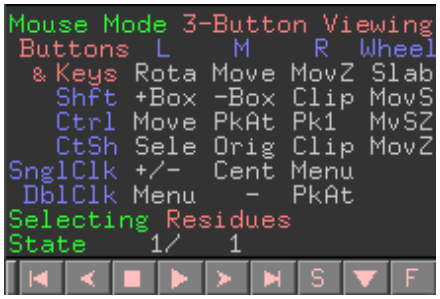
PyMOL

Open the pdb-file

- PyMOL -> File -> Open (*.pdb/*.cif/*.pse)
- **fetch** pdbID (for example: **fetch** 1k1g)

Interface

A => actions
S => show (representation)
H => hide (representation)
L => label
C => coloring



Mouse mode => 3-Button Viewing/Editing
(PyMOL -> Mouse …. options for mouse modes)

State => assembly 1/20 (NMR structures)
1/1 (crystall structures)

F => full screen mode

S => show sequence (PyMOL -> Display -> SequenceMode)

NMR vs crystal structure

NMR
-> hydrogen atom

- **set all_states, on**
- **intra_fit** *name*
- **split_states**

Crystal structure
-> no hydrogen atoms PyMOL -> Actions -> add hydrogens

- **hide** *(solvent)*
- **remove** *what*

Representation

- **split_chains**

Rename chain/selection

- **set_name** *old name, new name* (**set_name** 1k1g_A,protein)
  (**set_name** 1k1g_B, RNA)

Hide

PyMOL -> Hide (H) -> lines/sticks/cartoon/ribbon/labels/…

- **hide** *what* (**hide** lines)

Show

PyMOL -> Show (S) -> lines/sticks/cartoon/ribbon/labels/…

- **show** *what* (**show** cartoon)

- **dss** (defines secondary structure based on backbone geometry and hydrogen bonding patterns)

Color

PyMOL -> Color (C) -> by element/chain/side chain/representation/

Label

PyMOL -> Label (L) -> residues/chains/atom names

Label appearance:

PyMOL -> Settings -> Label -> Size/Font

- **set label_color**, *color*
- **set label_size,** 10 (points, default is 14)

To move label:

PyMOL -> Mouse -> 3-Button Editing => ctrl + left mouse button

Clear label:

PyMOL -> Label (L) -> clear

Save

Save session:

PyMOL -> File-> save session (save session as) (*name*.**pse)**

Save molecule: save molecule/ selection as pdb/cif file (coordinates)

PyMOL -> File-> Save Molecule (whole molecule/selection)

Save image:

PyMOL -> File-> Save Image -> PNG

Image

PyMOL -> Display -> background/shadows/colors/grid/quality/reflection/…

PyMOL -> Settings -> Label/Cartoon/Surface/Transparency/….

Rendering
PyMOL -> Settings -> Shadows/….

Ray button

Selection

- **select** *name* (**select** RNA)

Residue: (resn, r. or i.)

- **select resn** *res* *(**select resn** arg)* or **select r.** residue
- **select resn** res+res+res (**select resn** *arg+lys)* or **select r.** res+res+res
- **select resi** *156-162*

Atom type:

- **select name** *atom type* (**select name** ca) or **select n.** *atom type*

Complex characterisation

Distance measurements:

PyMOL -> Wizard -> Measurement

pick first atom => pick second atom units: Angströms

- **distance** *1. residue number/atom type*, *2. residue number/atom type*
  (distance 177/O, 511/H62)

measurement editing -> A, S, H, L, C options

Find close contacts:

- **indicate** *molecule/residue 4.0* (**indicate** RNA 4.0)

Electrostatics:

PyMOL -> Actions (A) -> generate -> vacuum electrostatics

Find polar contacts:

PyMOL -> Actions (A) -> find-> polar contacts