Advanced Visualization with Pmv

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Croucher ASI 2011, Hong Kong

Overview

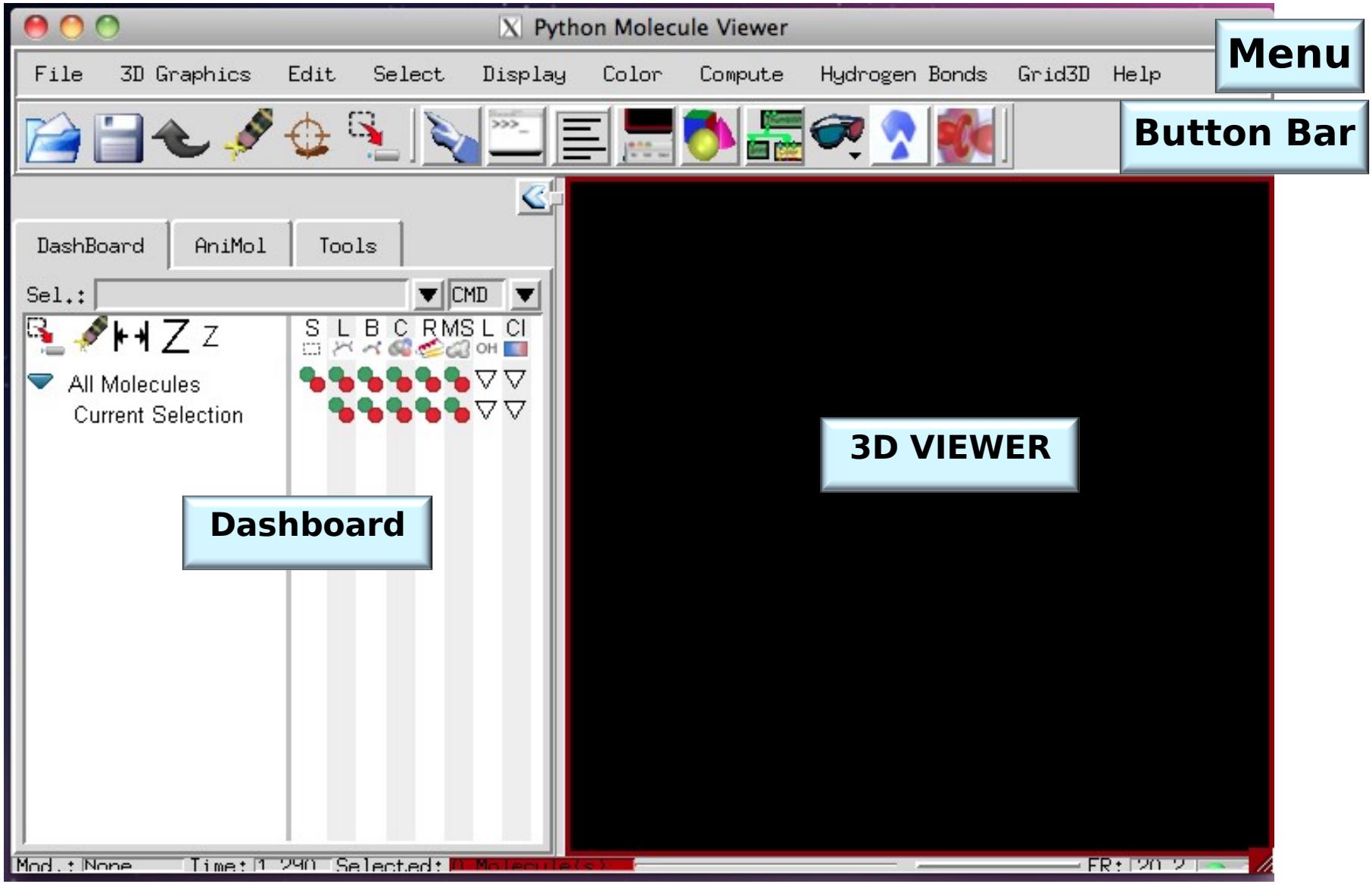
- Introduction to Pmv
- The Dashboard Panel
- Examples
  - The Tools Panel
  - (The AniMol Panel)

Obtaining Pmv

Freely available from the MGL website

http://mgltools.scripps.edu/downloads

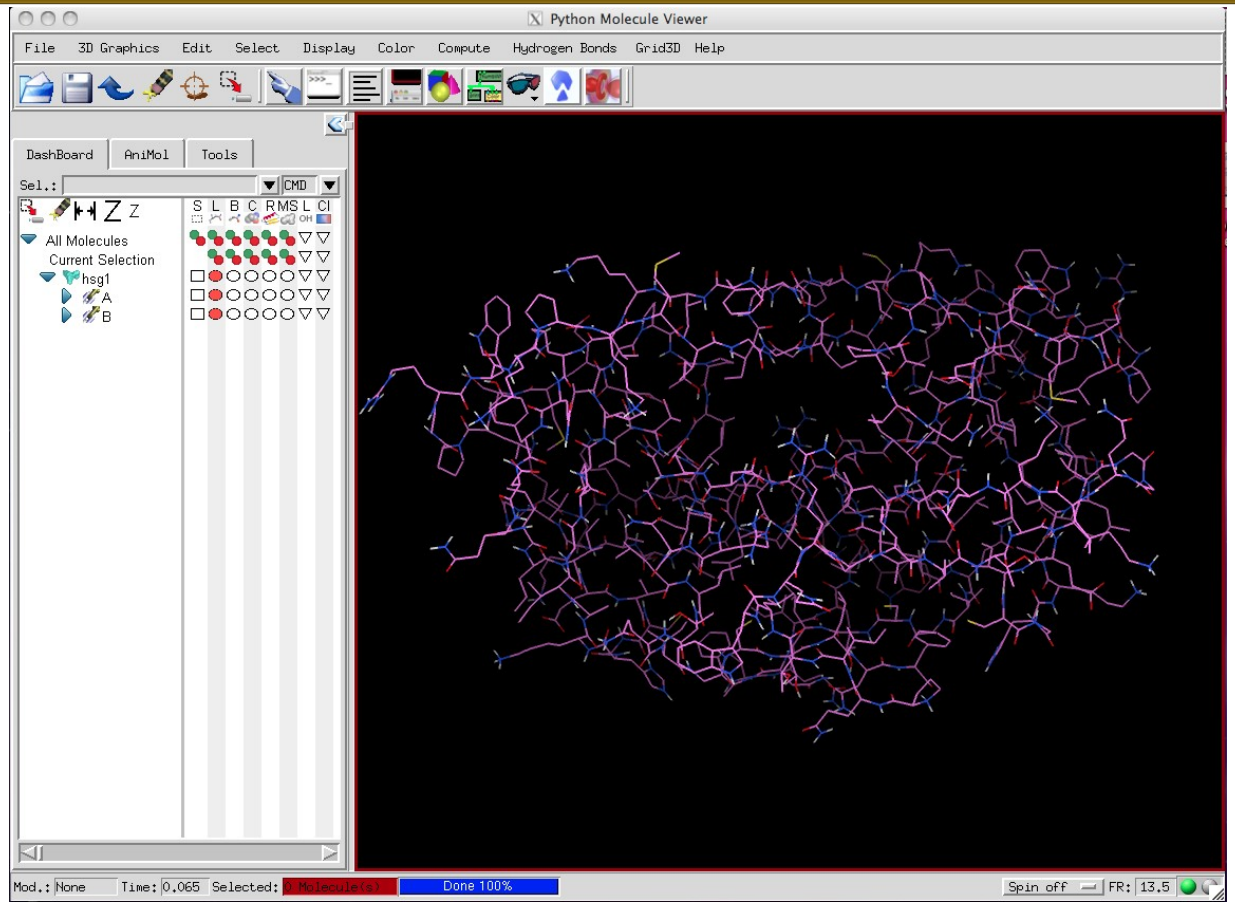
Starting Pmv



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: start Pmv

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: Pmv mouse

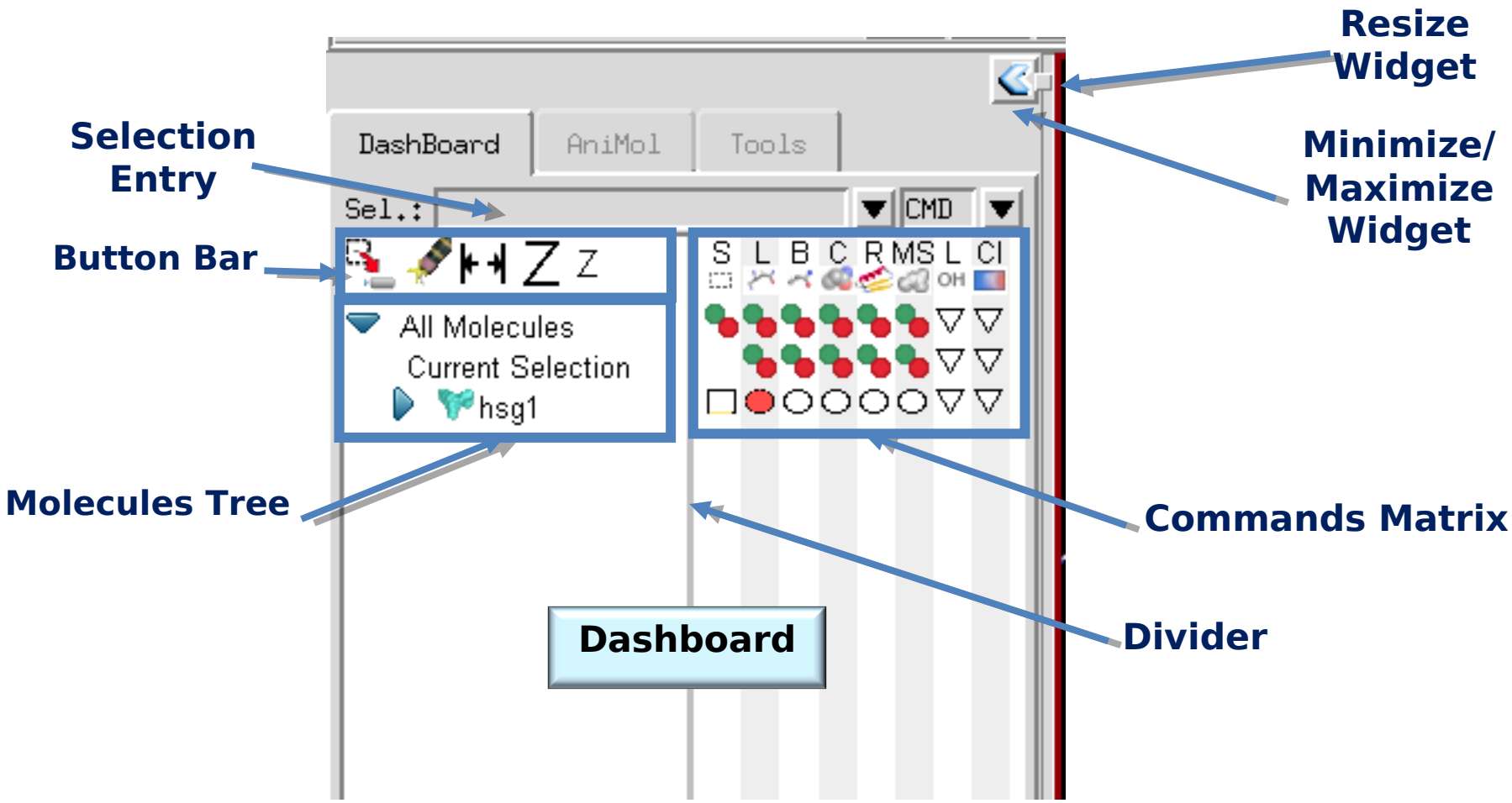
Button / Mod	Left	Middle	Right	Wheel
None	*Rotate*		*Translate left/right (X) and up/down (Y)*	*Zoom*
Shift	*Add to Selection*		*Translate in/out (Z)*	
Ctrl	*Remove from Selection*		*Center on Pixel*	

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)*

Pmv dashboard

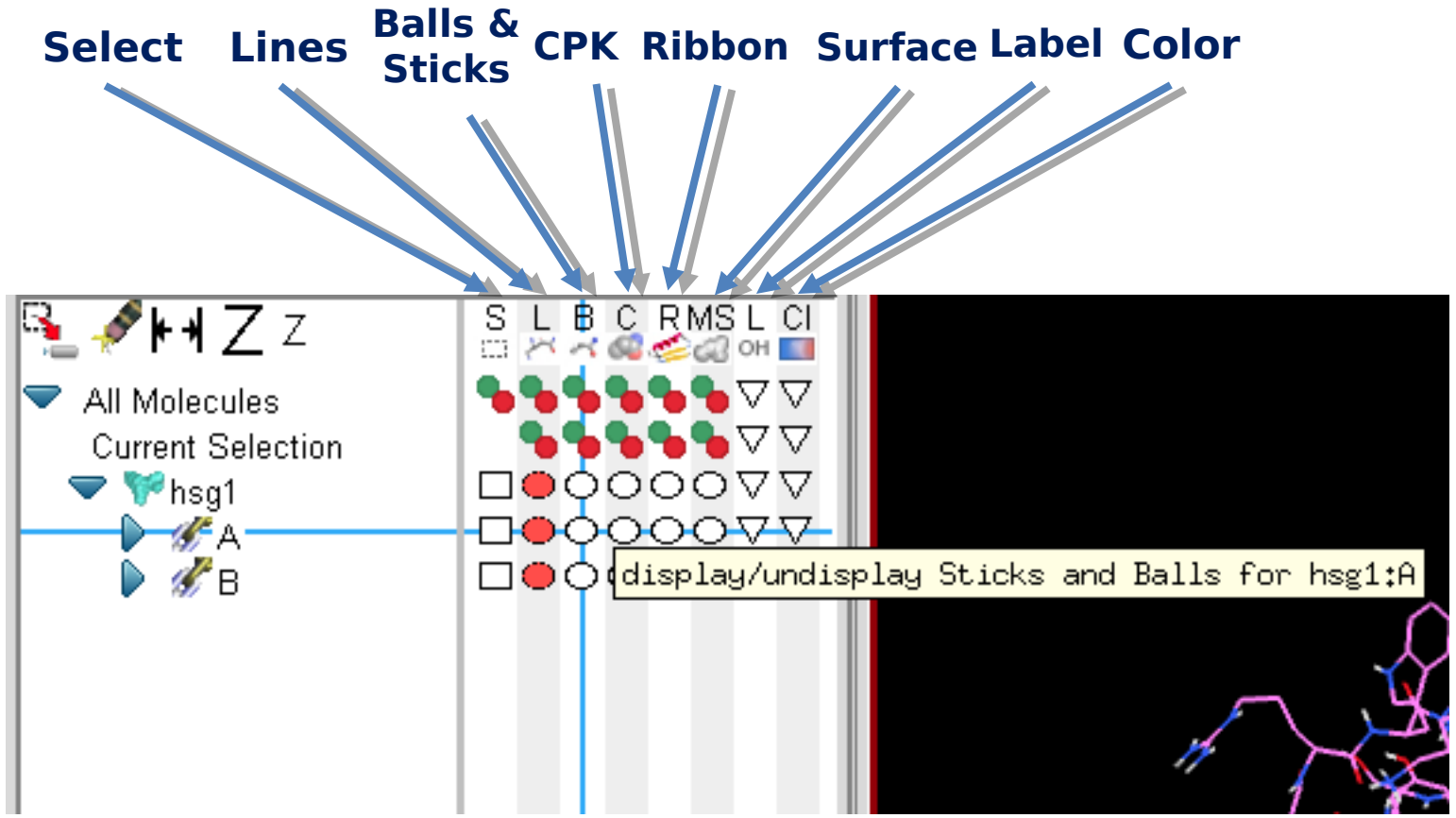


Exercise: Pmv dashboard

Task: dashboard

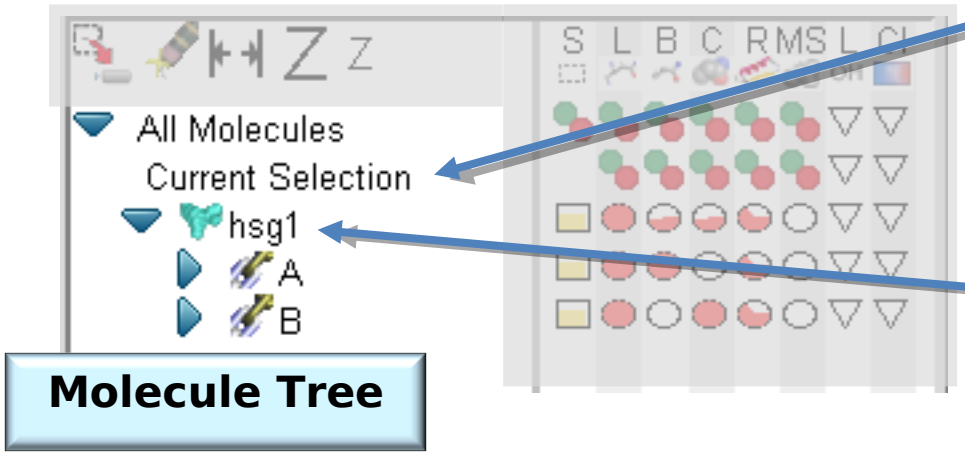
1 – hoover mouse over glyphs and read tool tips
2 – expand/collapse molecule tree
3 – make the dashboard wider
4 – move the divider right and left. Notice the labels in the molecule tree change upon mouse button release
5 – minimize dashboard
6 – restore dashboard
7 – find the button that sets the dashboard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

Dashboard Command Matrix



Notes:
- Tool tips on all command buttons

Dashboard Molecule Tree

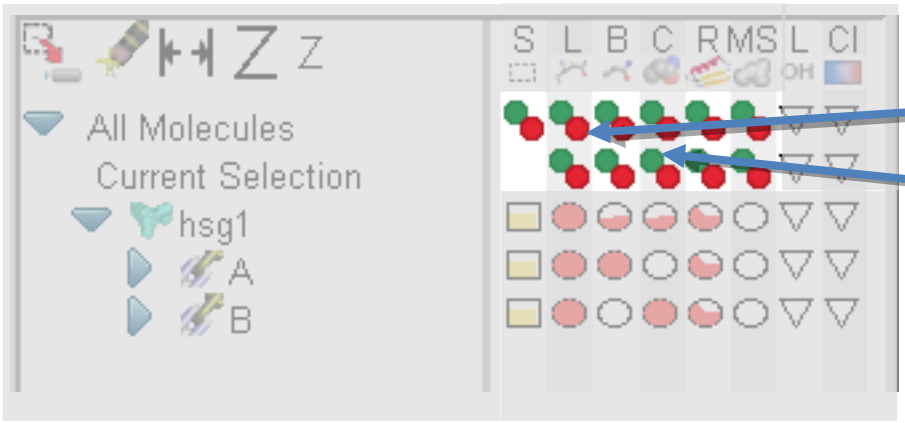


sets: cannot be expanded
represent molecular fragments
From the molecules loaded in Pmv

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

Dashboard Command Buttons

On/Off Command Buttons



Left click to:

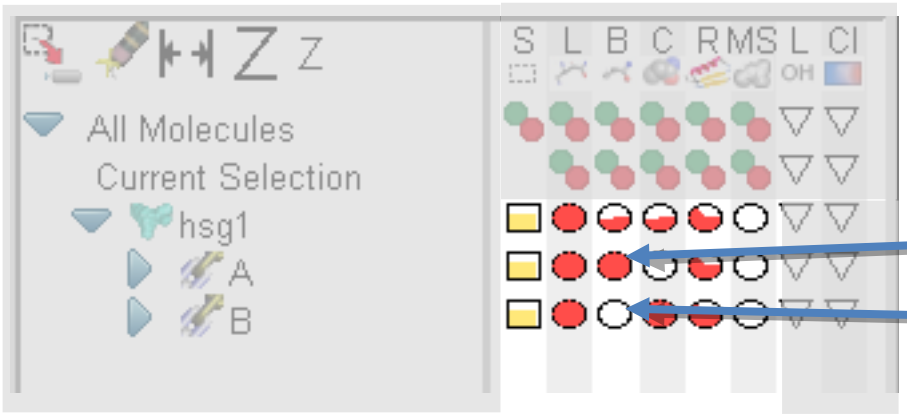
Un-display lines for all molecules

Display CPK for the current selection

Notes:
- **No state**
- **Left mouse click to activate button**
- **Right mouse click on green button 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

Toggle Command 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 Balls and Sticks and 50% as CPK)
- Cycle from “partial” to “full”, to “empty”, to “full” etc.
- Used for molecules (i.e. hsg1)

Exercise: Display Lines

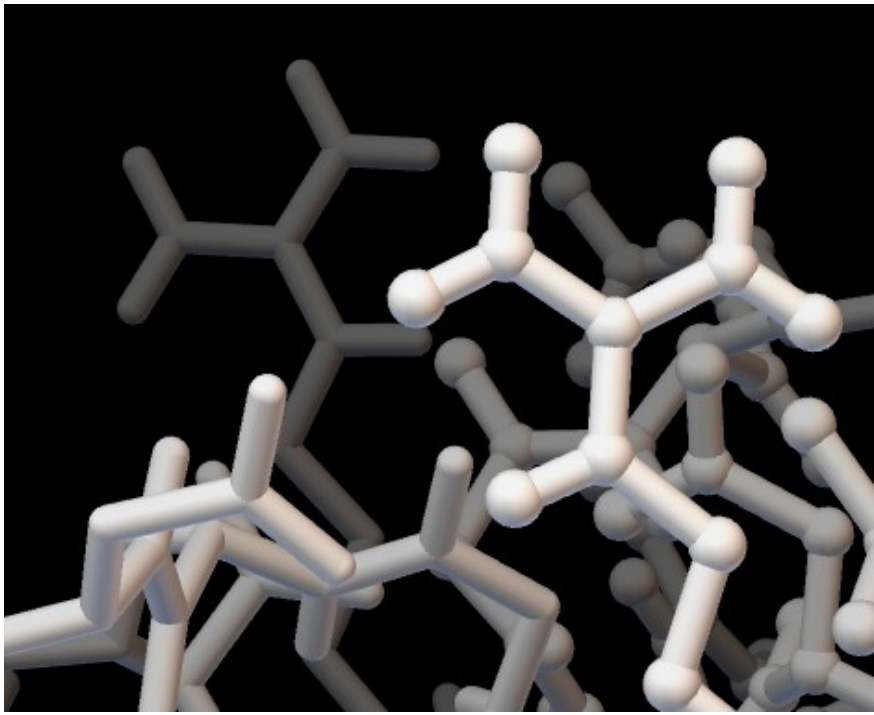
Task: display lines

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: display balls & sticks

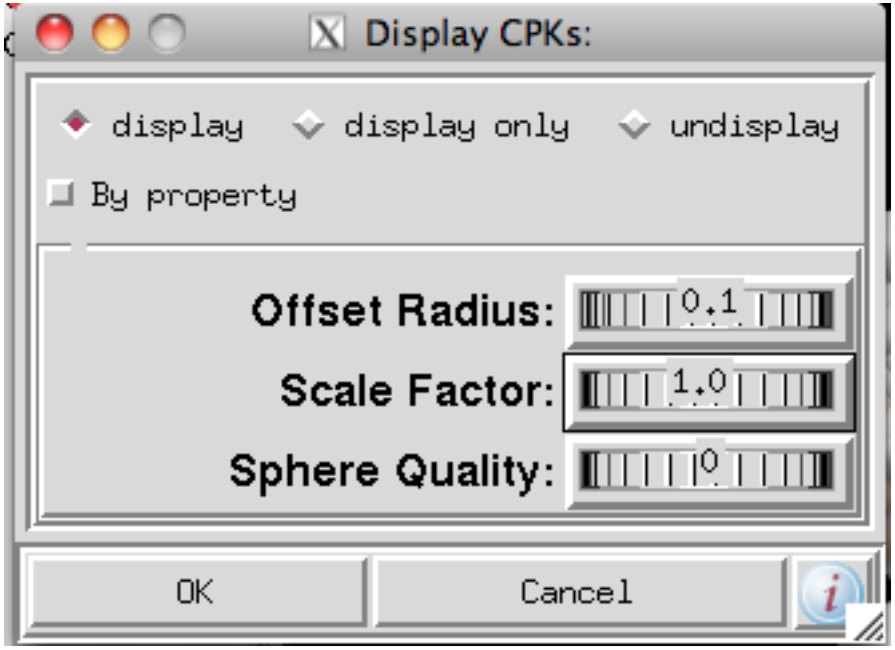
1 – display B&S for chain A
2 – right click on B&S for chain B and select “sticks and balls” instead of “licorice”



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

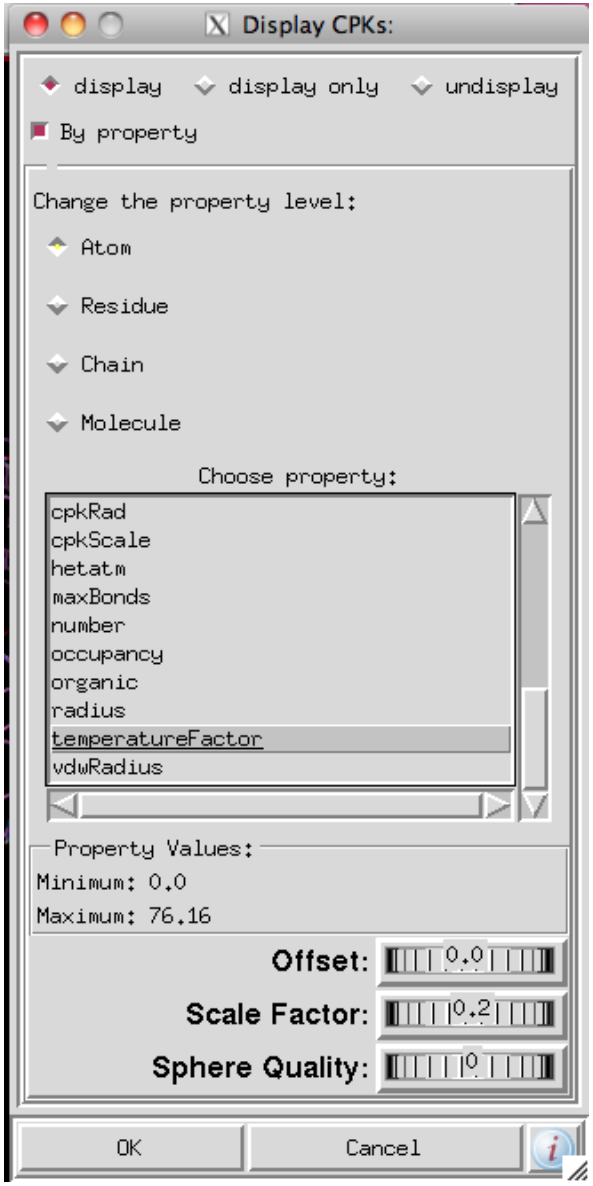


Radius = offset + atom radius*scale

Exercise: Display CPK

Task: display CPK

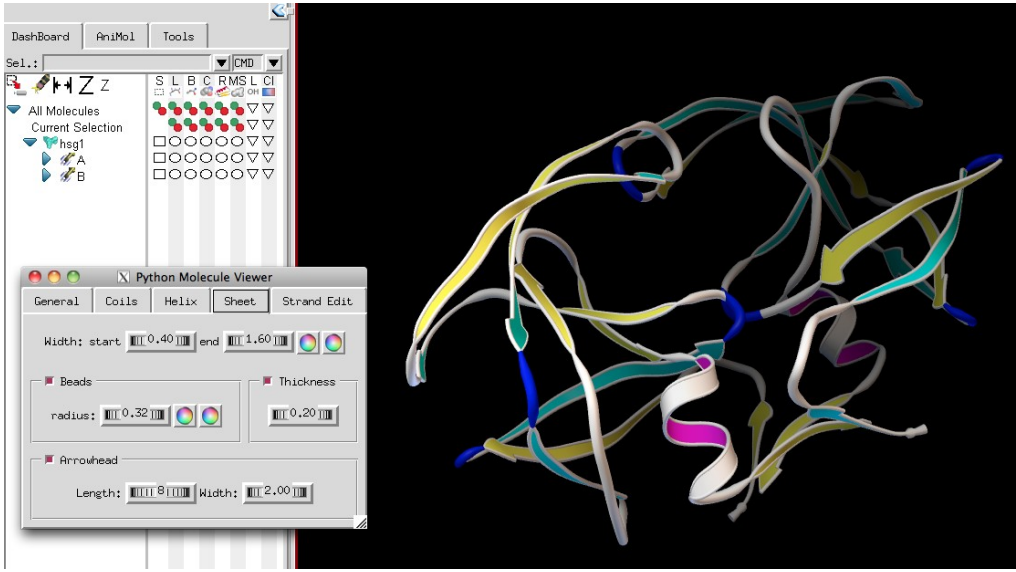
1 – click on “By Property” check button
2 – un display all CPK representations



Exercise: Display Ribbon

Task: display Ribbons

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



Task: display 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 – right click on surface for hsg1 and set probe radius to 3.0
4 – un-display surface for hsg1
5 – display surface for chain A
6 – display lines for hsg1

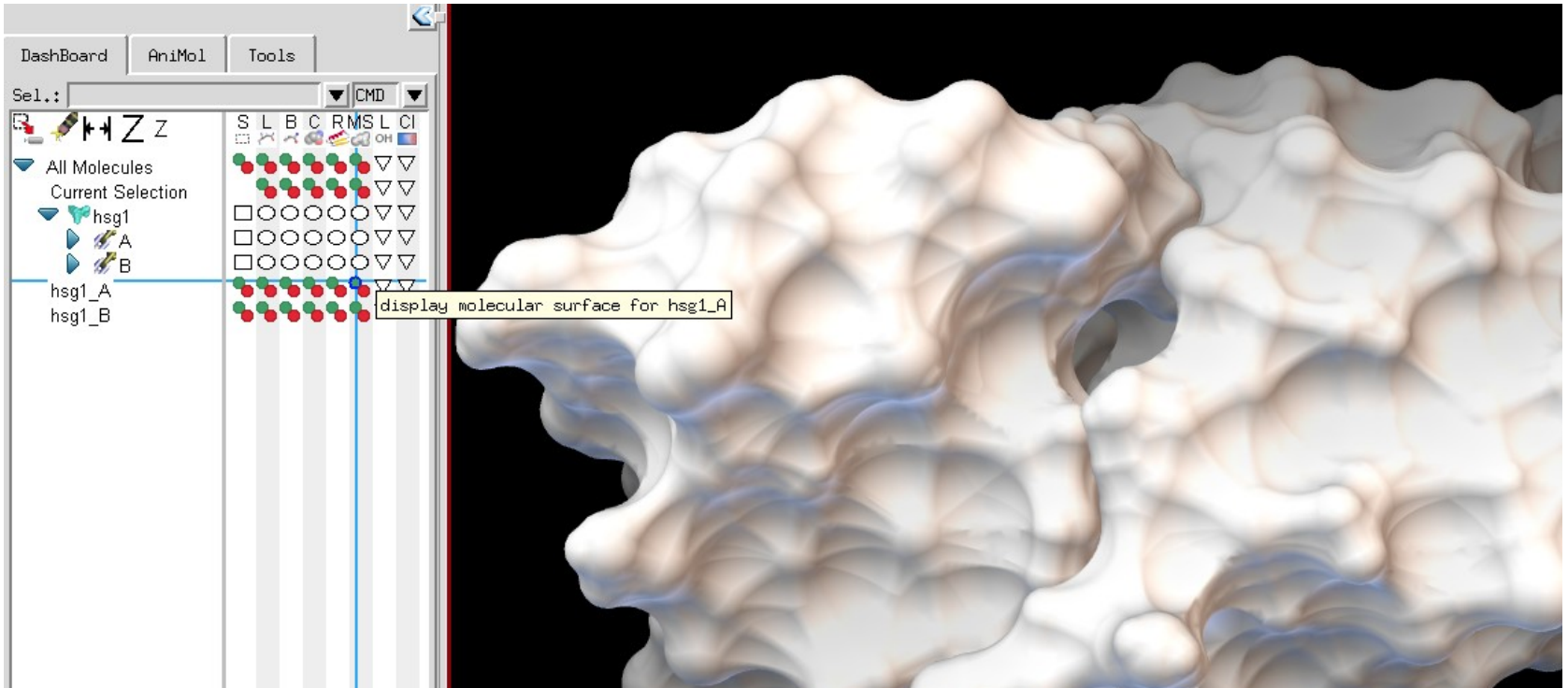
NOTE the surface is open

Exercise: Display Surfaces

Task: display closed surfaces

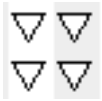
To close the surface:
1 – right click on the “hsg1” label in the molecule tree
2 – select “Make sets for chains”
3 – compute surface for the 2 created sets

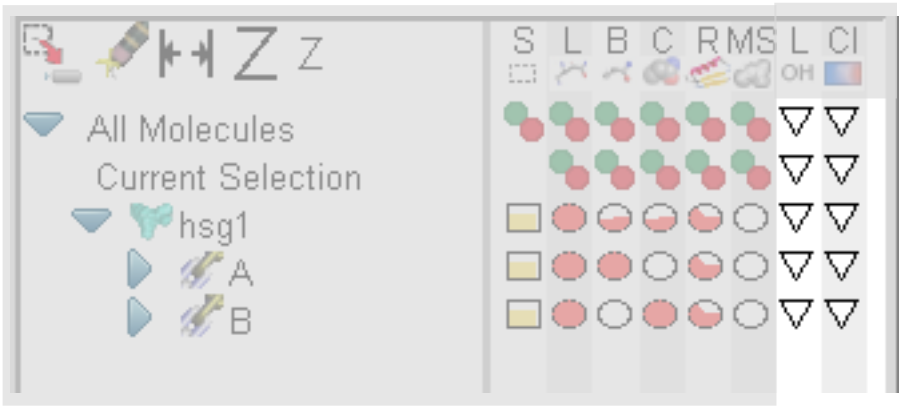
Hide all surfaces



Dashboard Command Buttons

Menu Buttons



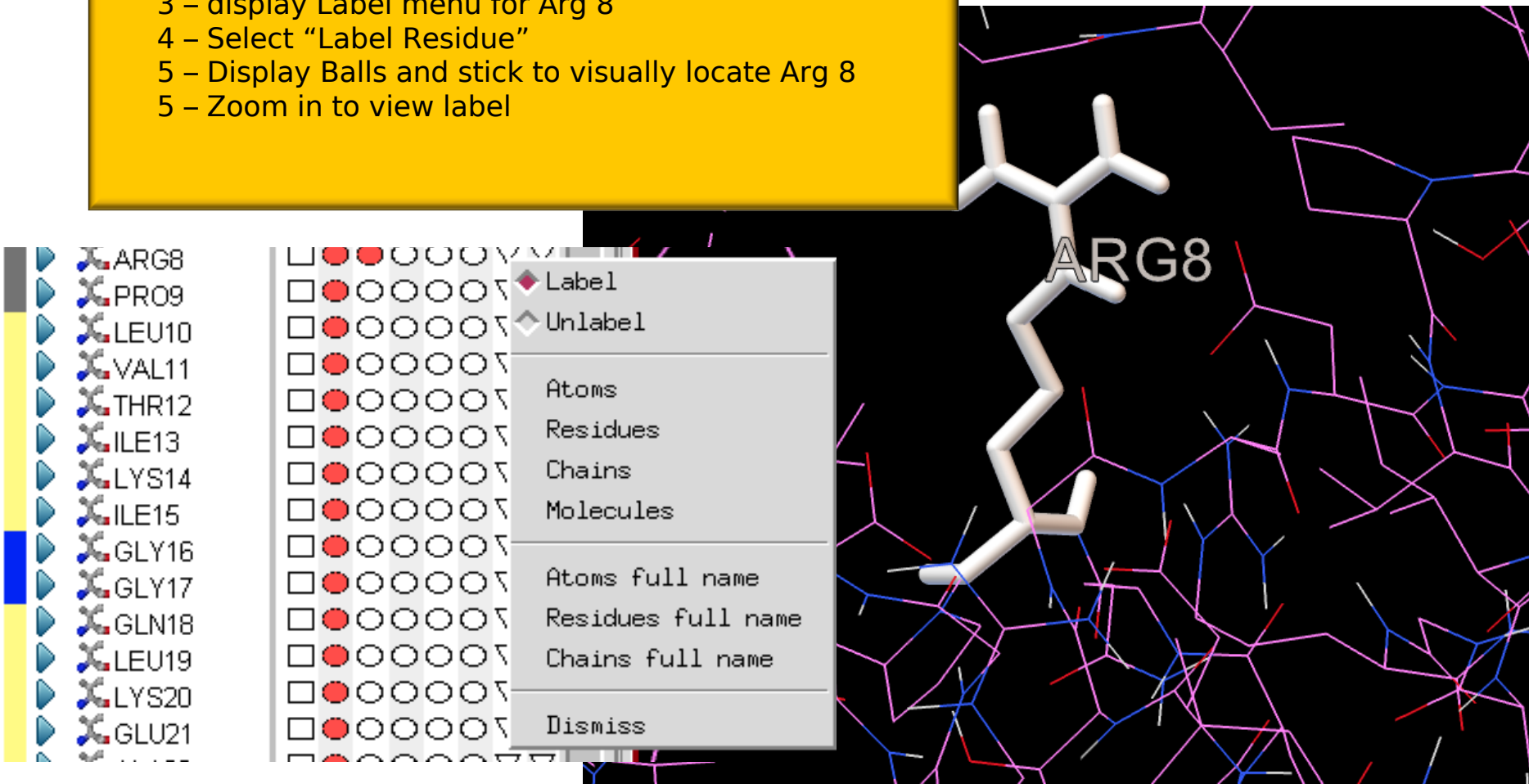


- **Left mouse click to display menu**

Exercise: Label Residue

Task: use label menu on Arg8 in chain A

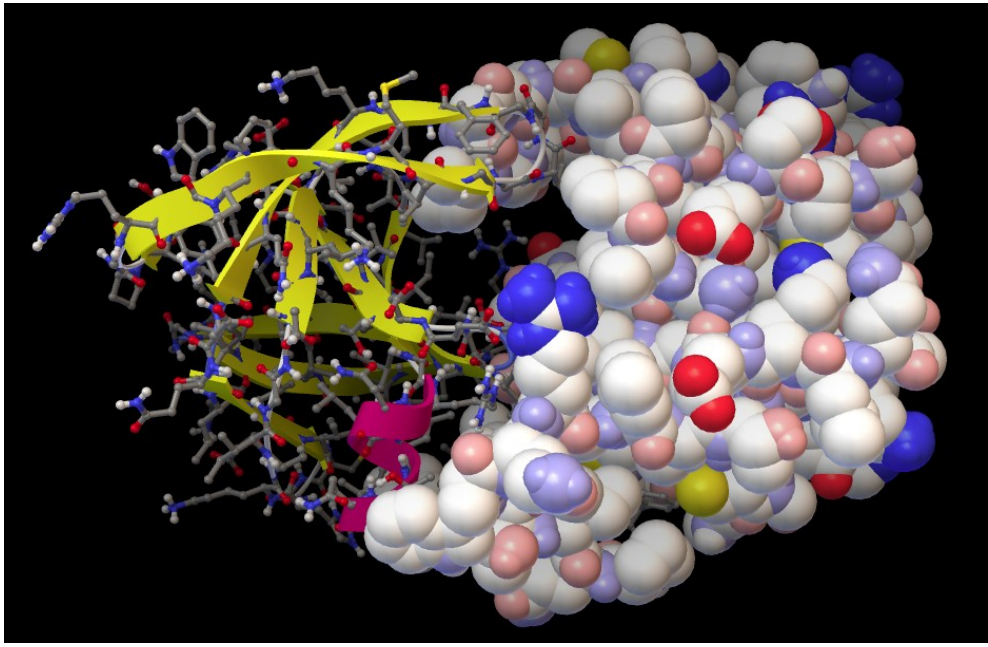
1 – un-display all representations except for lines
2 – expand the Molecule tree to find Arg8 in chain A
3 – display Label menu for Arg 8
4 – Select “Label Residue”
5 – Display Balls and stick to visually locate Arg 8
5 – Zoom in to view label

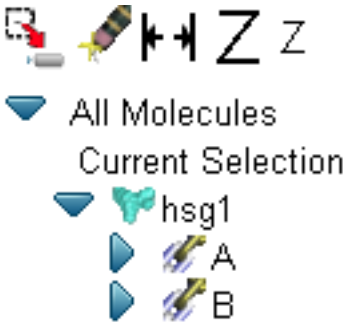


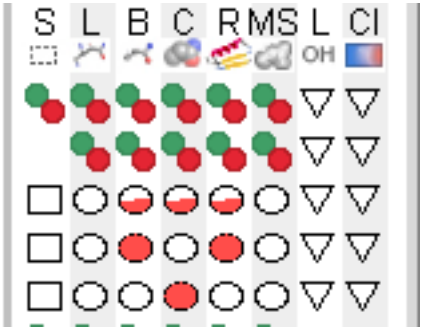
Exercise: Color Menu

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 sec. structure



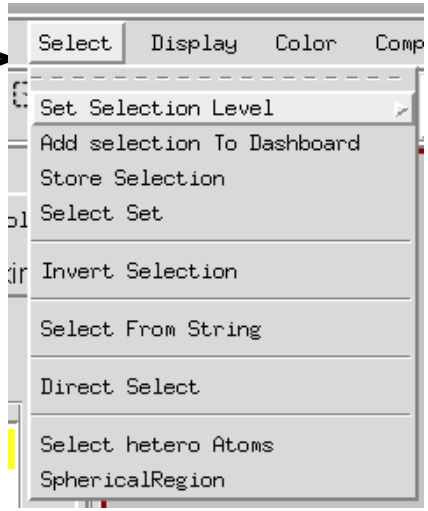


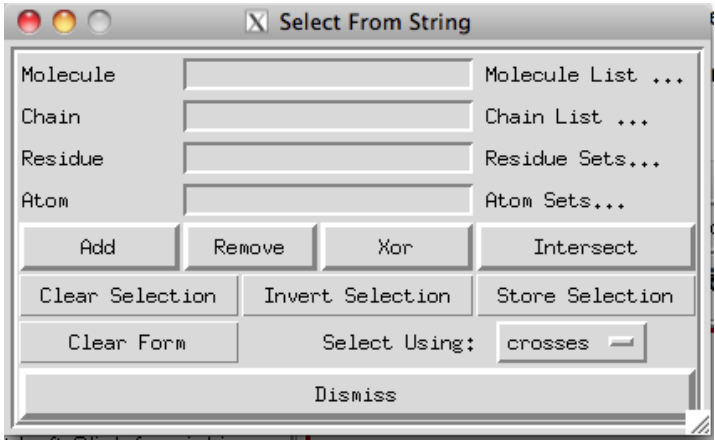


Note: Coloring schemes are disabled until a geometry is selected

Pmv selections

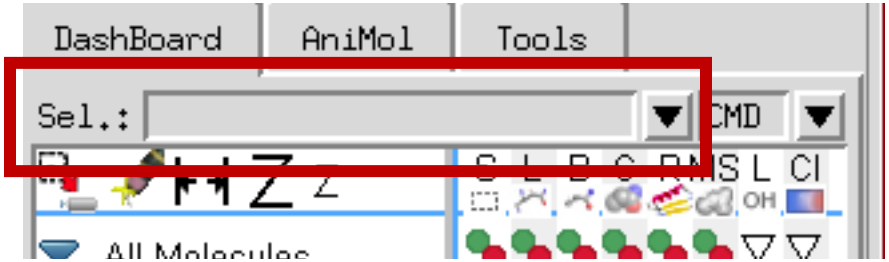
- Pmv menu commands operate on selection
- Shift left click and drag in 3D Viewer
- Powerful selection mechanisms
  - Menu Select ->





Pmv selections

- Powerful selection mechanism
  - Dashboard string selector



  - 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

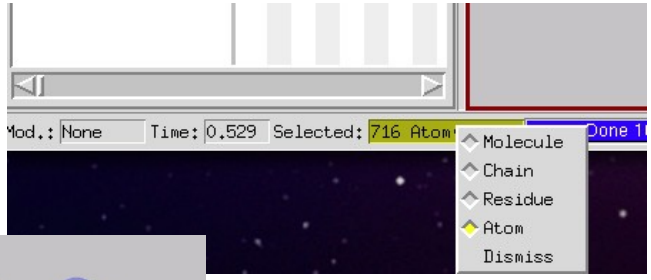
“Mol1, Mol2:::C,N,CA,O” selects backbone heavy atoms in molecules Mol1 and Mol2

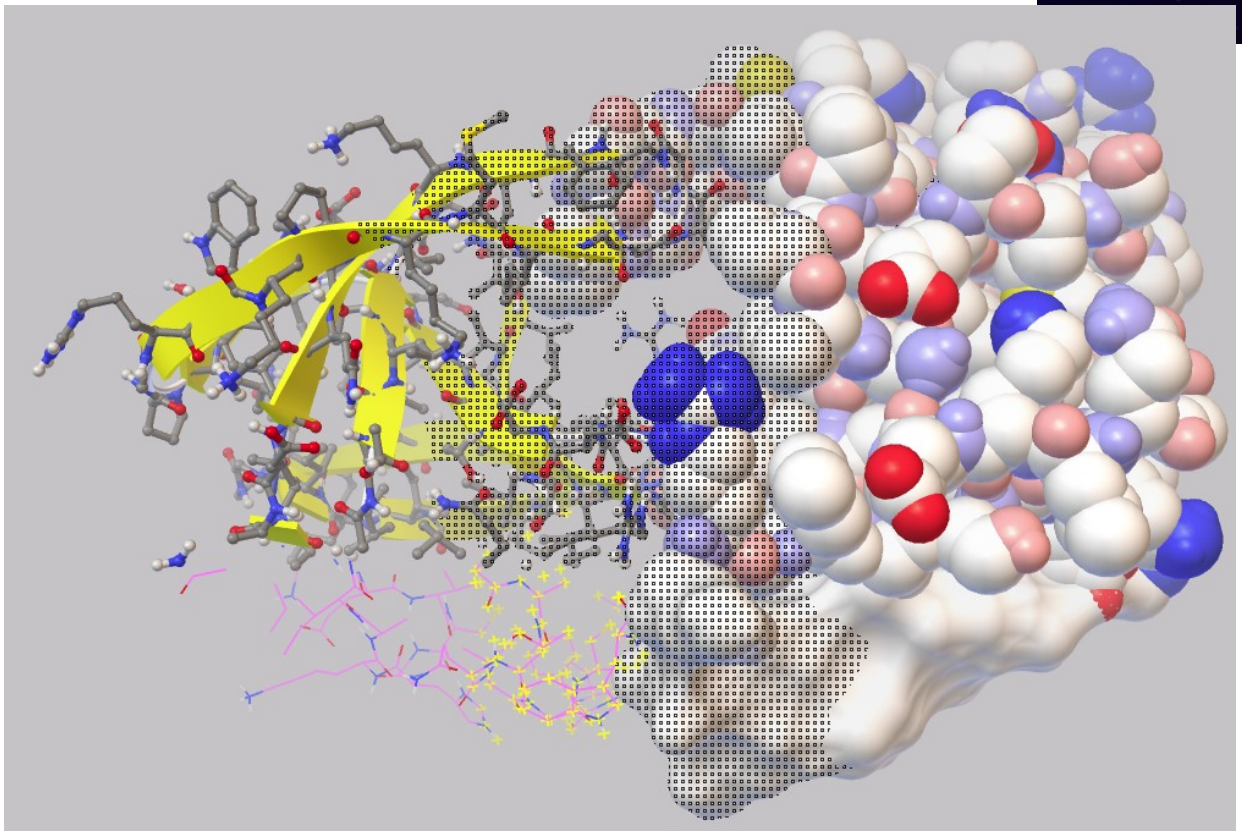
“::ALA35-THR45” selects a range of residues

http://mgldev.scripps.edu/docs/mgltools/1.5.6/Selection

Pmv selections

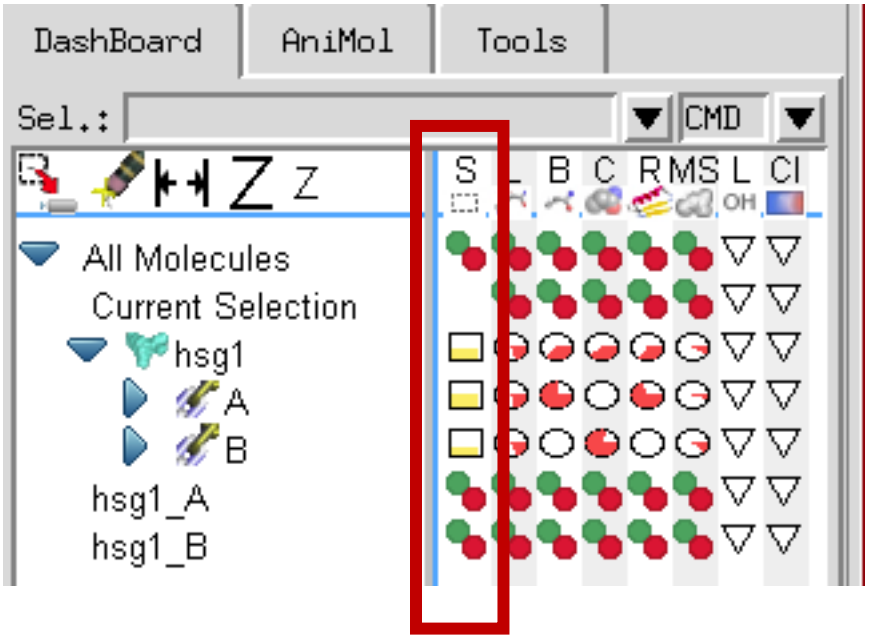
- Selection levels: molecule, chain, residue, atom
- Visual feed back of selected atoms on all representations





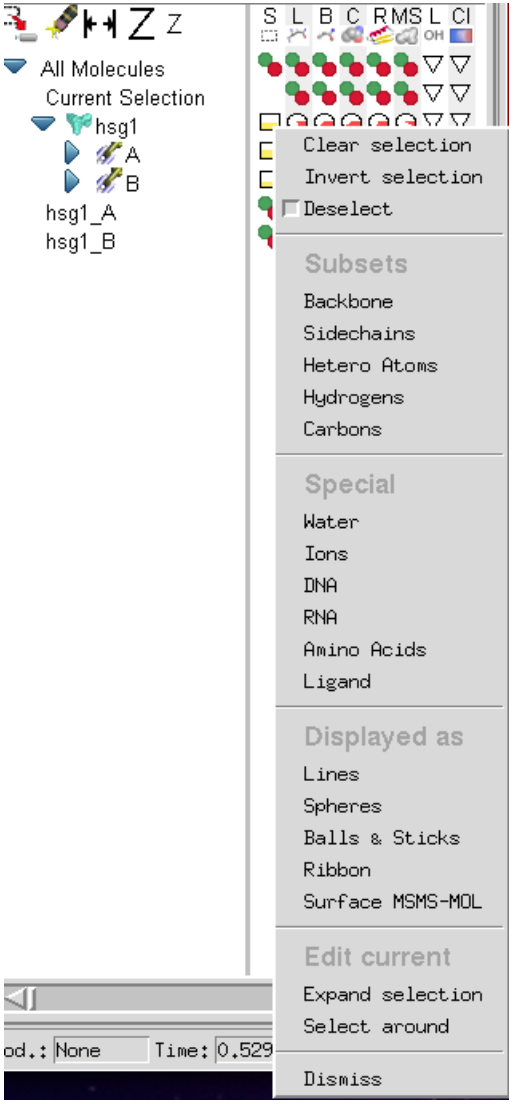
Pmv selections

- Powerful selection mechanism
  - Dashboard select column



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



Exercise: selections

Task: Apply different coloring schemes to various representations

1 – load indinavir.pdb
2 – select indinavir
3 – select atoms in hsg1 withing 4A of indinavir atoms
4 – set selection level to residue
4 – display B&S for selected side chains

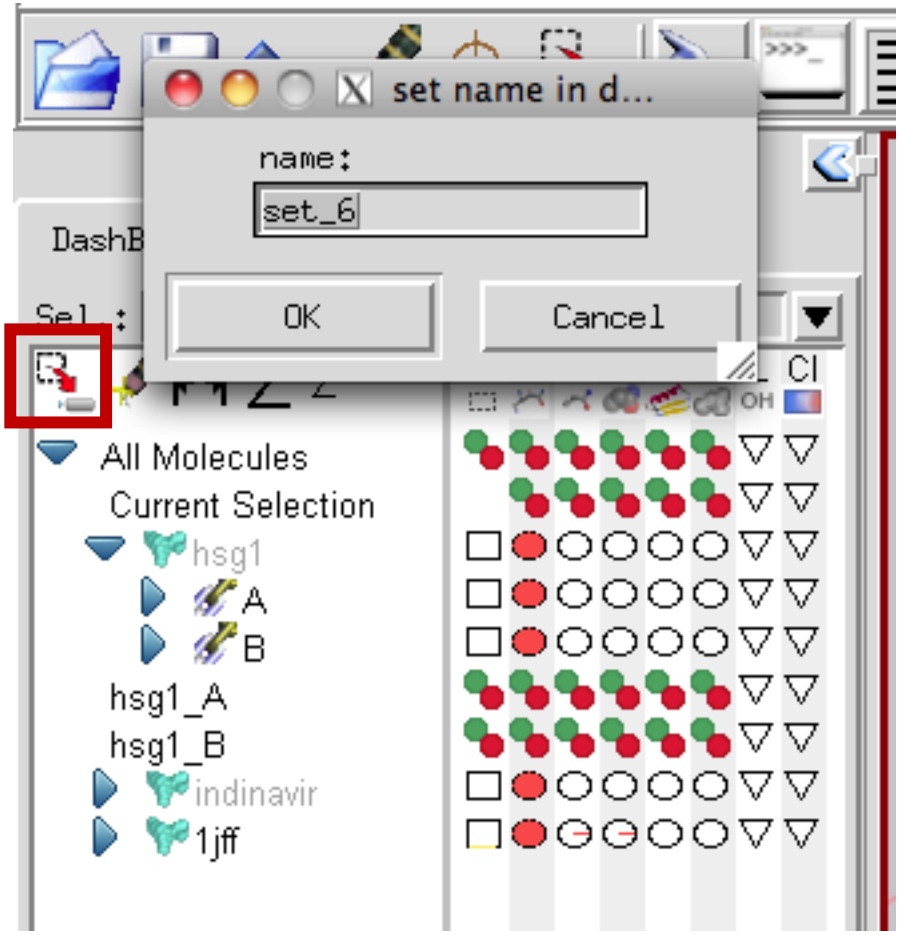
Exercise: selections

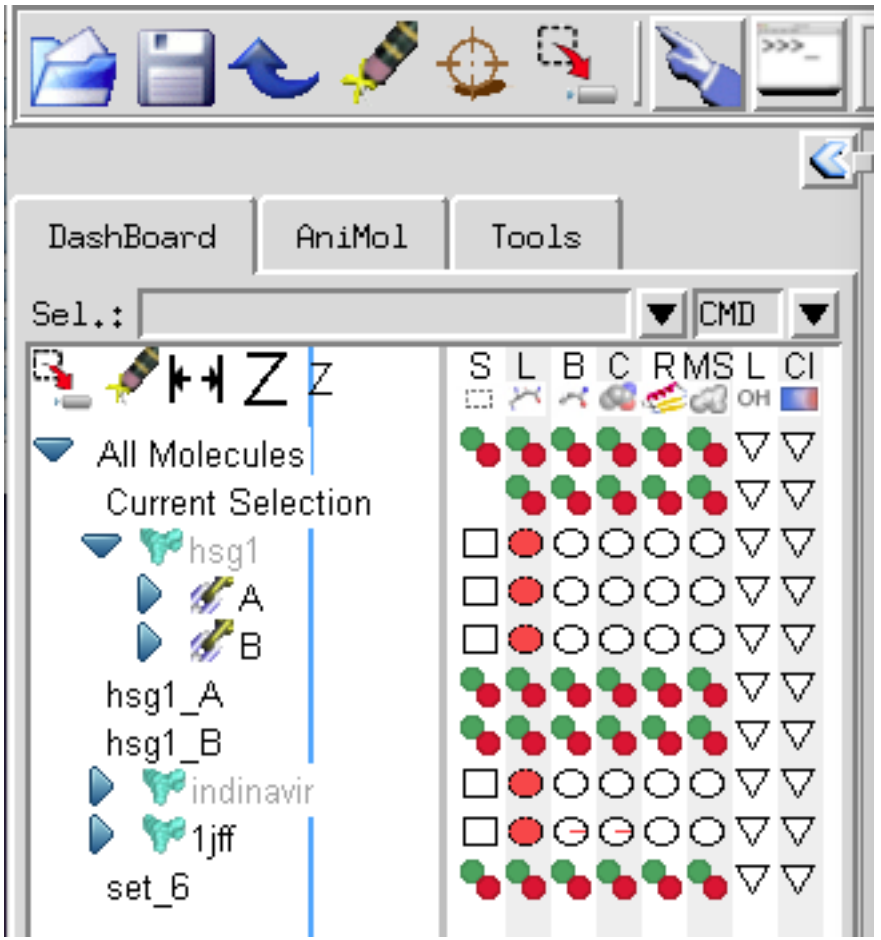
Task: Apply different coloring schemes to various representations

1 – double click on hsg1 name to hide molecule
(or right click on the name and select “hide” in menu)
2 – hide inidinavir
3 – fetch 1jff.pdb from web
4 – select ligands
5 – display B&S for ligands
6 – color ligands B&S by atom type
7 – display CPK for ions and color by atom type

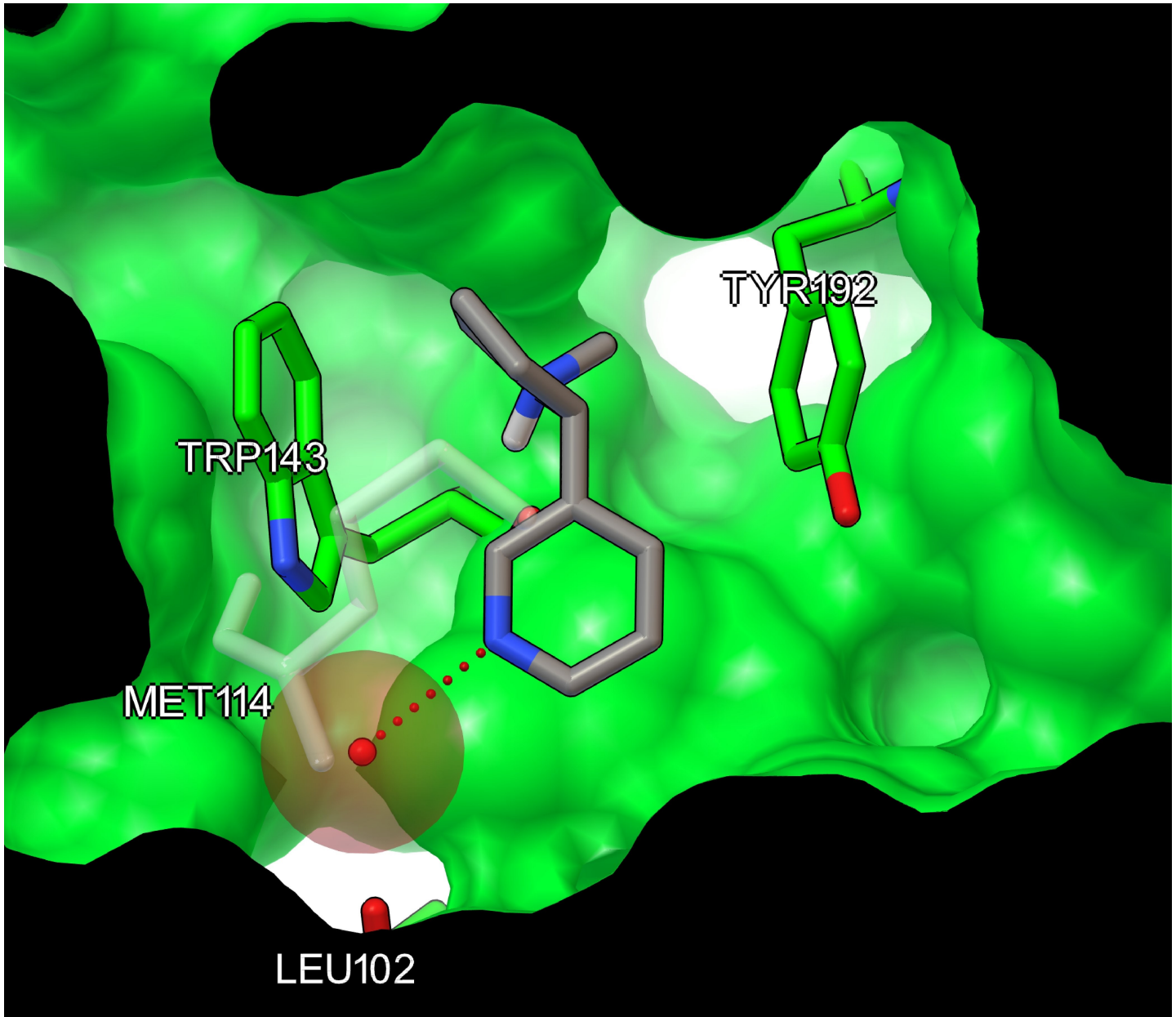
Dashboard User Sets

- Shortcut for operating on selections





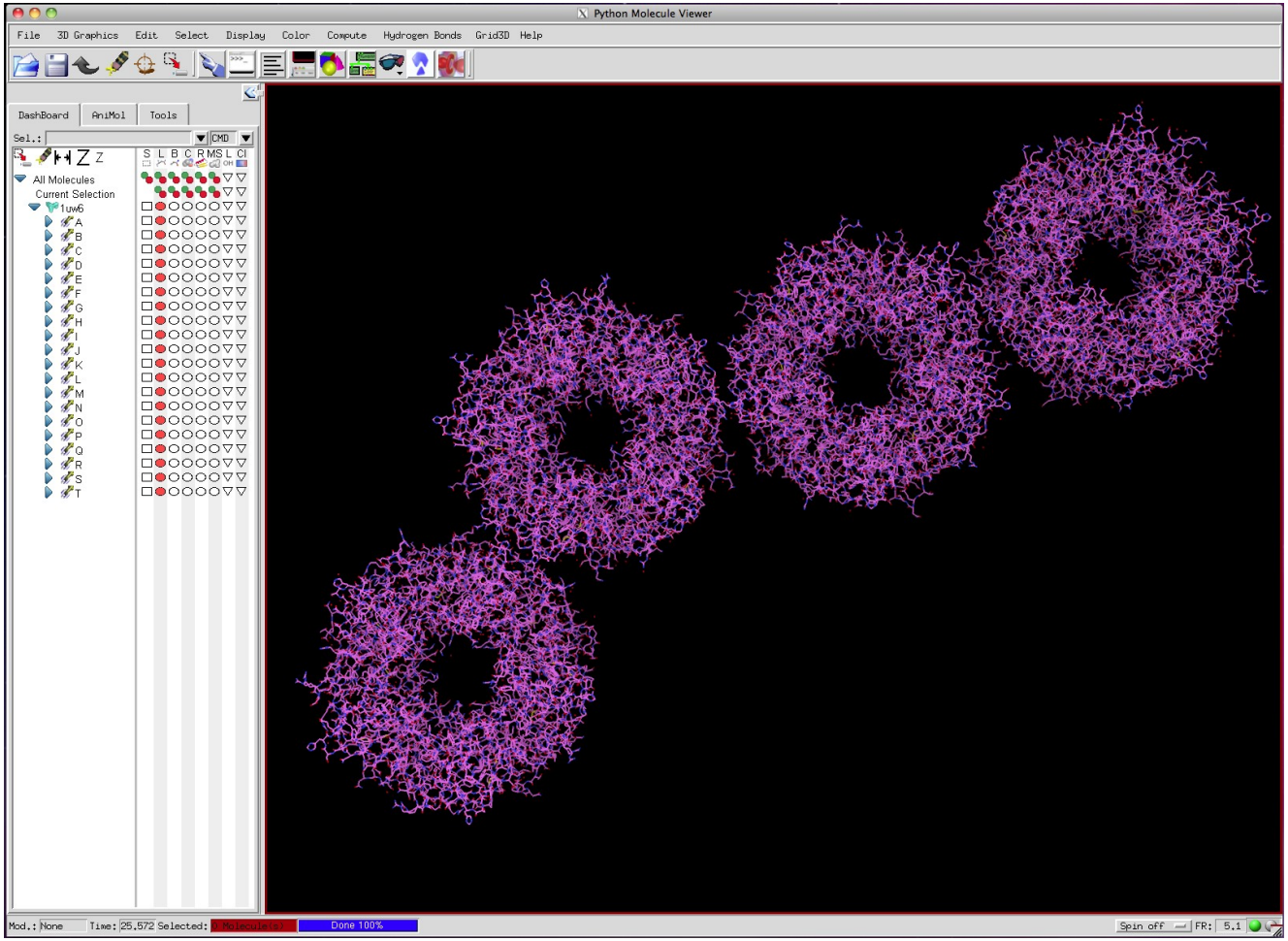
Example: 1uw6



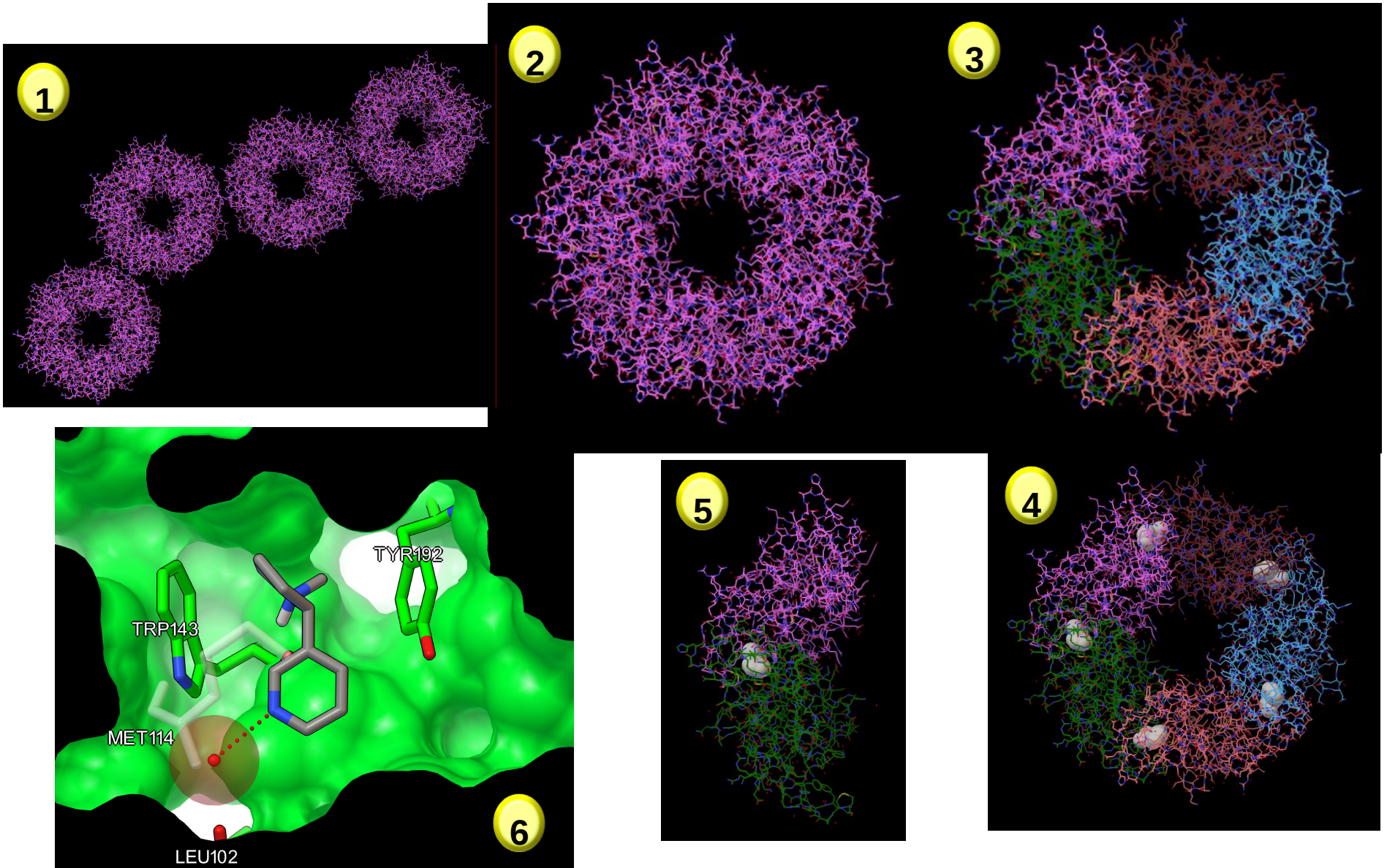
Exercise: selections

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

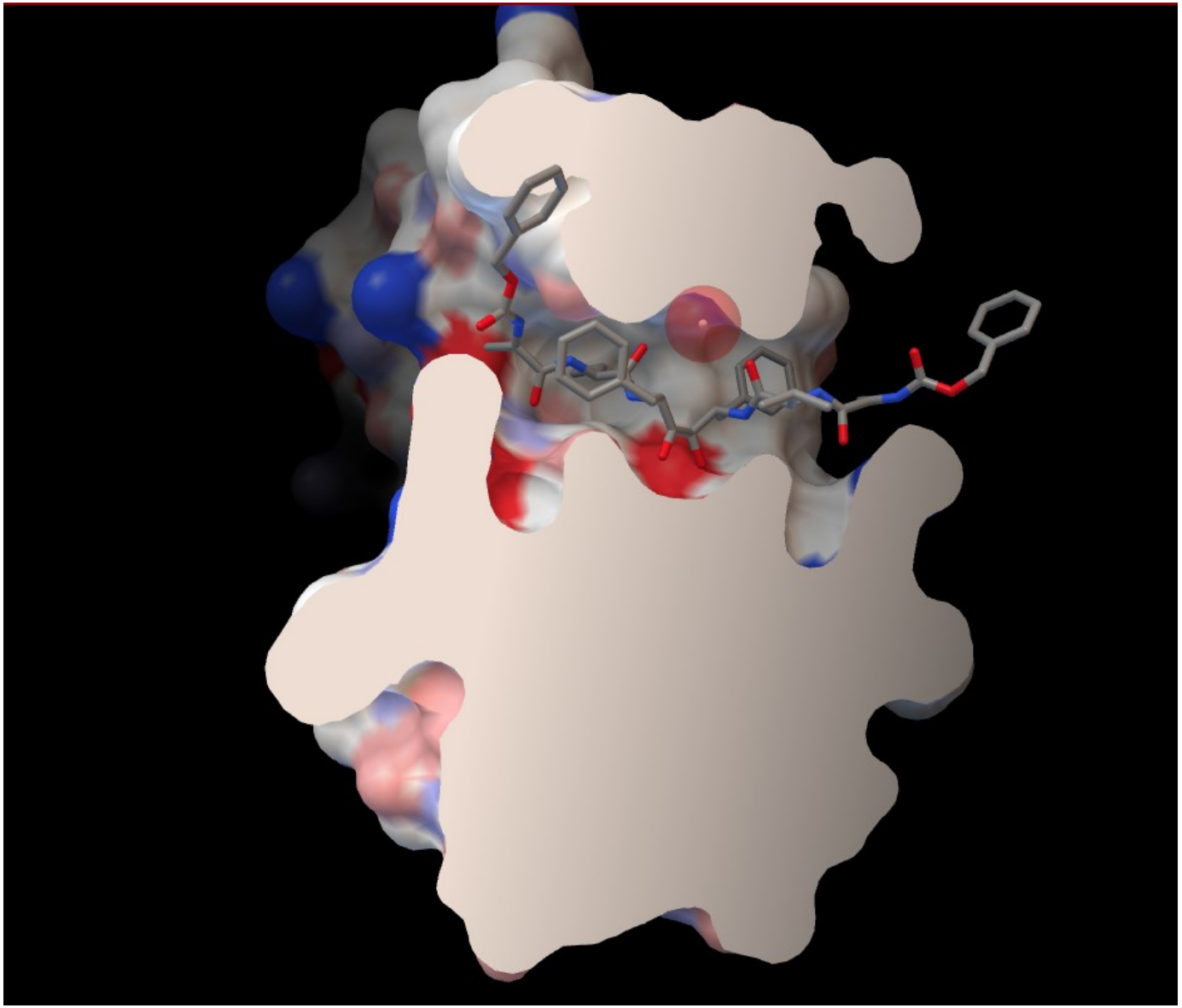
7 – select “binding with water”
8 – de-select “binding” set
9 – create “water” set

Exercise: selections

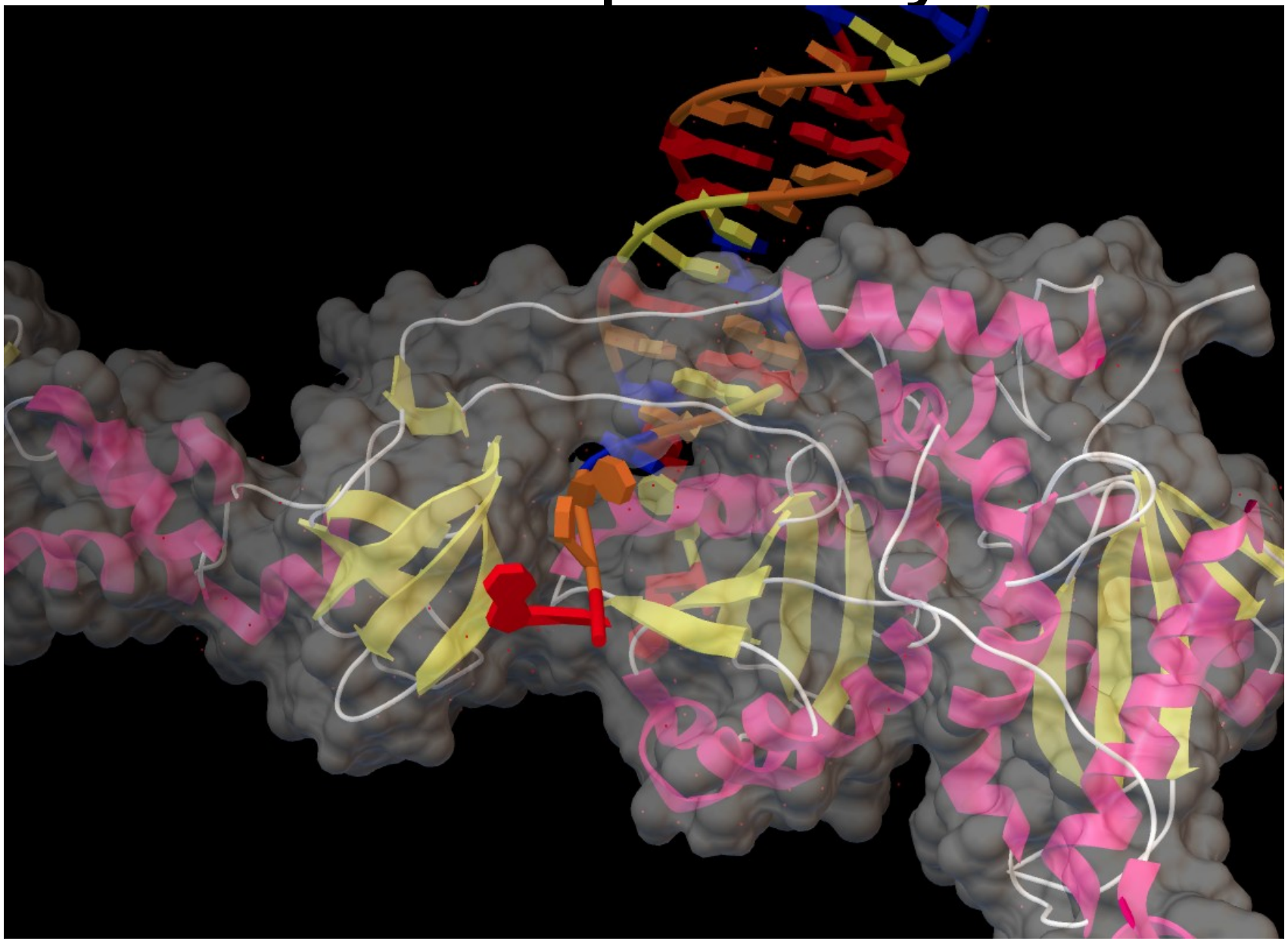
Task: compute surface

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



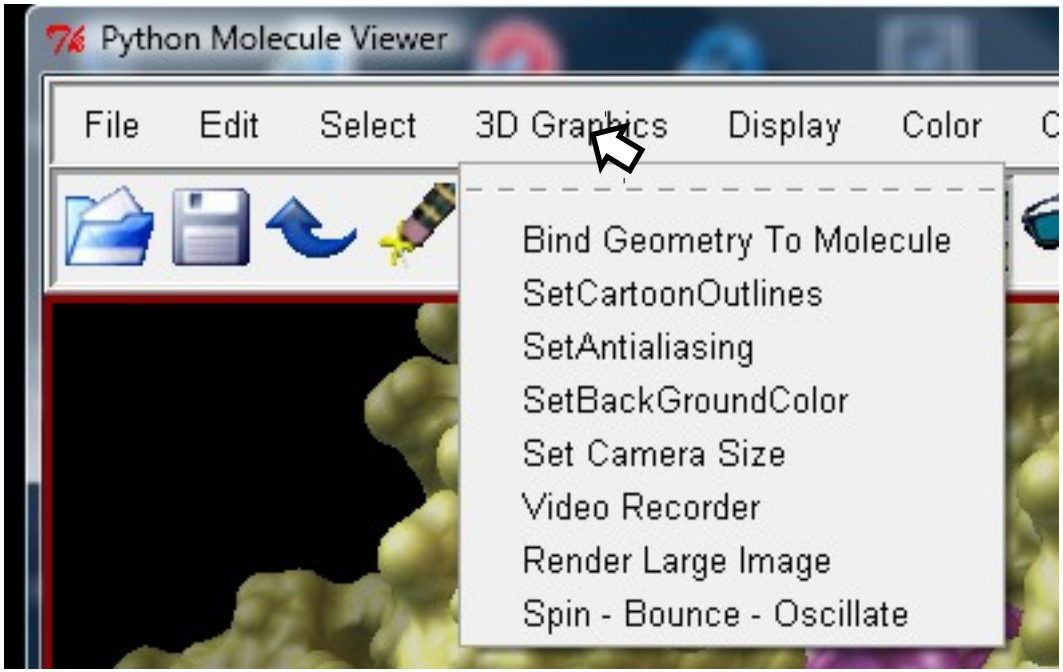
Example: 3oya



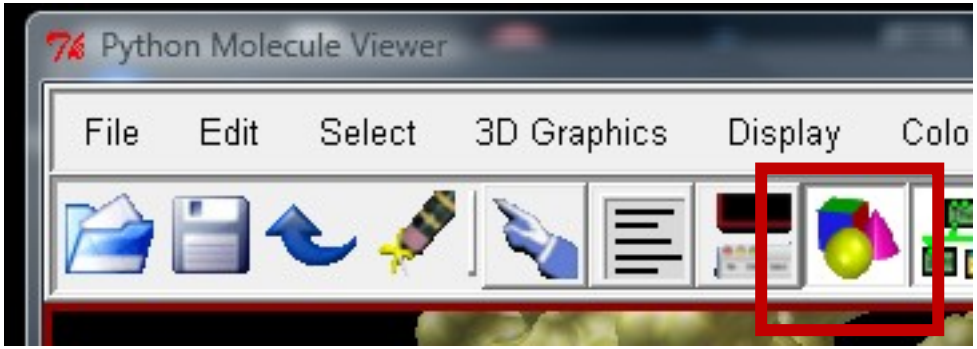
Feedback

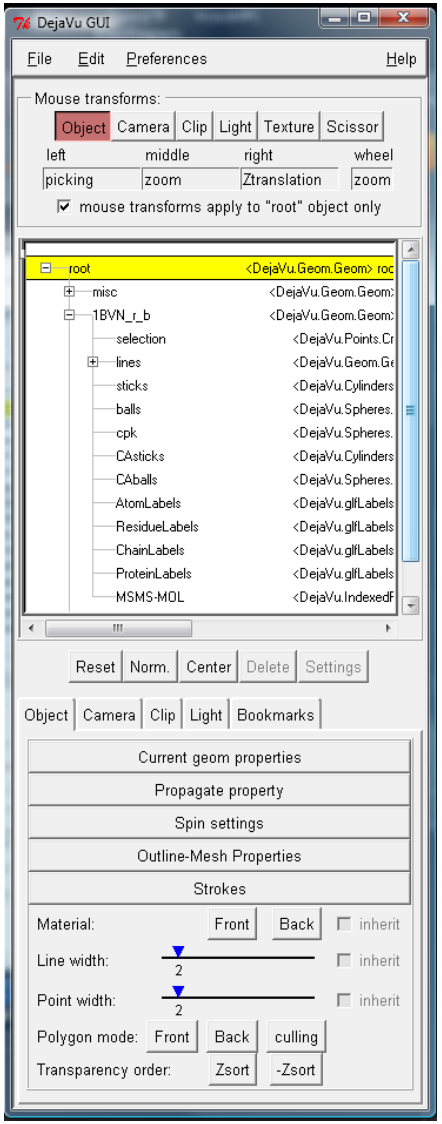
email: forli@scripps.edu

3D Visualization

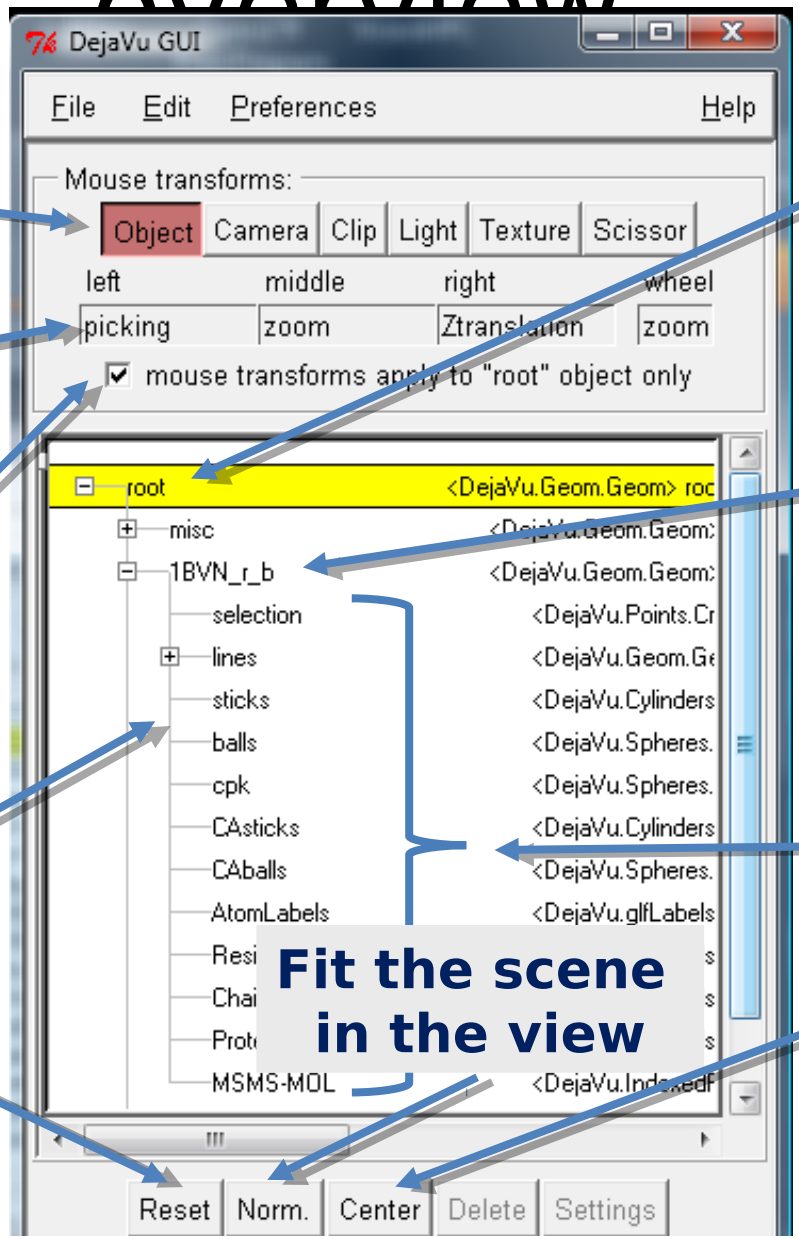


3D Visualization





3D Visualization: GUI overview



Bind Mouse to transform

Operations assigned to mouse buttons (changes with modifiers)

When checked 3D transformations apply to root

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

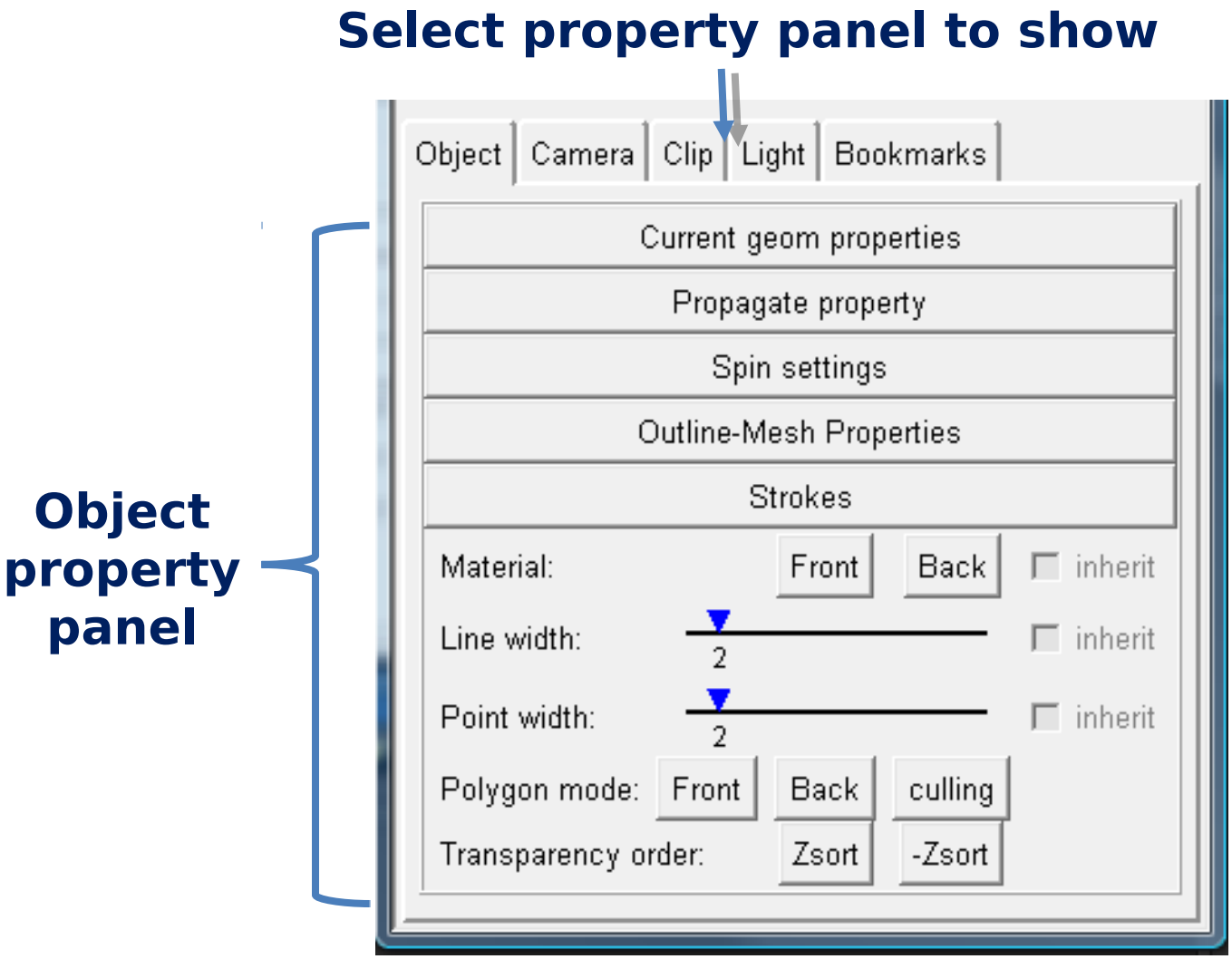
Geometry objects hierarchy

Reset tramsformation of current object

Fit the scene in the view

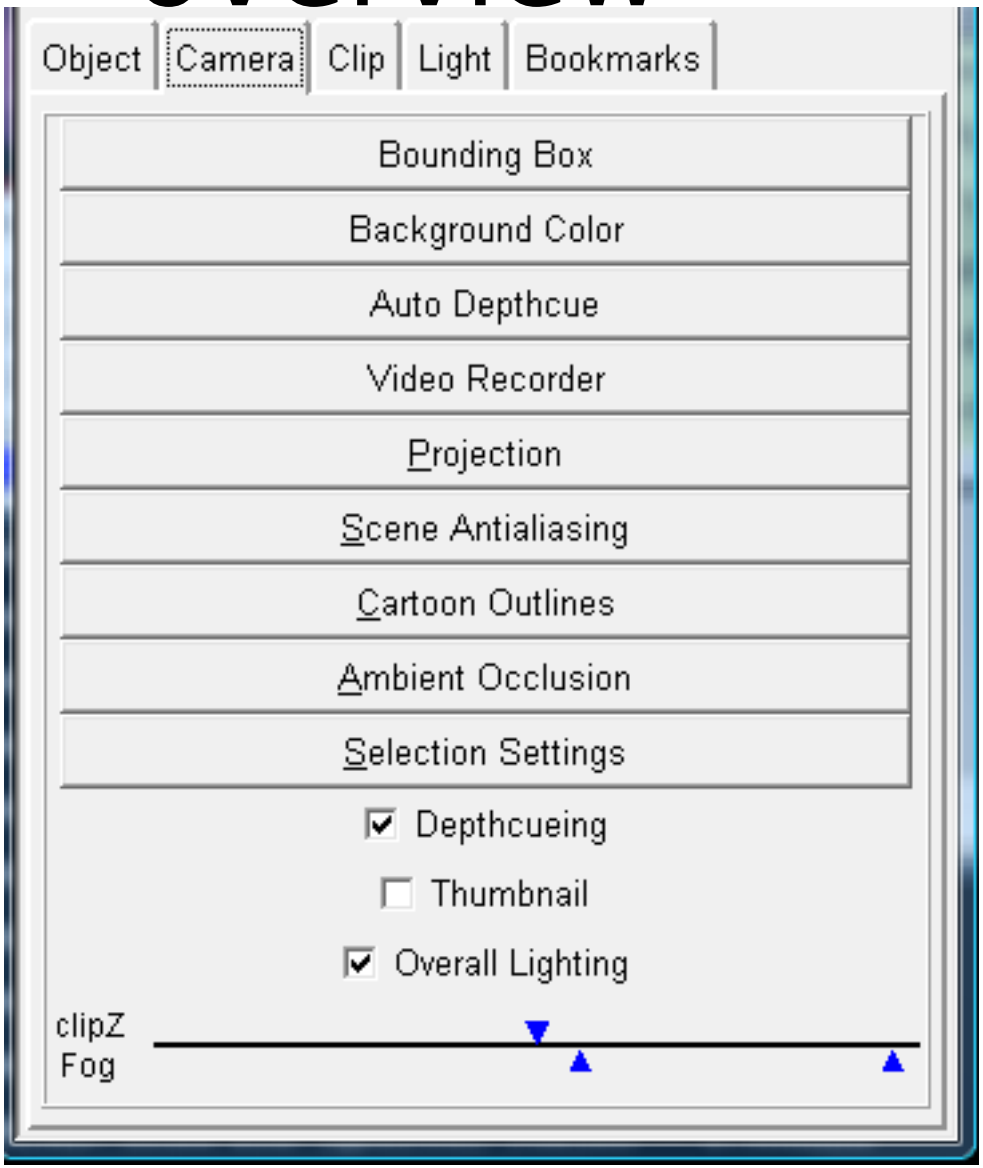
Set rotation center to center of the scene

3D Visualization: GUI overview

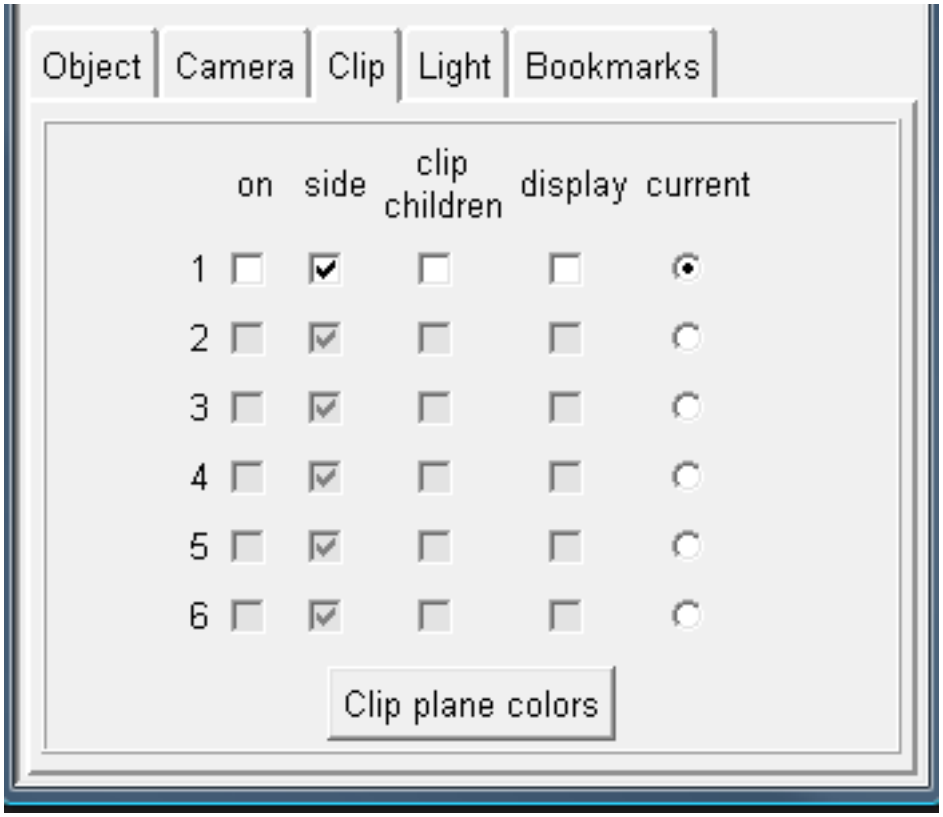


3D Visualization: GUI overview

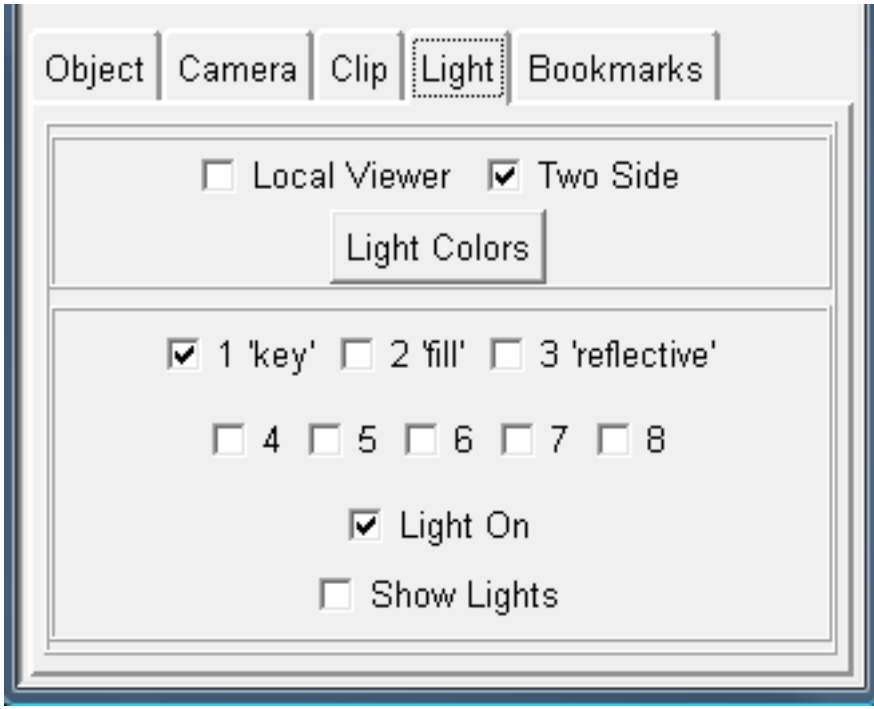
Camera property panel



3D Visualization: GUI overview



Clipping planes property panel

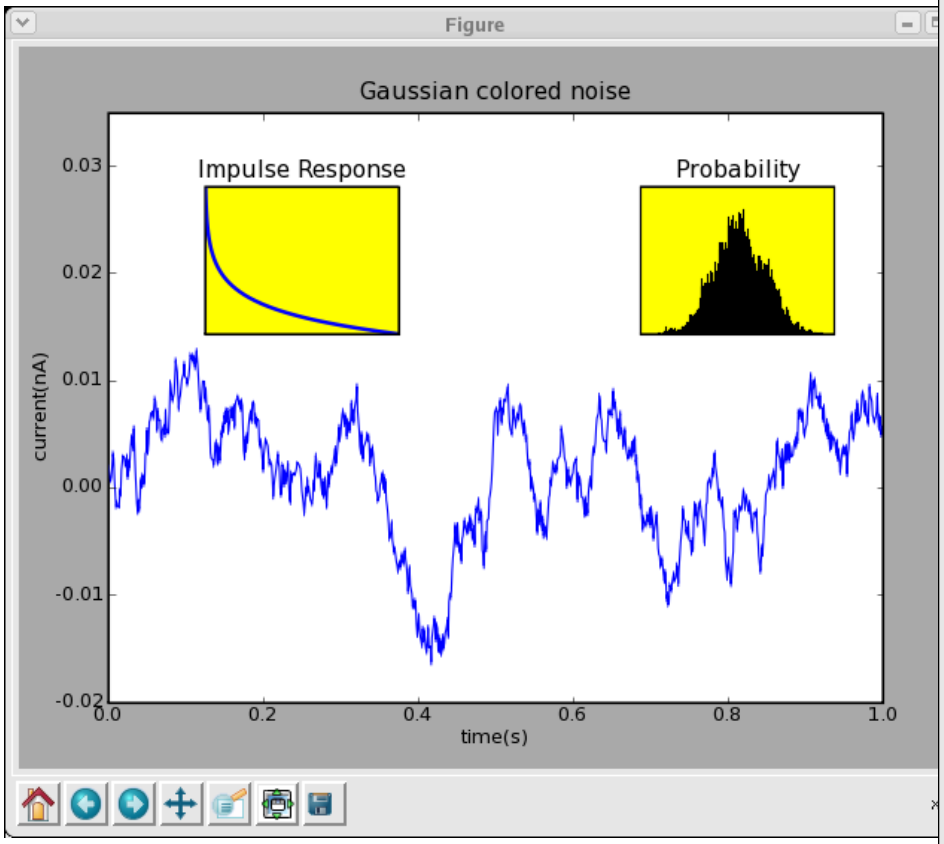


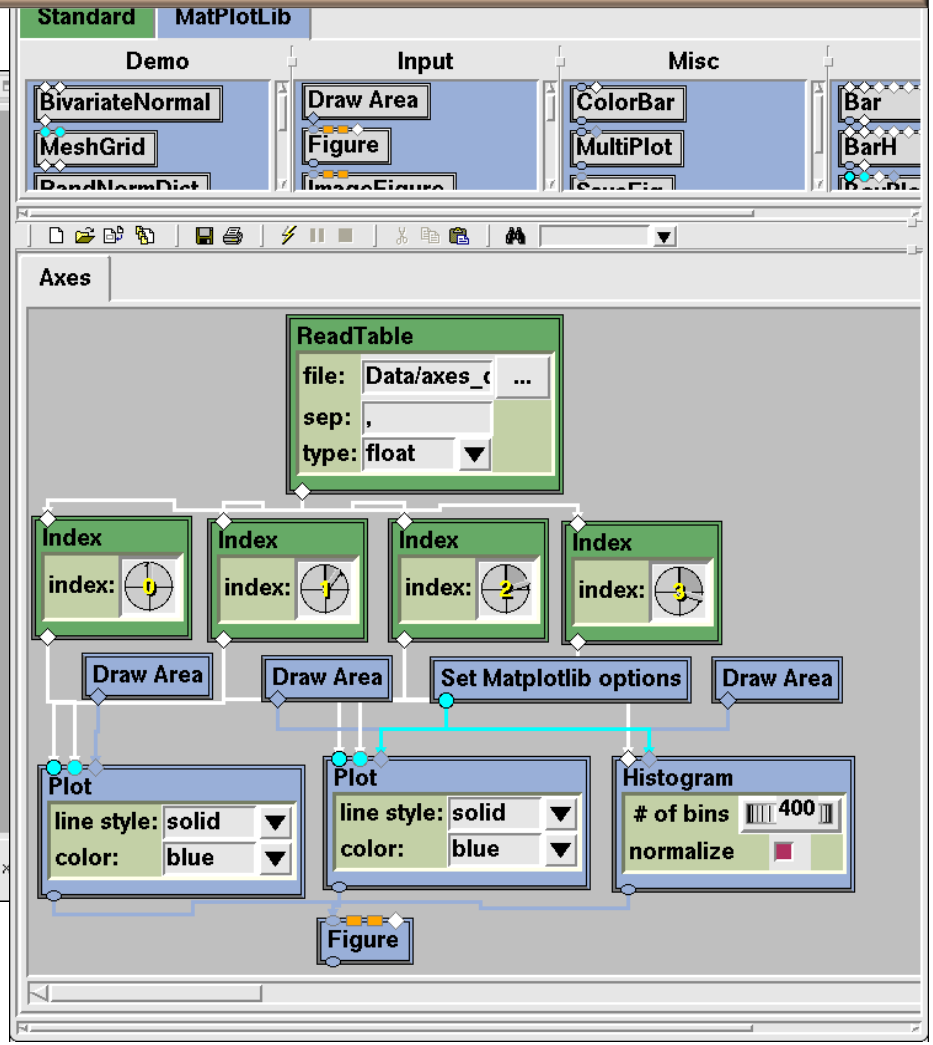
Lights property panel

2D plotting

http://mgltools.scripps.edu/packages/vision/matplotlib/vision-netwo

Desktop/doc/Examples/matplotlib





Matplotlib in DejaVu