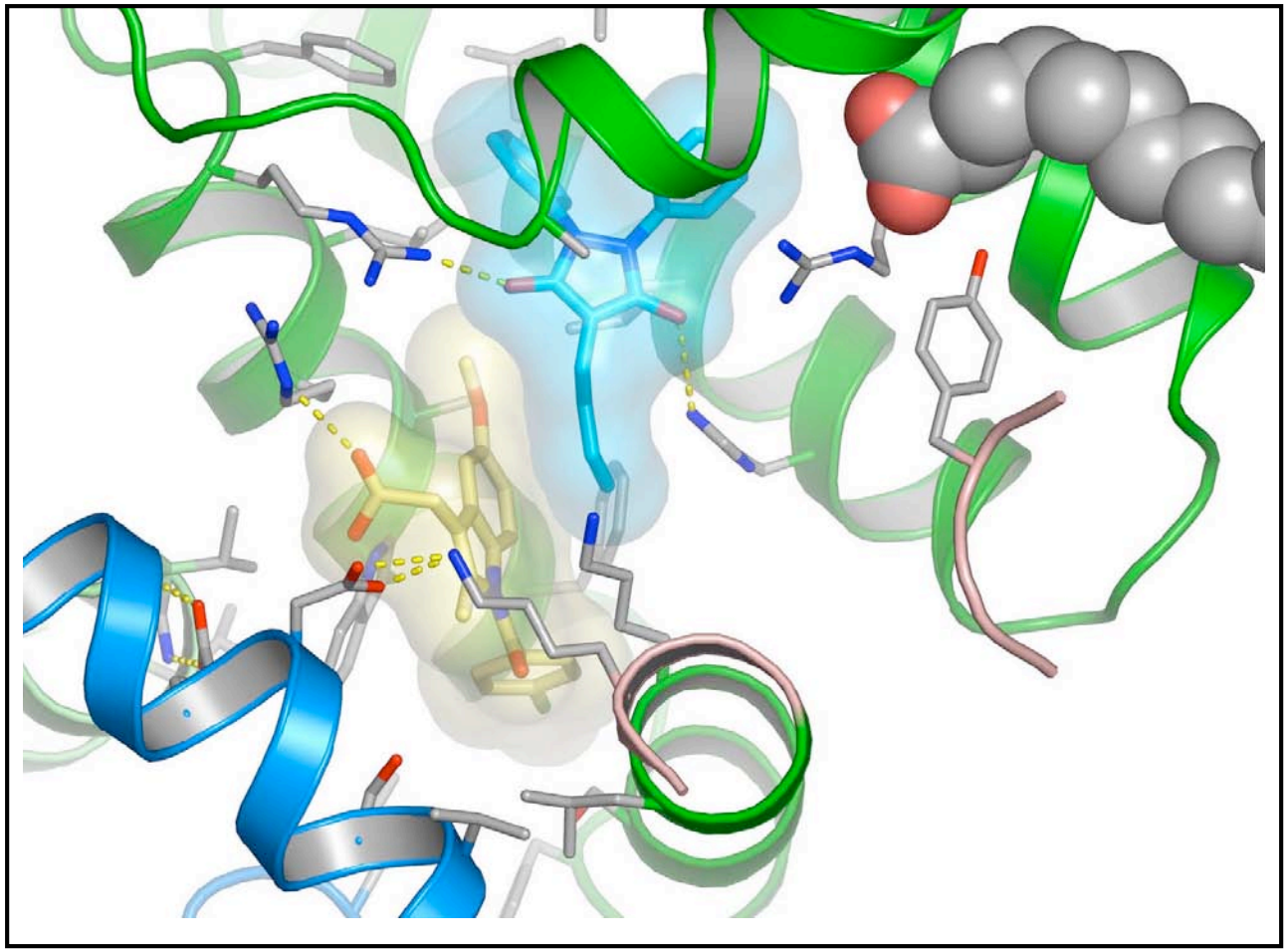
PyMol Tutorial



What are we going to cover

- Brief overview of the program
- Quick introduction to the basic features

- Just enough to get you started …
- You need to spend “hands on” time getting to know the program

Introduction to PyMol

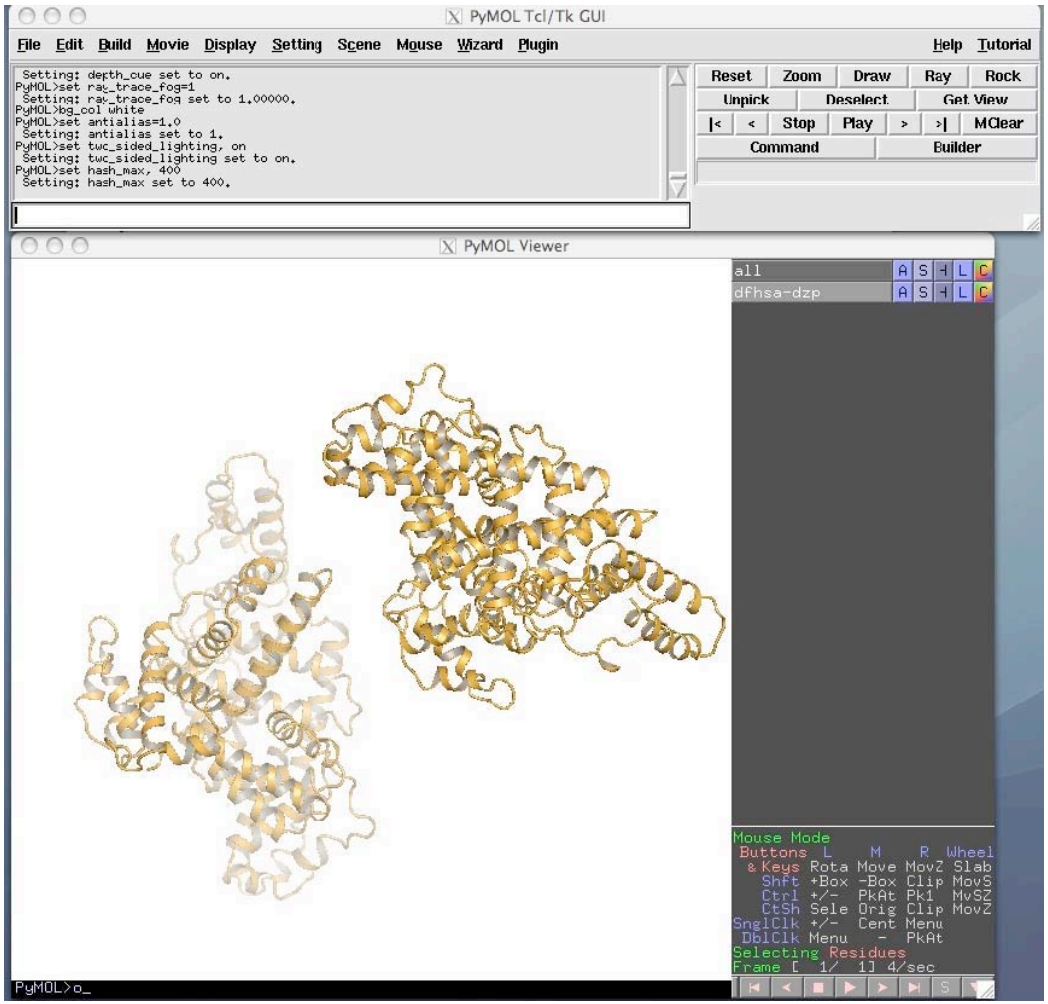
- What is pymol for?
  - Looking at pdb files (protein, nucleic acid, ligands, etc.)
  - Making publication quality figures (of models and maps)
  - NOT for model building

- Where can I get it?
  - pymol.sourceforge.net
  - Current version: 0.99
  - pymol.sourceforge.net/html/ -for the manual

- Other important links
  - www.rcsb.org — Protein data bank
  - 144.16.71.146/rp — Ramachandran plotting tool
  - www.igs.cnrs-mrs.fr/Caspr2/RMSDcalc.cgi — Structure alignment site (RMSD calc)

Starting the program

- Locate the application icon and click on it.
  - For windows users look under the program files section of the windows start menu
  - Use the PyMol + Tck-TK GUI +console icon
  - You should see a command window and a graphics window

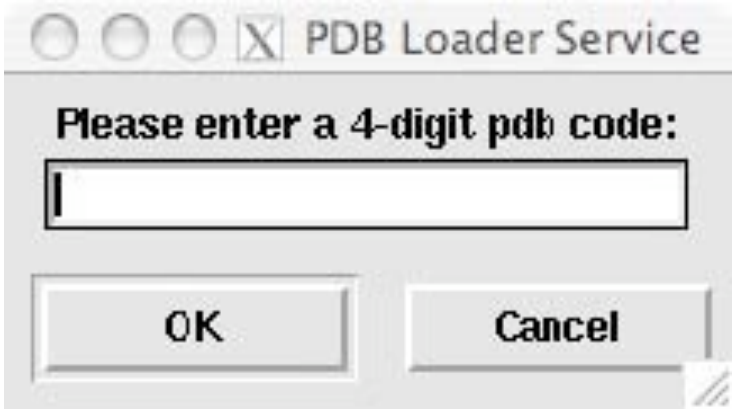


Part 1 – loading, moving and displaying

- How do I?
  - Load a pdb file
  - Change display settings
  - Create an object
  - Use the mouse to move, zoom, slab, rotate
  - Use the object menus: A, S, H, L, C
  - Navigate contextual menus
  - Display the sequence
  - Select residues
  - Save my work

How do I load a PDB file

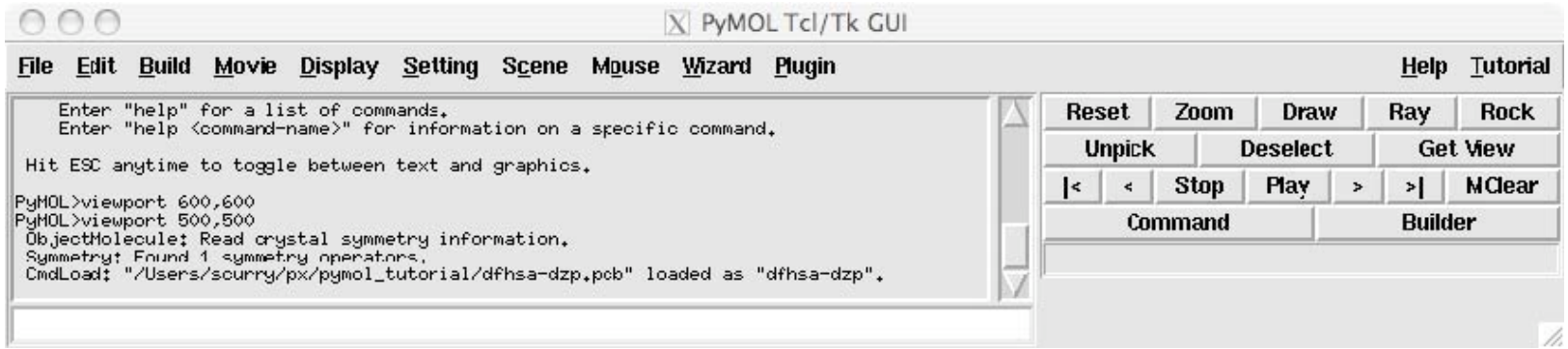
- Download a pdb file directly into pymol
  - Make sure you are connected to the internet
  - Plugin > PDB loader service
  - Typew in the PDB ID (e.g. 1AB9)
  - Object appears with this PDB ID



- Load a “local” pdb file
  - File > Open …
  - Select a pdb file
  - Object appears with the same name as the pdb file

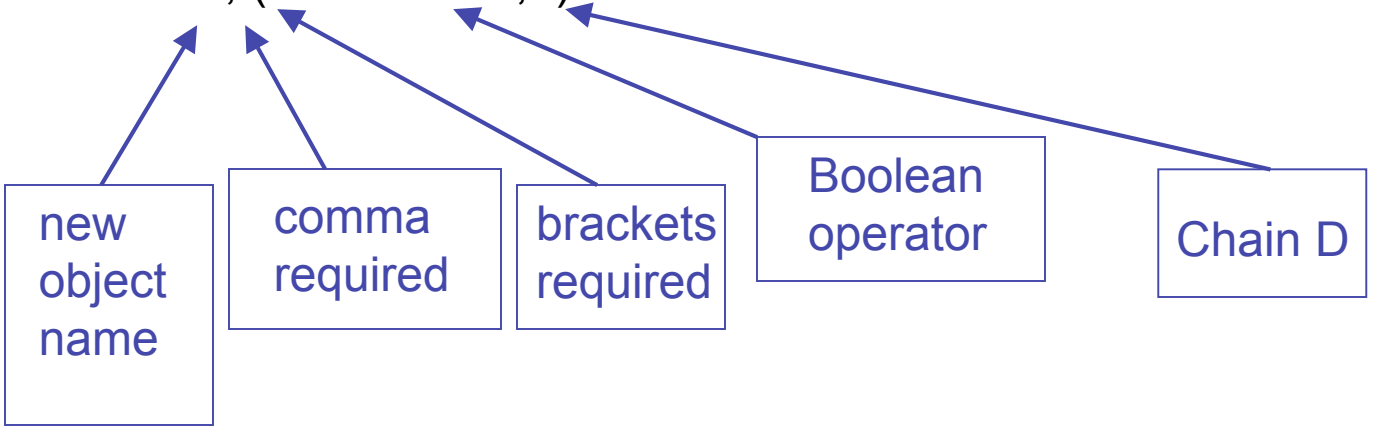
Useful display settings

- Display > Background > white --- set the background colour
- Display > orthoscopic view --- no perspective distortion



Creating new objects

- To create an object containing just chain A of 1AB9
  - Type in command (or graphics window):
    create D, (1AB9 and c;d)



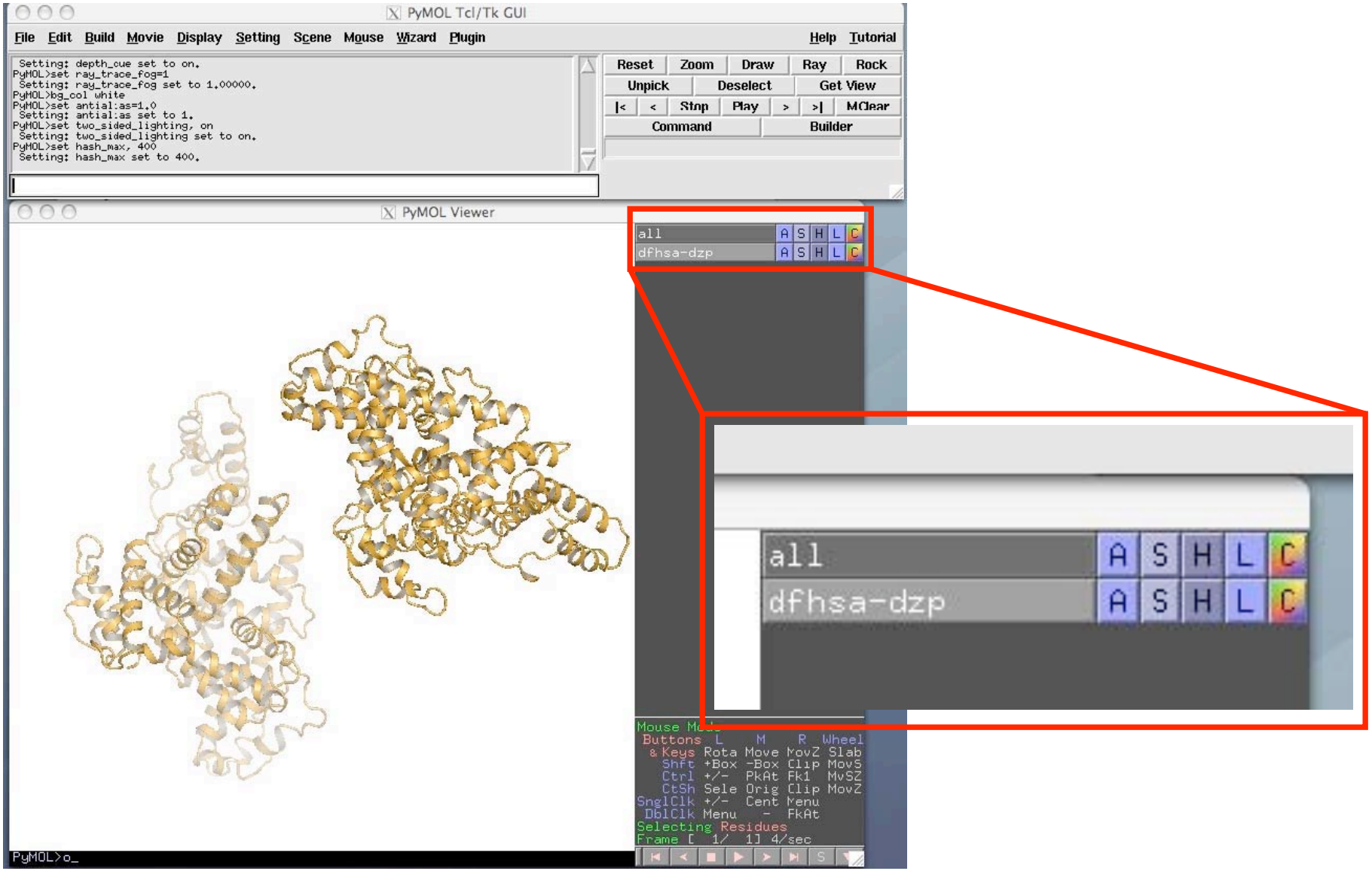
Using the mouse in the graphics window

- Unmodified controls
  - Left – rotate molecule (x, y and, at edges, z)
  - Middle – translate molecule (x, y)
  - Right – zoom (= Move Z)
  - Wheel – slab/clip

- With shift key
  - Right – up/down: clip front
    – left/right: clip back

Menu at bottom right

Object menus: A, S, H, L, C

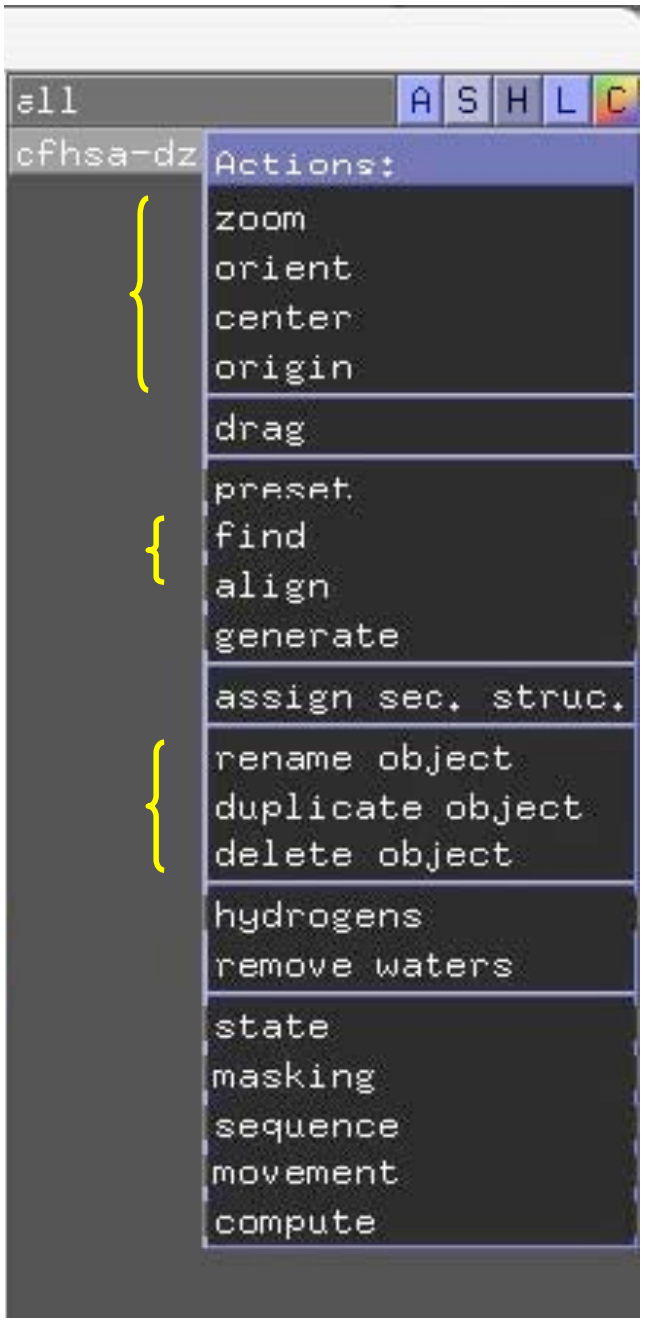


A is for Action

Navigation Tools

Analysis tools

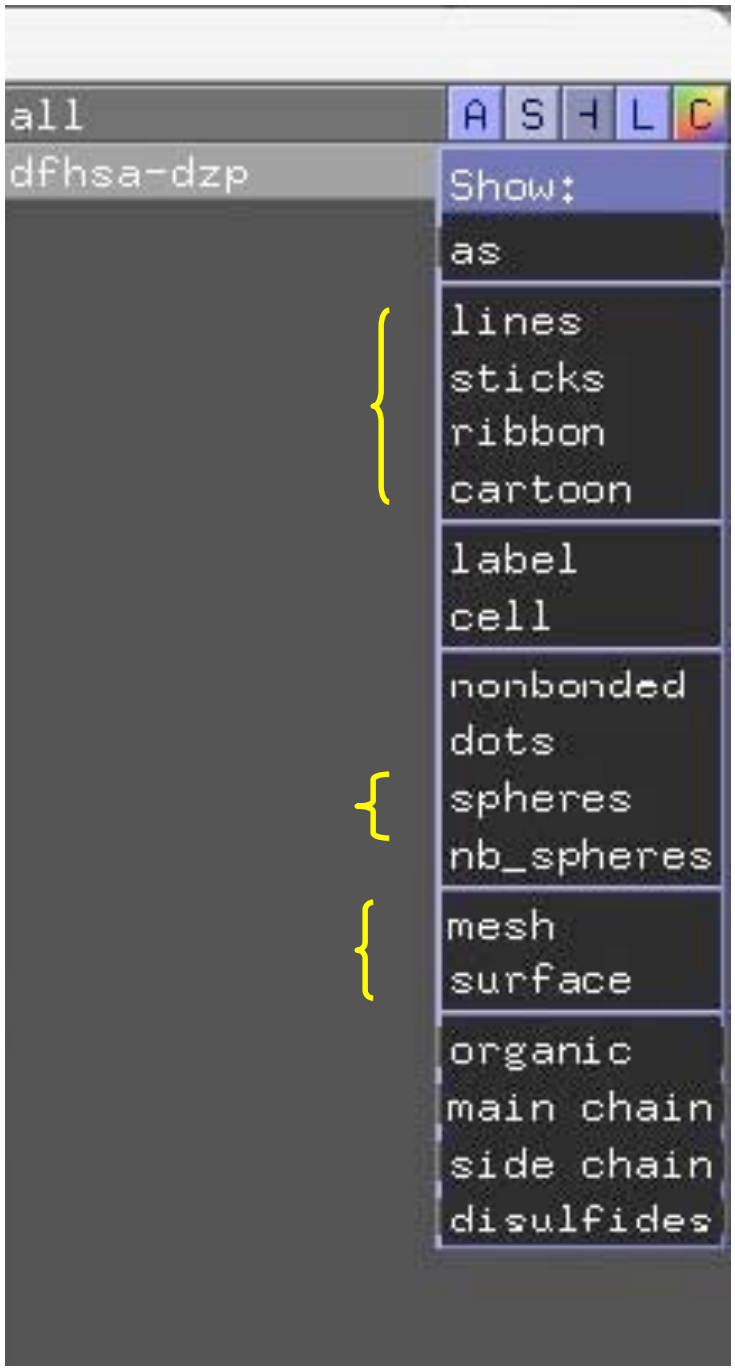
Object manipulation



NB: some of these have sub-menus

S is for Show

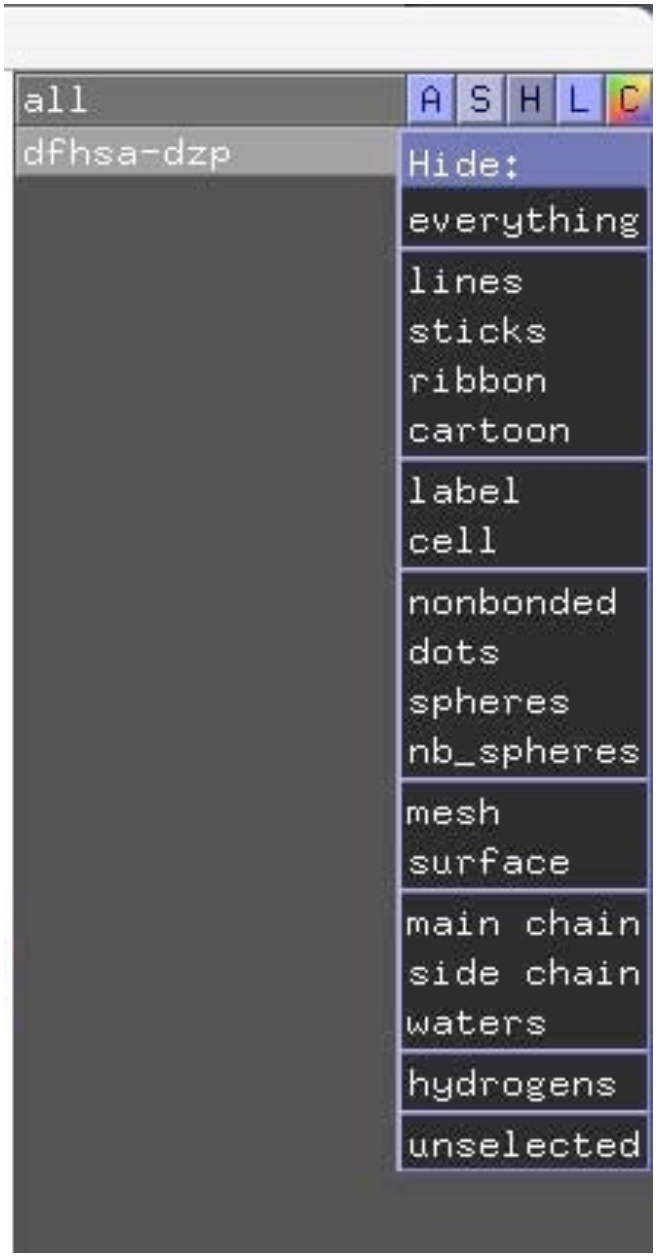
Useful representations



H is for Hide

Same content as Show menu

Use Show and Hide to toggle things on and off



L is for Label

Useful for keeping track of key residues

C is for Color

Lots of options

Mostly self-explanatory

Color menu gives names
of ready-made colors that can be
used in scripts

Display the sequence

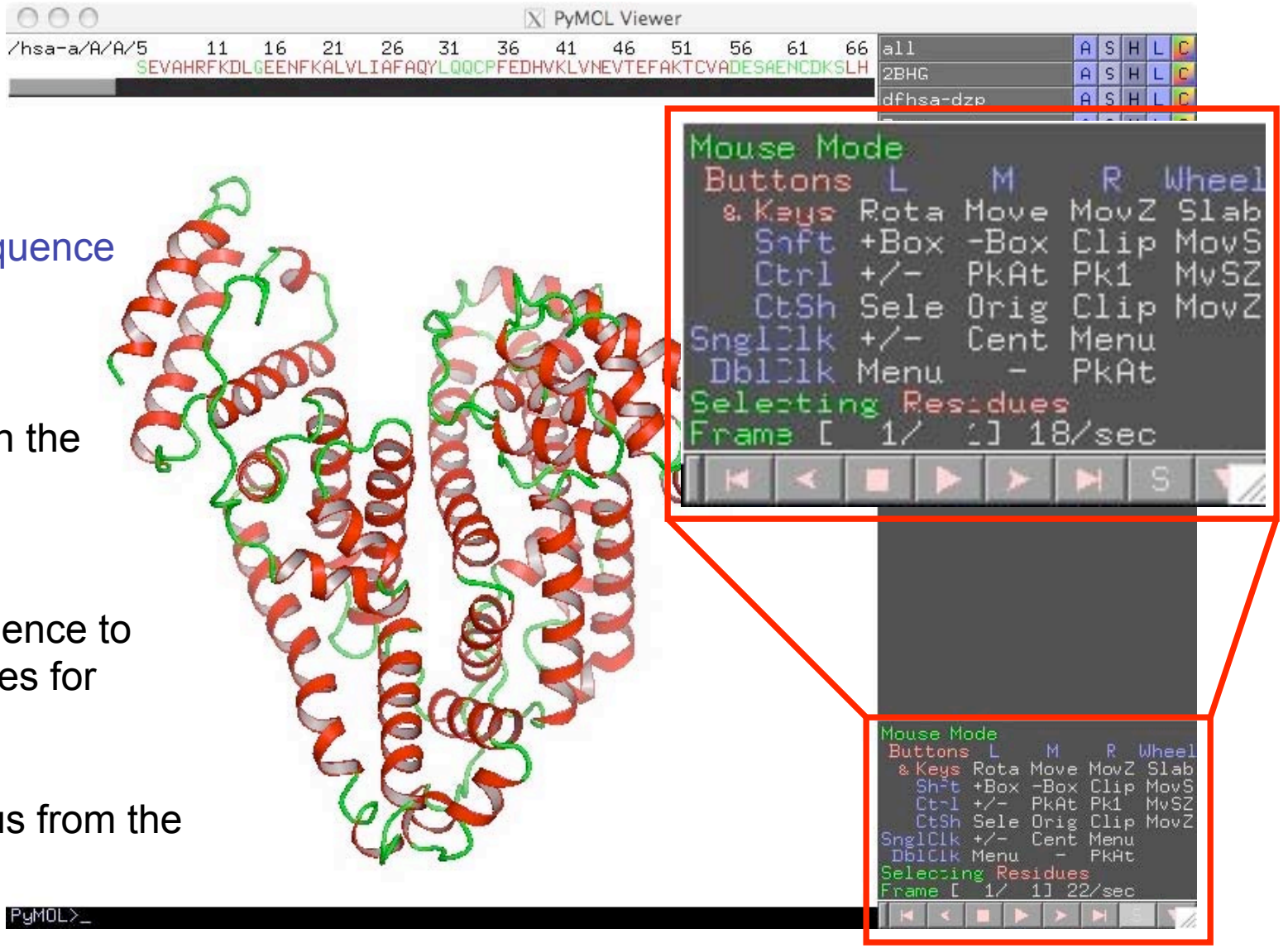
From menu:
Display > sequence

Or

Click on “S” in the mouse menu

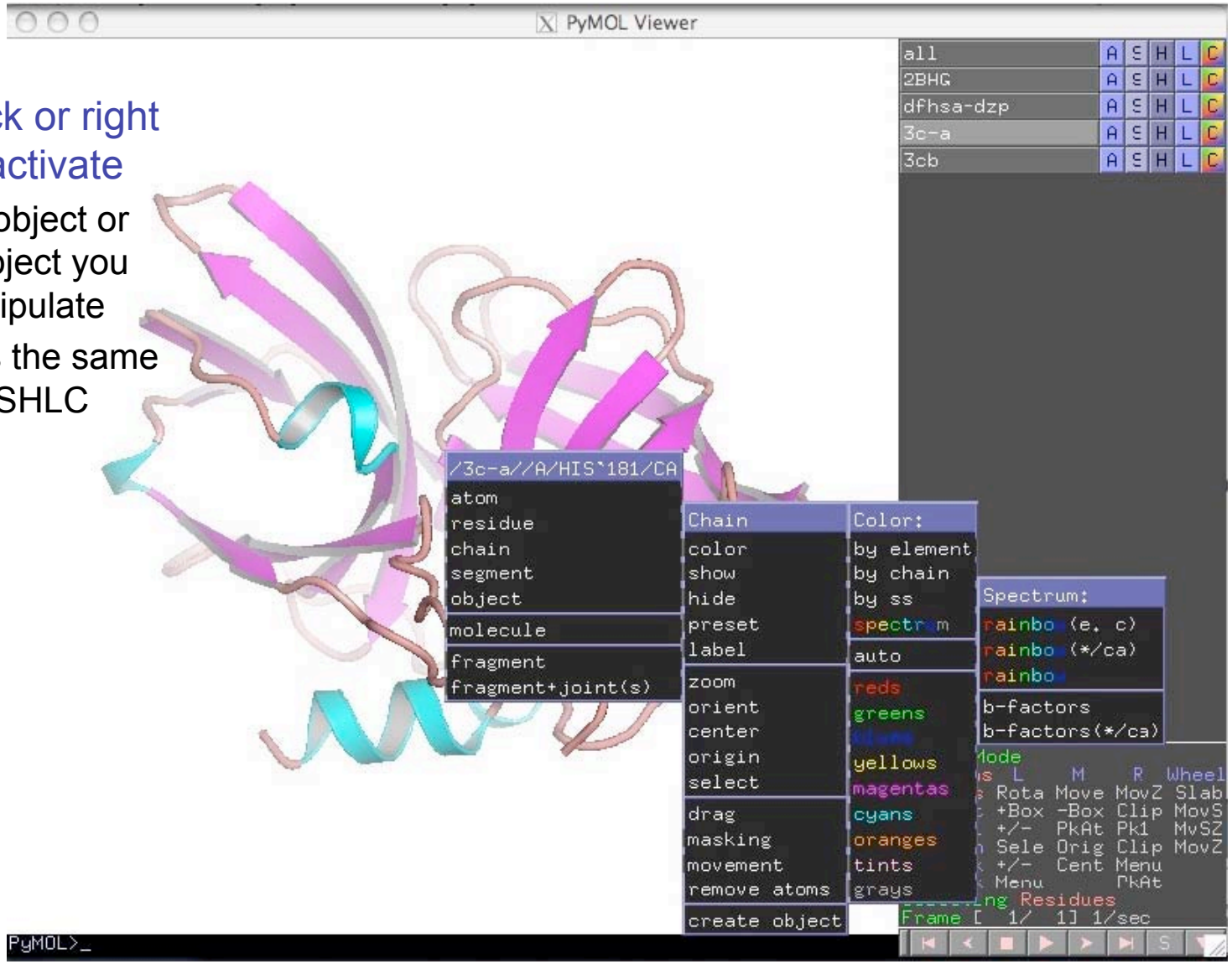
Use the sequence to Select residues for Modification

Access menus from the sequence



Contextual menus

- Left double click or right single click to activate
  - Click on an object or part of an object you want to manipulate
  - More or less the same menus as ASHLC

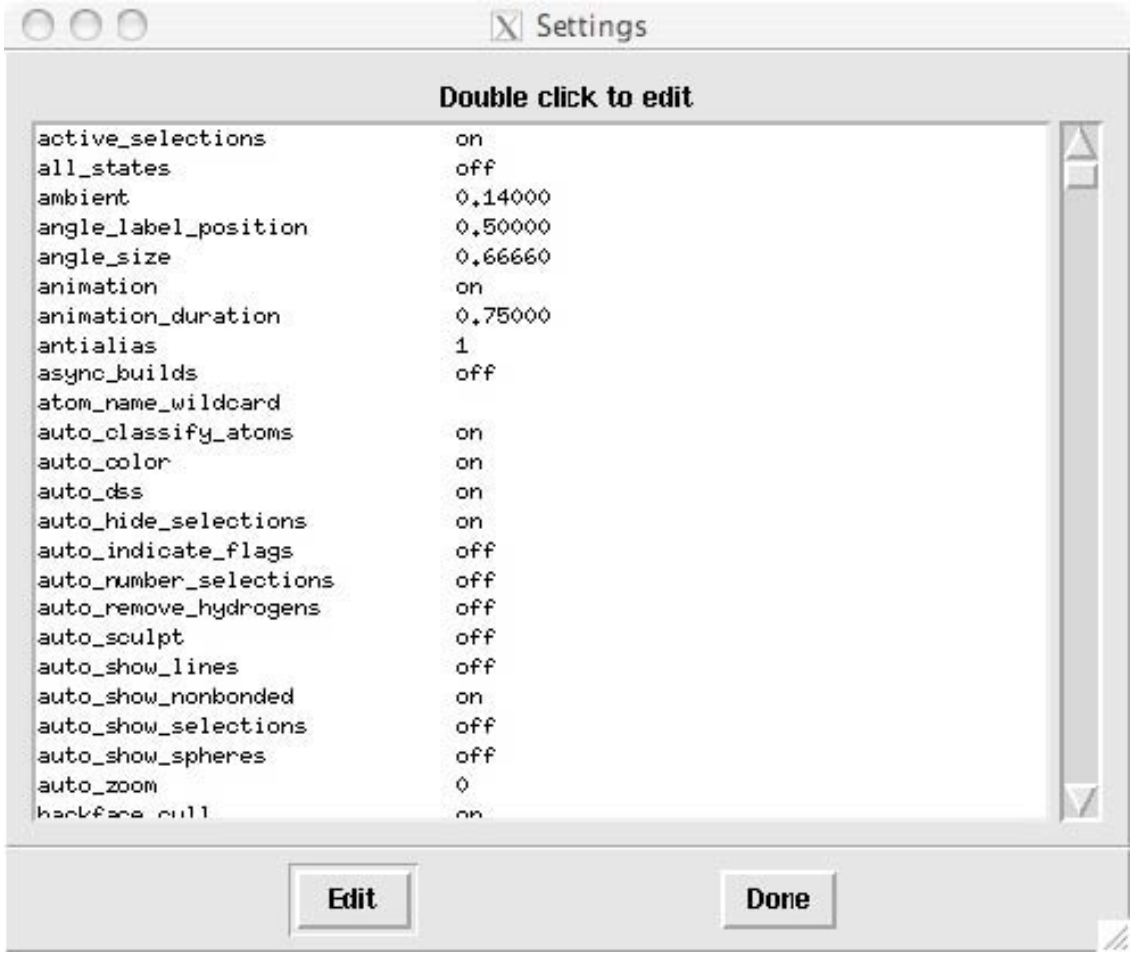


The Settings menu

Settings > edit all …

Lots of options!

Make educated guesses and see what happens



Saving your work

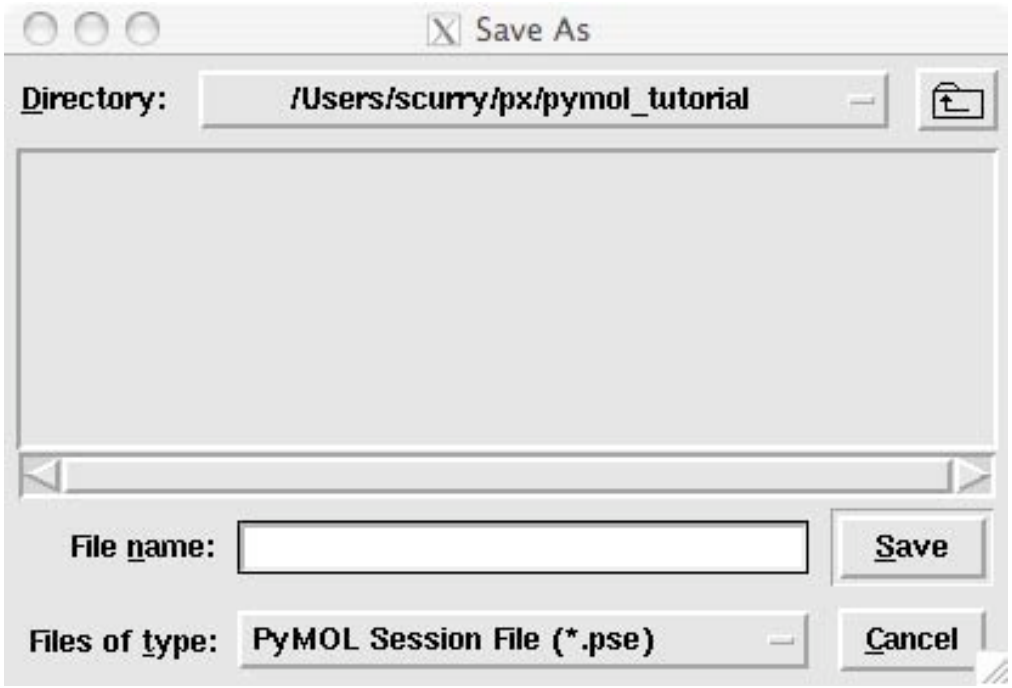
File > save session …

Enter filename as “file.pse”

Will save all your current settings (display objects, maps, etc.)

When you return to PyMol, load this file:

File > Open



Part 2 – Structural analysis

- Selection syntax
- Displaying Biochemical Properties
  - Selecting secondary structues
  - Calculating dihedral angles
  - Polar Contacts and Hydrogen-bonding
- Alignment of two or more structures

Selection syntax

resi 99-105	residues 99-105 inclusive
(i;99:105) (i = residue id number)	
resn tyr	all Tyrosine residues
(r;tyr)	(r = residue name)
resn tyr or resn phe	all tyr and phe residues
r;tyr+phe	all tyr and phe residues
Chain A	chain A
(c;a)	(c = chain)
Name N	all atoms named “N” (=main-chain nitrogen)
(n;N)	(n = atom name)
(n;CA)	all atoms named ”CA” (=alpha carbon)
	(get to know the atom names in pdb files)
(n;c+o+n+ca)	all backbone atoms
(n;c,o,n,ca)	all backbone atoms
Elem C	all carbon atoms
(e;C)	(e = element)

Selection Algebra

Operator	**Short Form**	**Effect**
not s1	!s1	Selects atoms that are not in object s1
s1 and s2	s1 & s2	Selects atoms included in both s1 and s2
s1 or s2	s1|s2	Selects atoms included in either s1 or s2
s1 around X	s1 a. X	Selects atoms with centers within X Angstroms of the center of any atom in s1
s1 expand X	s1 e. X	Expands s1 by all atoms within X Angstroms of the center of any atom in s1
s1 within X of s2	s1 w. X of s2	Selects atoms in s1 that are within X Angstroms of s2
neighbor s1	nbr. s1	Selects atoms directly bonded to s1

Atom Selection Macros

- Macros make it possible to represent a long atom selection phrase such as:

  select 1AB9 and segi PROB and chain B and resi 35 and name ca

In a more compact form

  select /1AB9/PROB/b/35/ca

/object-name/segi-identifier/chain-identifier/resi-identifier/name-identifier

If you do not need one to these identifiers, just leave that space blank

select /1AB9//b/35/ca

Displaying Biochemical Properties

- Selecting secondary structues
  - Select helix, (ss h)
  - Select sheet, (ss s)
  - Select loop, (ss l+"")
- Manually assigning secondary structure
  - alter 11-40/, ss='S'
  - alter 11-40/, ss='H'
  - alter 11-40/, ss='L'

  to set residues 11-40 to beta strand, alpha helix, and loop respectively

Measurement Wizard

wizard > measurement

- Pretty much self explanatory
- Select measurement mode from pull-down menu
- Use the mouse to pick the atoms involved in the distance, angle or torsion angle you are interested in as prompted in the upper left hand corner of the graphics window
- When finished, click done

Calculating dihedral angles

- The get_dihedral function requires four single-atom selections to work:

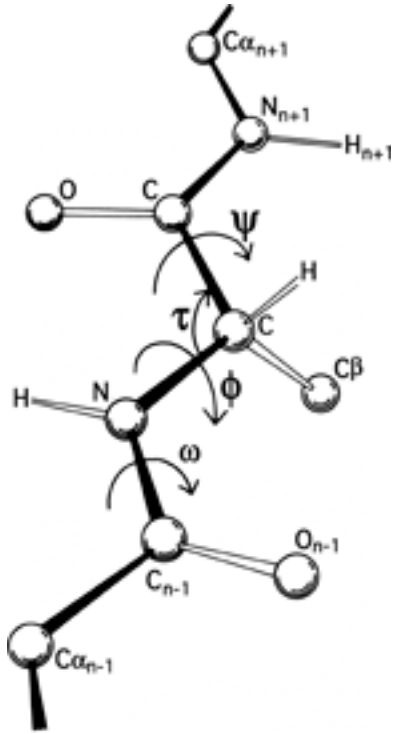
get_dihedral 1AB9//B/16/c,1AB9//B/17/n, 1AB9//B/17/ca, 1AB9//B/17/c

Returns the phi angle for residue 17 in chain B of 1AB9

For the psi angle you would use N_i, CA_i, C_i, N_{i+1}

get_dihedral 1AB9//B/17/n,1AB9//B/17/ca, 1AB9//B/17/c, 1AB9//B/18/n

- Alternatively you can use the measurement tool under the wizard tab and manually select the four atoms involved in each dihedral



Polar Contacts

- Using the PyMol menus one may display Polar Contacts. These are defined as

  set h_bond_cutoff_center, 3.6

  with ideal geometry and

  set h_bond_cutoff_edge, 3.2

  with minimally acceptable geometry

- These settings can be changed *before* running the detection process

Hydrogen-bonding

- Easy Hydrogen Bonds

```
dist name, s1, s2, mode=2
```

- More complicated Hydrogen Bonds –

```
h_add 1AB9
select protein, chain A or chain B or chain C
select substrate, chain D
select don, (elem n+o and (neighbor hydro))
select acc, (elem o or (elem n and not (neighbor hydro)))
dist HBA, (substrate and acc), (protein and don), 3.2
dist HBD, (substrate and don), (protein and acc), 3.2
delete don
delete acc
hide (hydro)
```

Structural Alignment

- Requires at least 2 structures to be loaded into pymol

```
align 1NES, 1AB9
```

- PyMol will first do a sequence alignment and then try to align the structures to minimize the RMSD between the aligned residues
- When the alignment runs it will print out some information:

```
Match: read scoring matrix.
Match: assigning 388 x 370 pairwise scores.
MatchAlign: aligning residues (388 vs 370)...
ExecutiveAlign: 1393 atoms aligned.
ExecutiveRMS: 68 atoms rejected during cycle 1 (RMS=2.34).
ExecutiveRMS: 82 atoms rejected during cycle 2 (RMS=1.41).
Executive: RMS =    1.095 (1243 to 1243 atoms)
```

- Restricting the alignment
  - Alignment of just the backbone atom

```
align 1NES and name n+ca+c+o,1AB9 and name n+ca+c+o
```

- For more difficult alignments try RMSD calc website