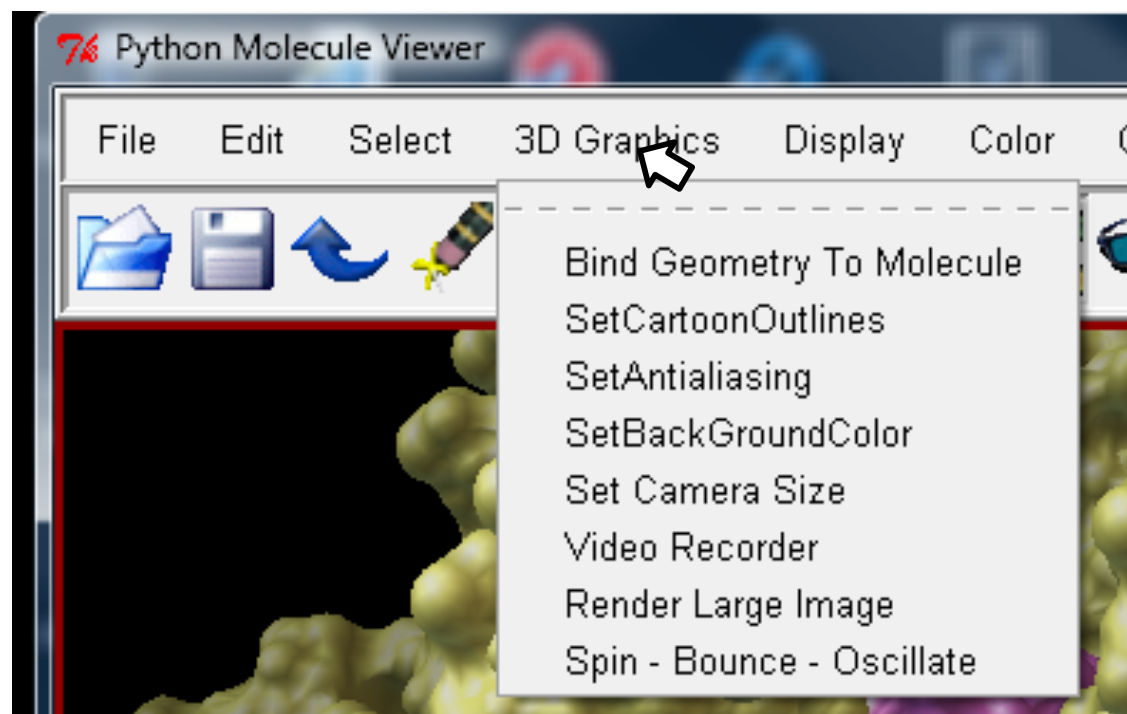




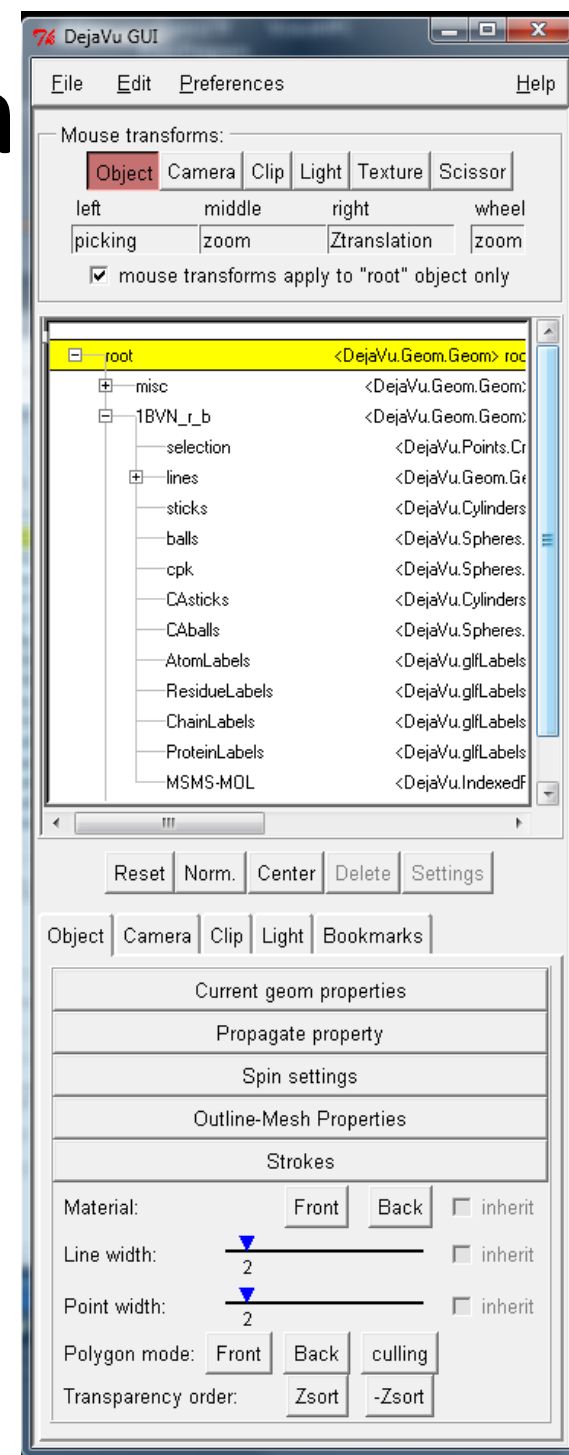
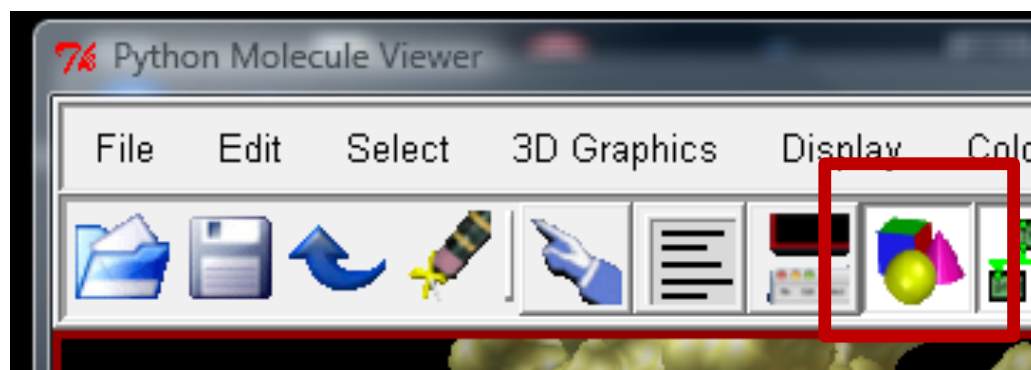
# Feedback

**email: [sanner@scripps.edu](mailto:sanner@scripps.edu)**

# 3D Visualization



# 3D Visualization



# 3D Visualization: GUI overview

The image shows a screenshot of the **DejaVu GUI** window. The window has a menu bar with **File**, **Edit**, **Preferences**, and **Help**. Below the menu bar is a section titled **Mouse transforms:** with tabs for **Object**, **Camera**, **Clip**, **Light**, **Texture**, and **Scissor**. Under the **Object** tab, there are buttons for **left**, **middle**, **right**, and **wheel**, each with a corresponding action: **picking**, **zoom**, **Ztranslation**, and **zoom**. A checkbox labeled **mouse transforms apply to "root" object only** is checked. Below this is a tree view showing the **Geometry objects hierarchy**. The root node is **root** (highlighted in yellow). It has a sub-tree **1BVN\_r\_b** which includes **selection**, **lines**, **sticks**, **balls**, **cpk**, **CAsticks**, **CAballs**, **AtomLabels**, **ResidueLabels**, **ChainLabels**, **ProteinLabels**, and **MSMS-MOL**. To the right of the tree view is a list of objects with their class names, such as **<DejaVu.Geom.Geom>**, **<DejaVu.Points.Cr>**, **<DejaVu.Geom.Ge>**, **<DejaVu.Cylinders>**, **<DejaVu.Spheres>**, **<DejaVu.Spheres>**, **<DejaVu.Cylinders>**, **<DejaVu.Spheres>**, **<DejaVu.glfLabels>**, **<DejaVu.glfLabels>**, **<DejaVu.glfLabels>**, and **<DejaVu.IndicedF>**. At the bottom of the window are buttons for **Reset**, **Norm.**, **Center**, **Delete**, and **Settings**. Blue lines with dots point from text annotations to specific GUI elements.

**Bind Mouse to transform**

**Operations assigned to mouse buttons (changes with modifiers)**

**When checked 3D Xforms apply to root**

**Geometry objects hierarchy**

**Reset Xform of current object**

**Root geom parent of all geometries and current object**

**Master geom for all geoms of a given molecule**

**Geoms created by Pmv cmds for that molecule**

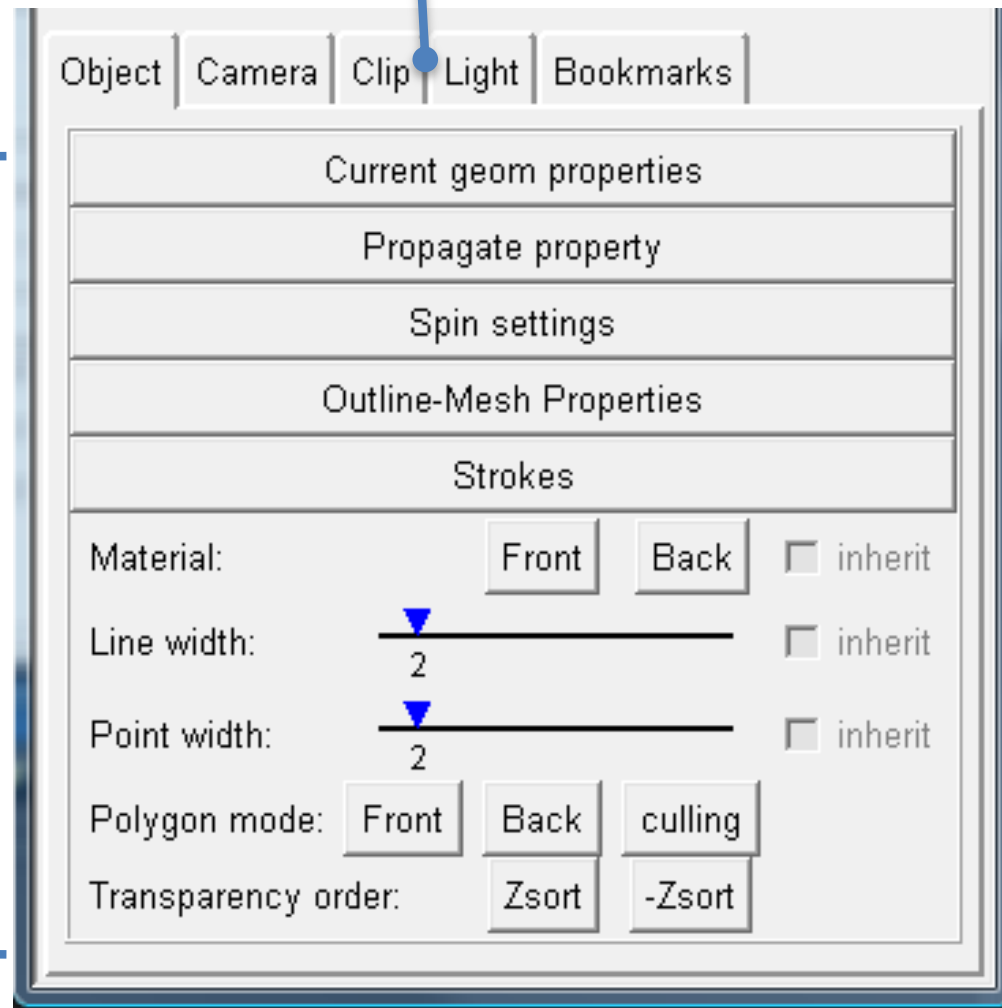
**Set rotation center to center of the scene**

**Fit the scene in the view**

# 3D Visualization: GUI overview

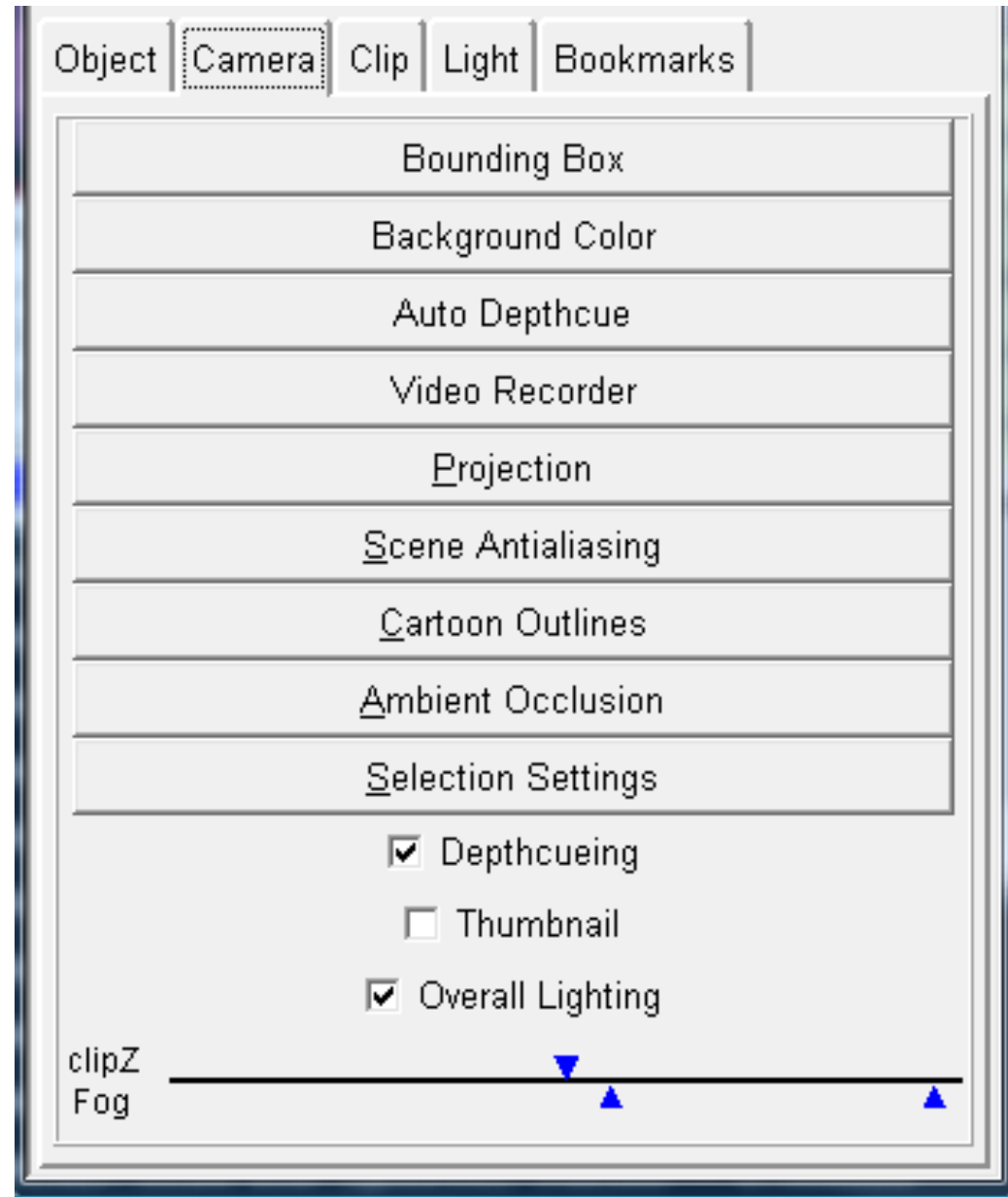
Select property panel to show

Object  
property  
panel



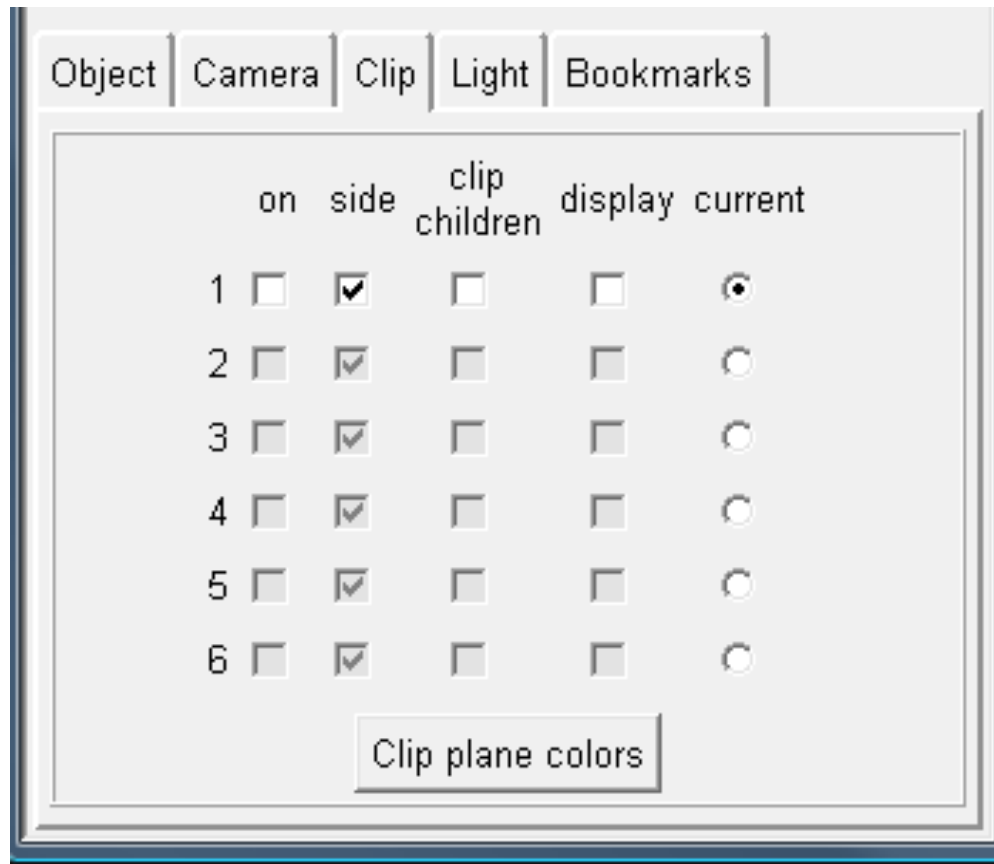
# 3D Visualization: GUI overview

**Camera  
property  
panel**





# 3D Visualization: GUI overview



**Clipping planes property panel**



**Lights property panel**