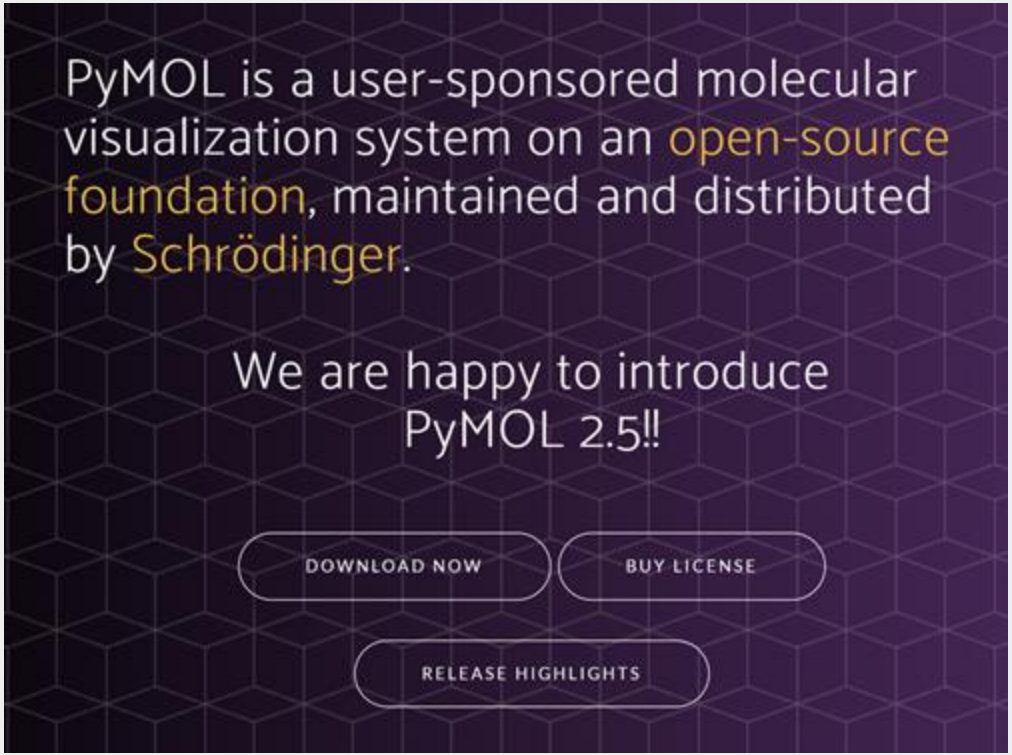


https://pymol.org/

Types of Structure Determination

NMR

- Can capture conformational heterogeneity
- Complexity increases exponentially with target size

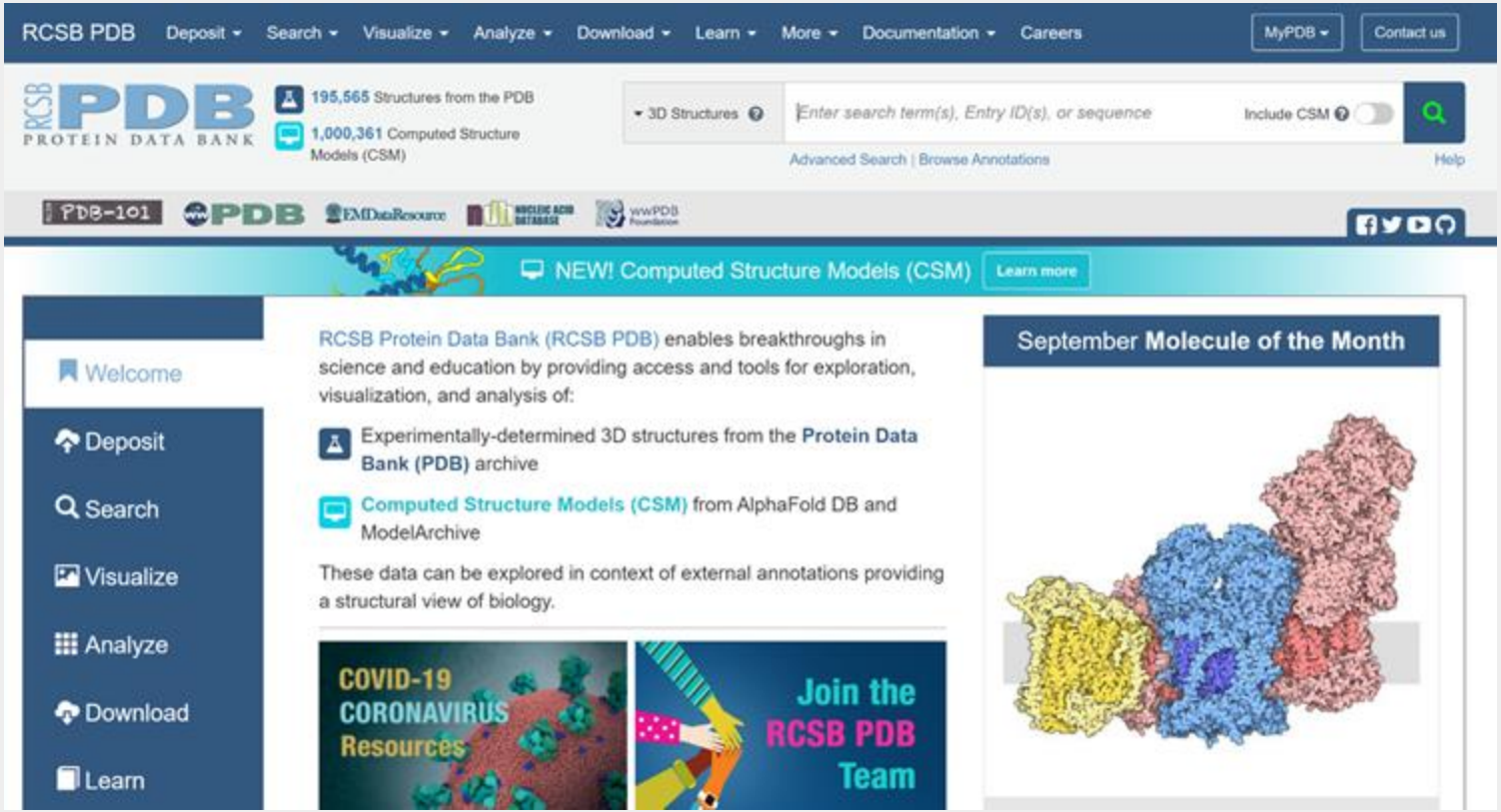
Cryo-EM

- Can capture some conformational heterogeneity
- Best for large complexes (>100 kDa)

X-ray crystallography

- Can capture some conformational heterogeneity
- Best for smaller complexes, but works with some large complexes

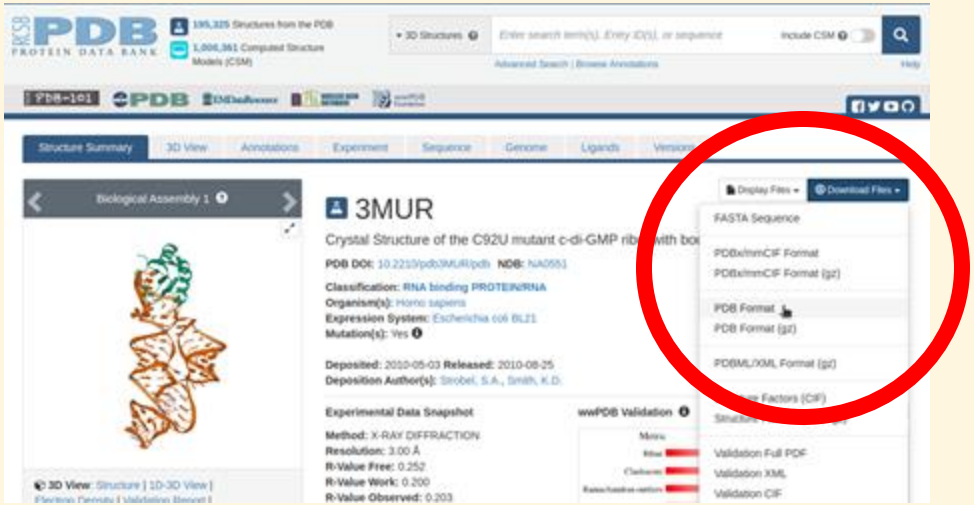
The PDB



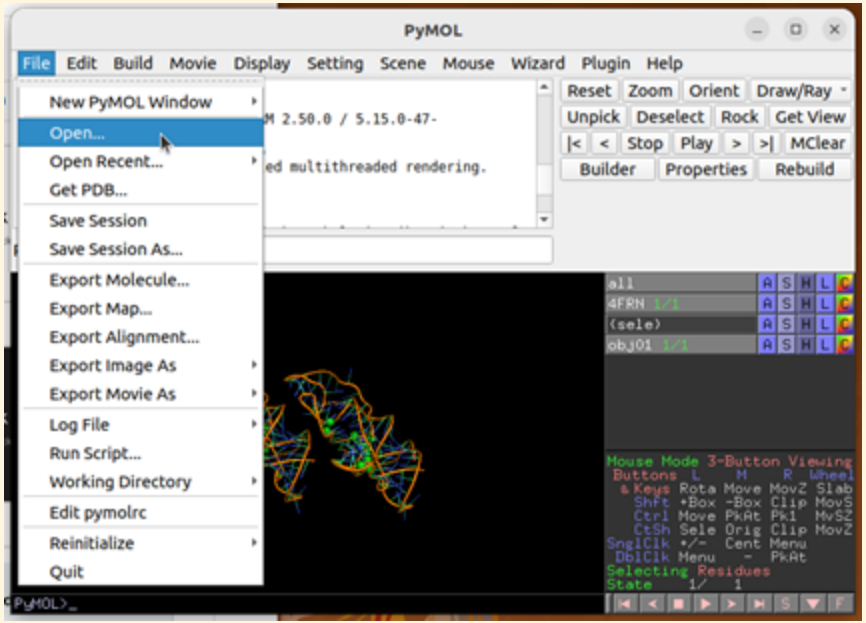
Almost all structure papers will have a PDB entry.
The PDBID is sometimes buried.
Check the Results, Methods, Data Availability, Supplemental information, etc.

Opening a structure

Download PDB file



File ⟶ Open…



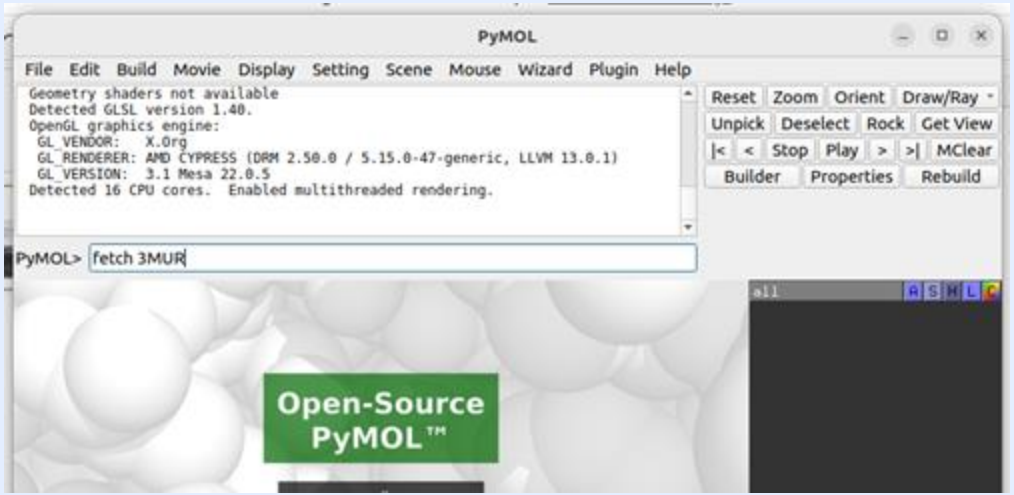
PyMol Wiki

https://pymolwiki.org/index.php/Main_Page

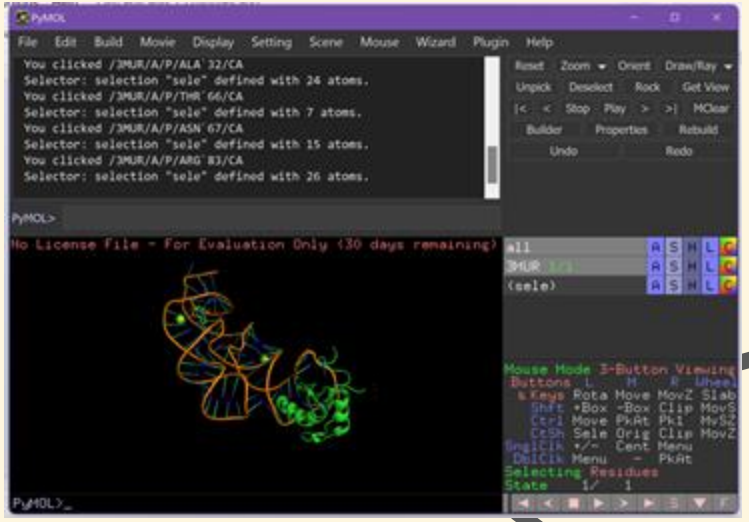
Opening a structure

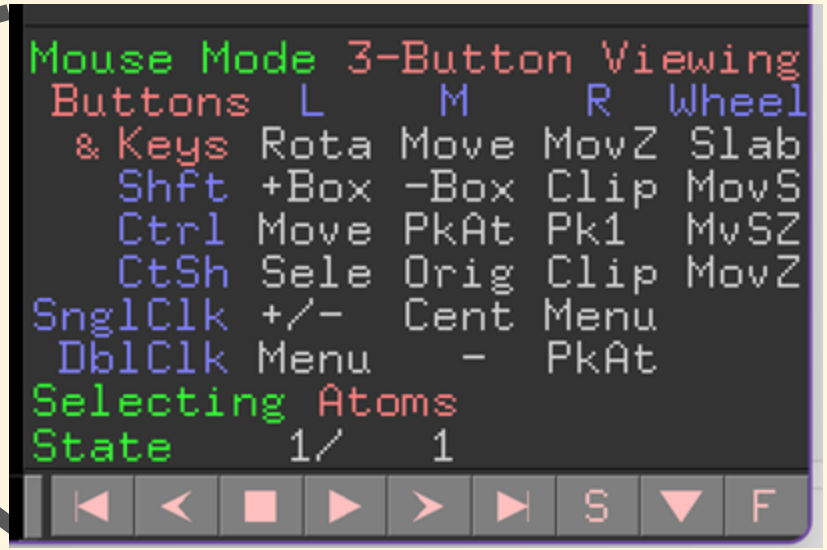
Find PDB Number

> fetch *PDB Number*



Moving the Structure





Warning: Clicking on the box will toggle between viewing and editing

GL_VENDOR: ATI Technologies Inc.
GL_RENDERER: AMD Radeon Pro 455 OpenGL Engine
GL_VERSION: 2.1 ATI-2.4.9
License Expiry date: 01-may-2019
Detected 8 CPU cores. Enabled multithreaded rendering.

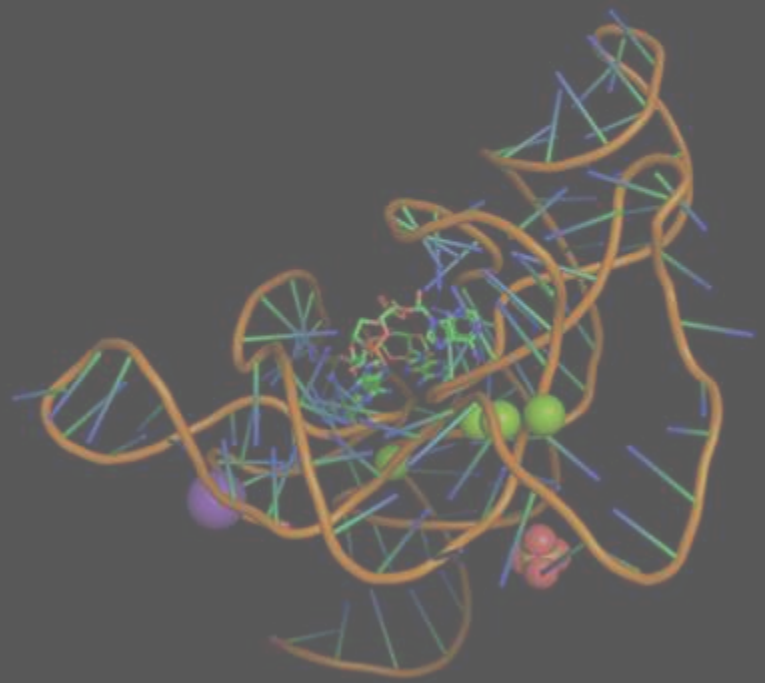
PyMOL>fetch 4QK8
please wait ...
TITLE Thermoanaerobacter pseudethanolicus c-di-AMP riboswitch
ExecutiveLoad-Detail: Detected mmCIF
CmdLoad: loaded as "4QK8".

PyMOL>

Reset Zoom Orient Draw/Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear
Builder Properties Rebuild

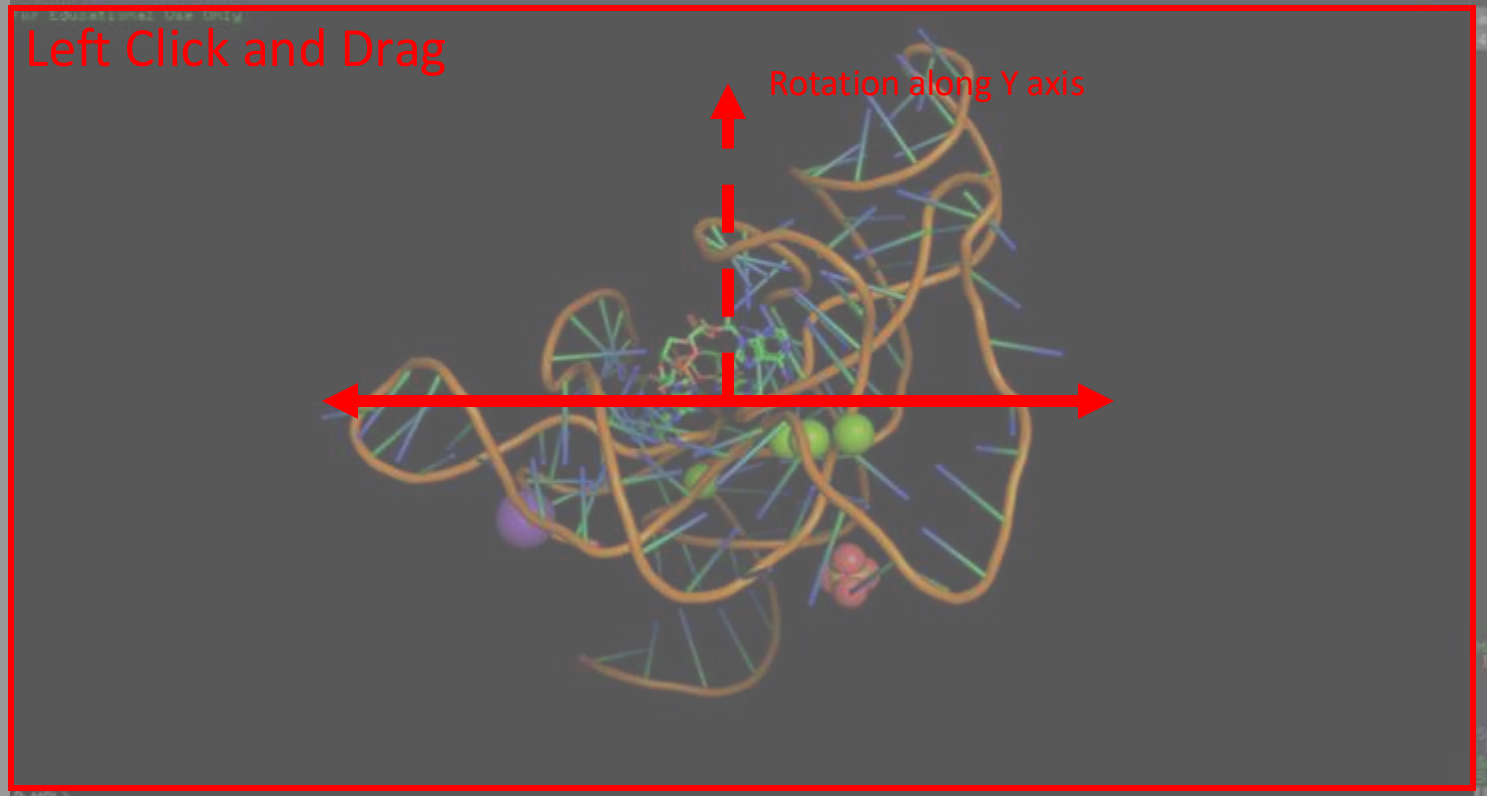
For Educational Use Only

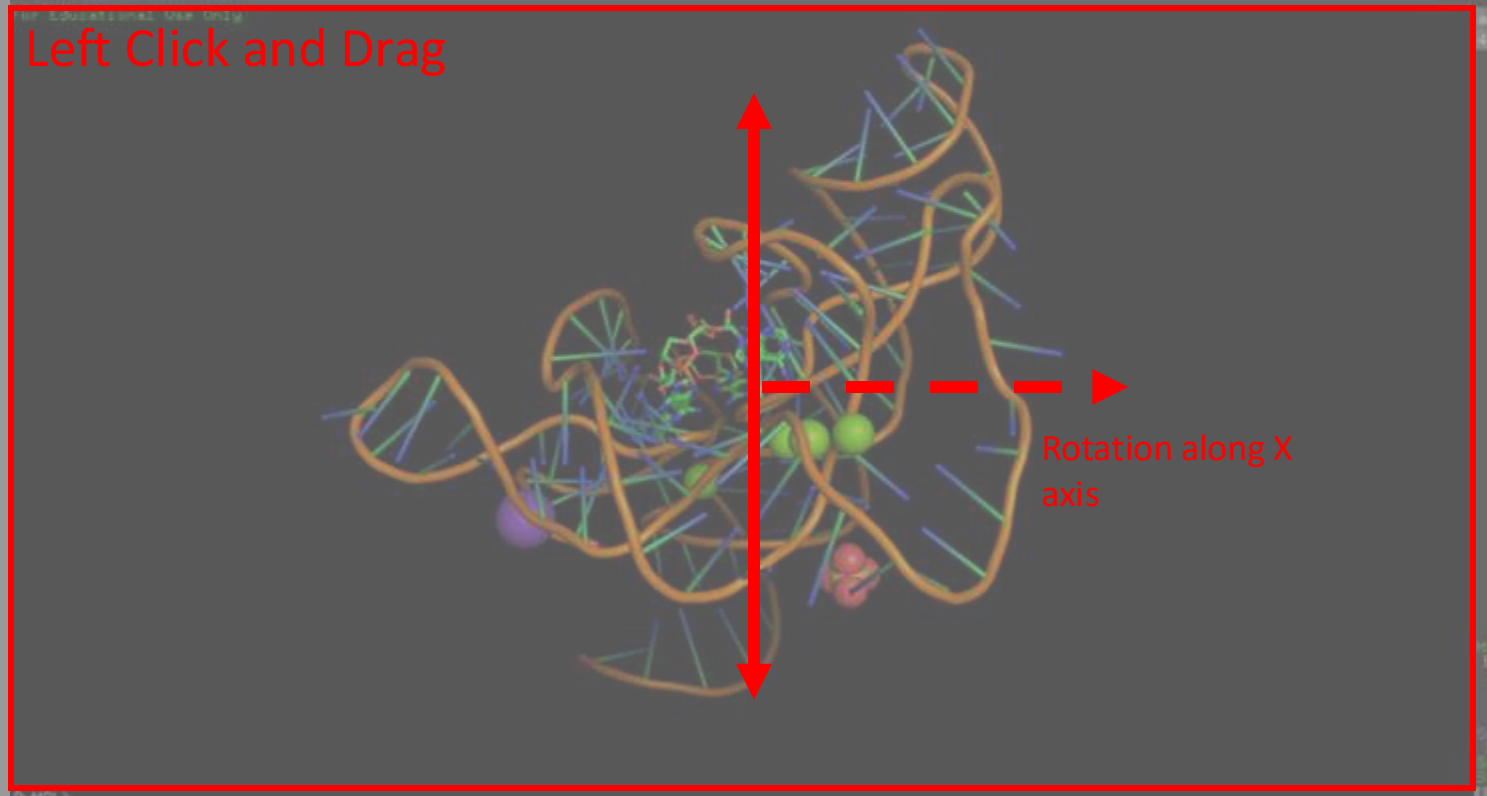
Display Area

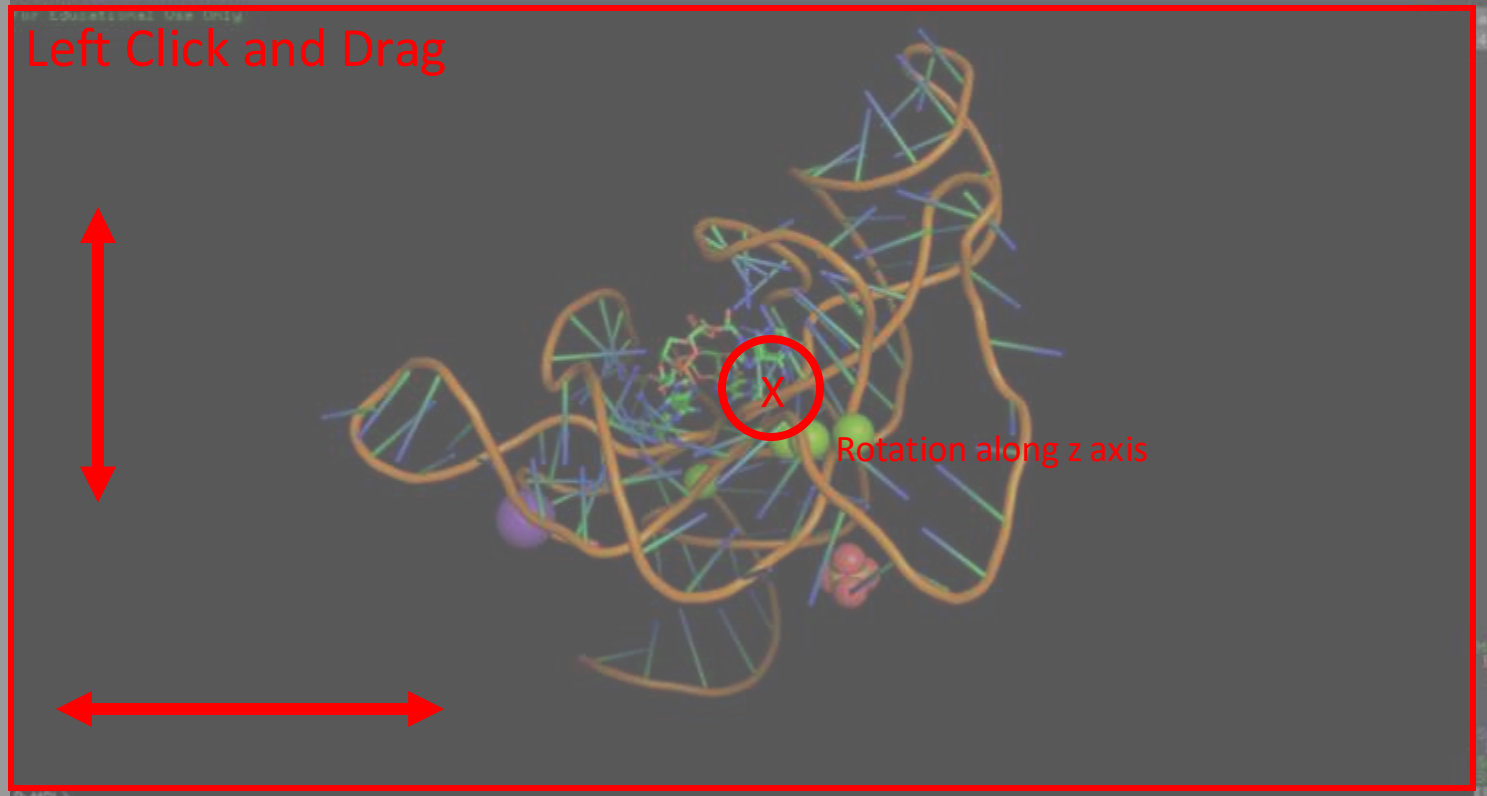


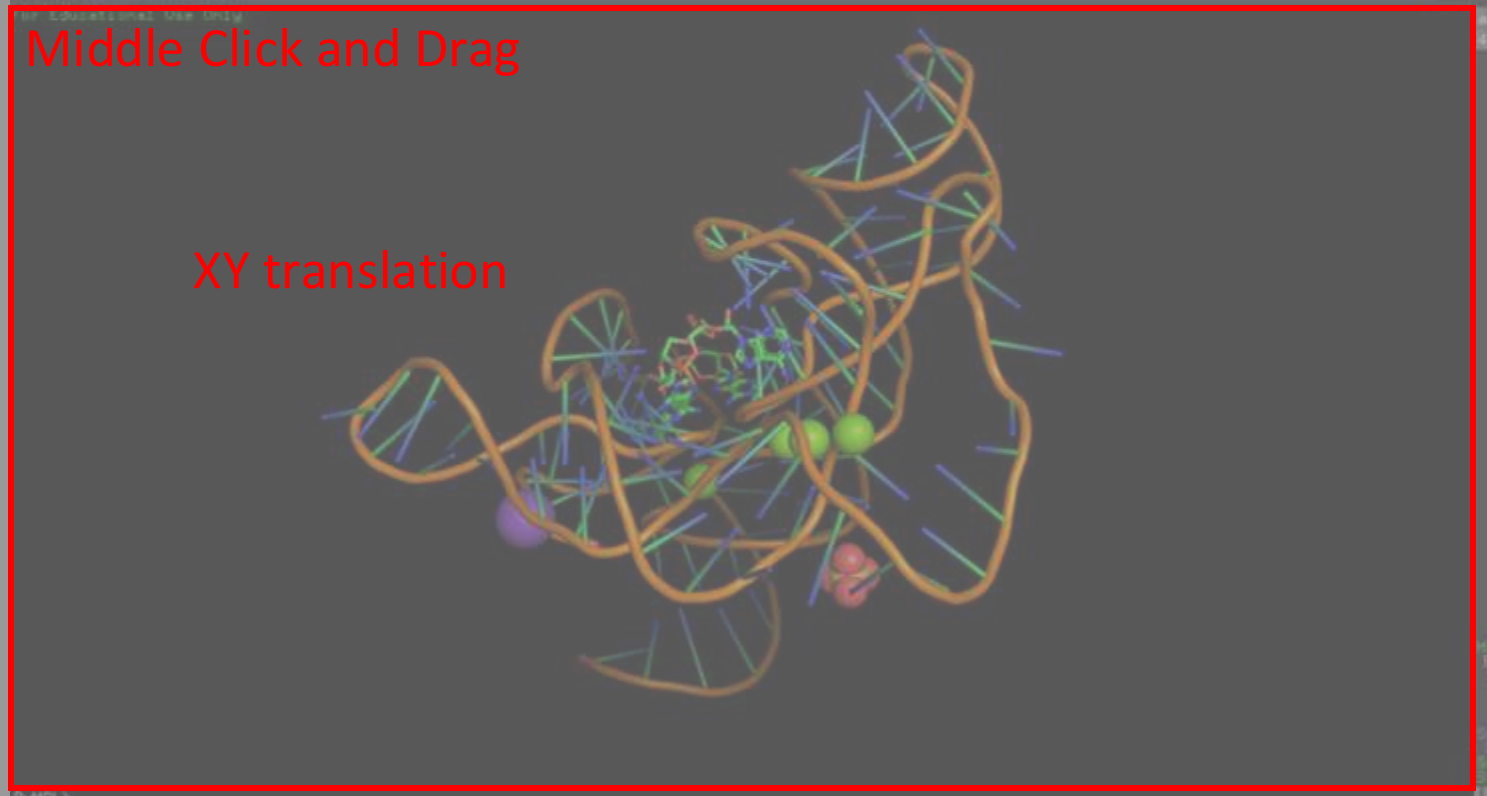
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
&Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl Move PkAt PkTg MvSZ
Ctrl+Shft Sele Orig Clip MovZ
PkCtrl */- Cent Menu
PkShift Menu - PkAt
Selecting Residues
State 1/ 1

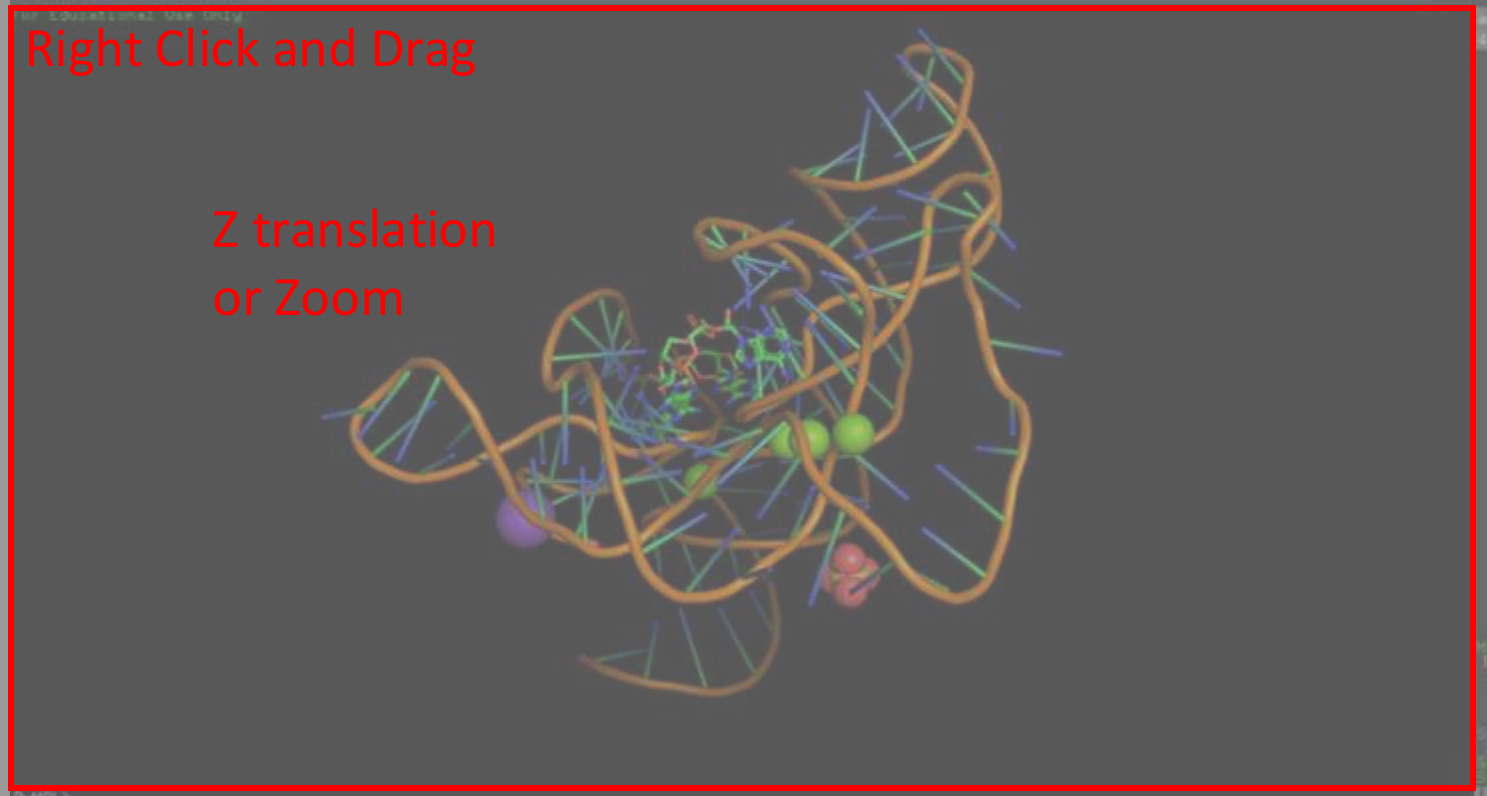
PyMOL>_

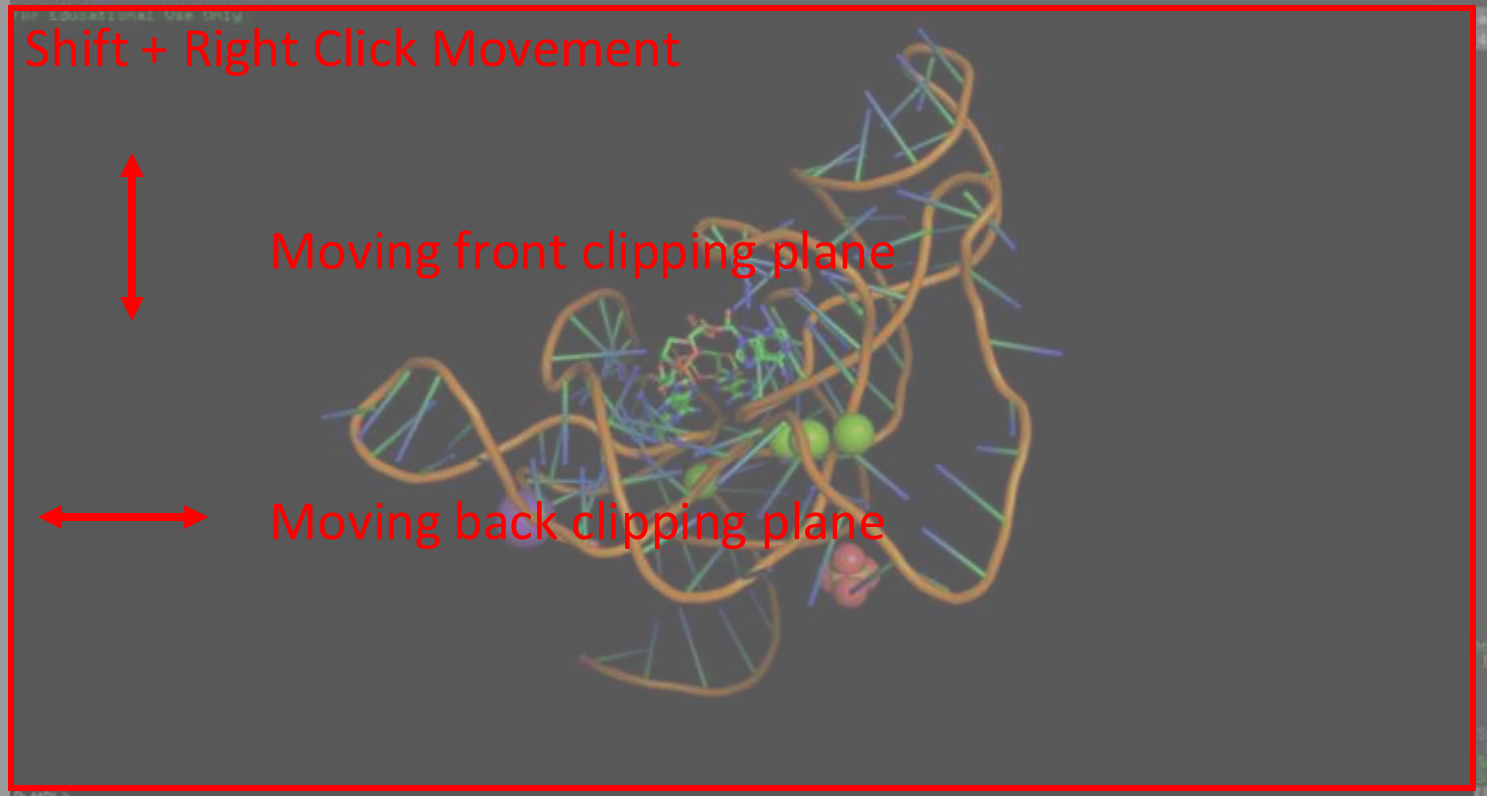

Left Click and Drag
Rotation along Y axis

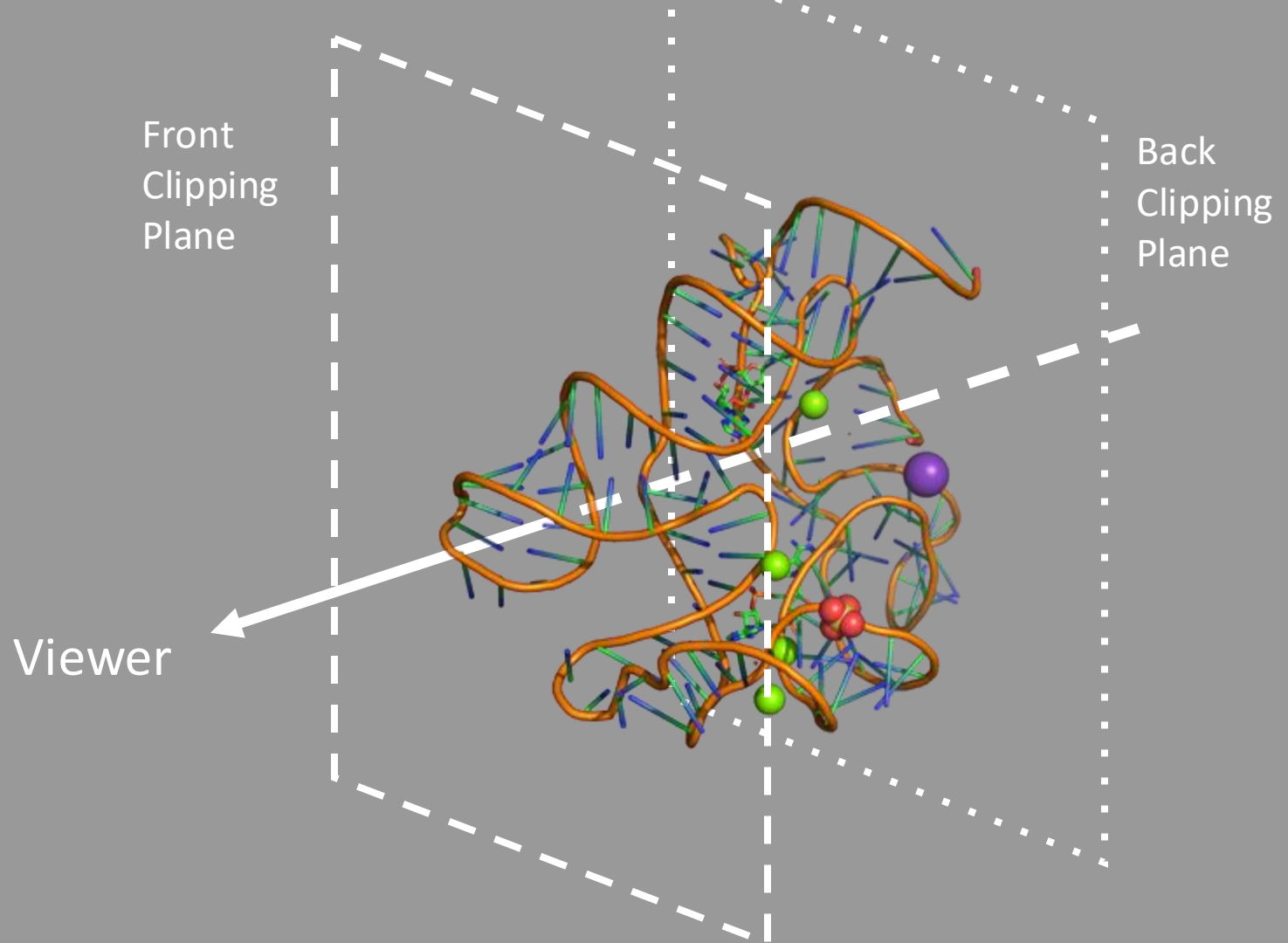

Left Click and Drag
Rotation along X axis


Left Click and Drag
X
Rotation along z axis


Middle Click and Drag
XY translation

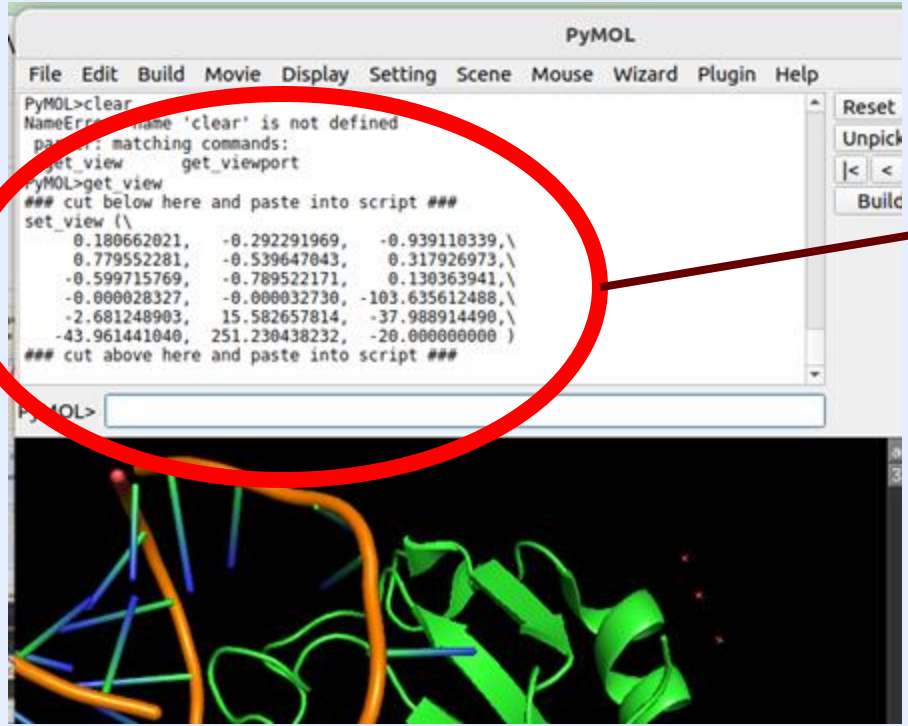

Right Click and Drag
Z translation
or Zoom


Shift + Right Click Movement
Moving front clipping plane
Moving back clipping plane


Front
Clipping
Plane
Back
Clipping
Plane
Viewer

Moving the Structure

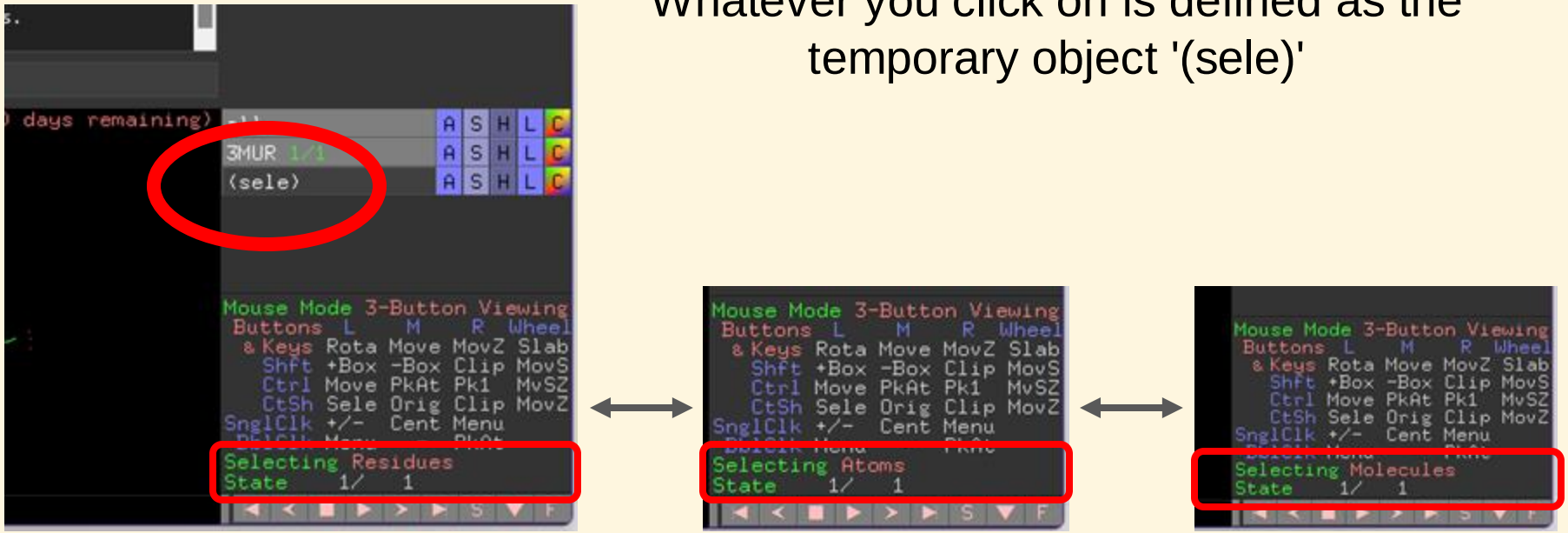
Move structure where you want and run:
> get_view



fetch *PDB Number*
set_view (\
0.180662021, -0.292291969, -0.939110339,\
0.779552281, -0.539647043, 0.317926973,\
-0.599715769, -0.789522171, 0.130363941,\
-0.000028327, -0.000032730, -103.635612488,\
-2.681248903, 15.582657814, -37.988914490,\
-43.961441040, 251.230438232, -20.000000000)

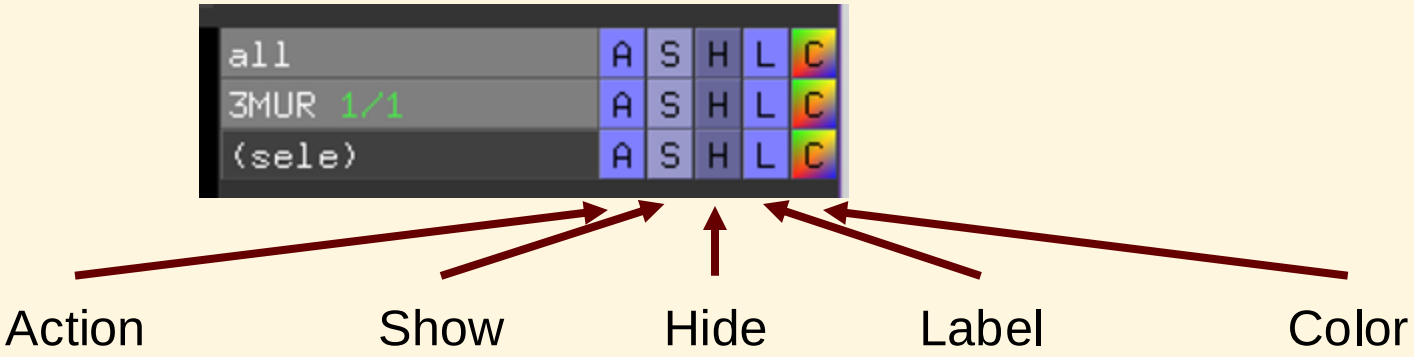
Selecting parts of the structure

Whatever you click on is defined as the temporary object '(sele)'

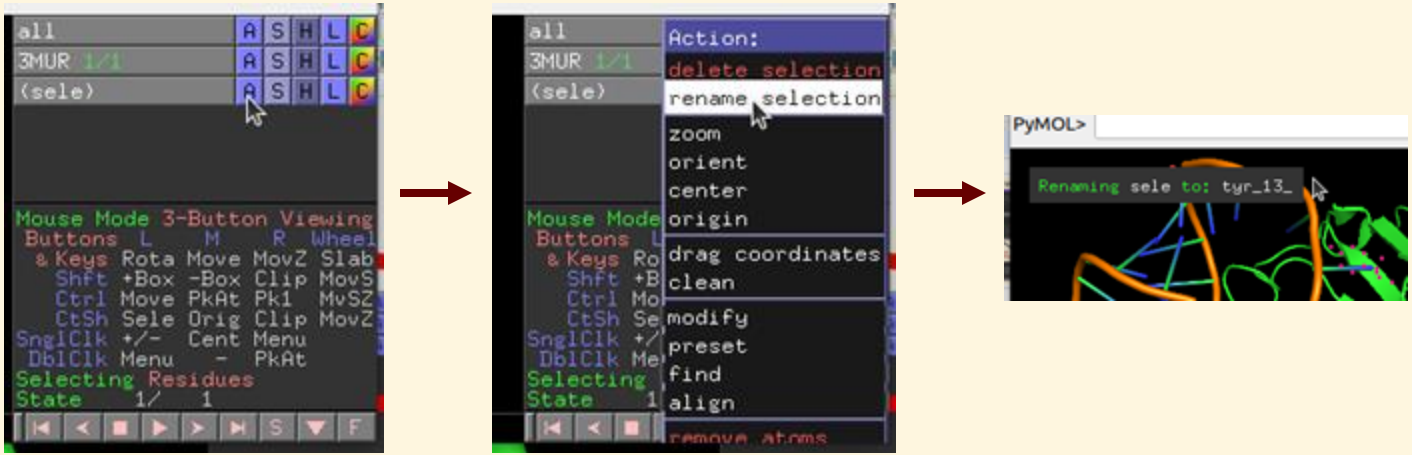


Clicking on the box changes what clicking selects

You can do stuff to selections!



Renaming a (sele) "saves it"



You can also define selections using the command line

When you select a residue it tells you what the name of that residue is

The name of the object

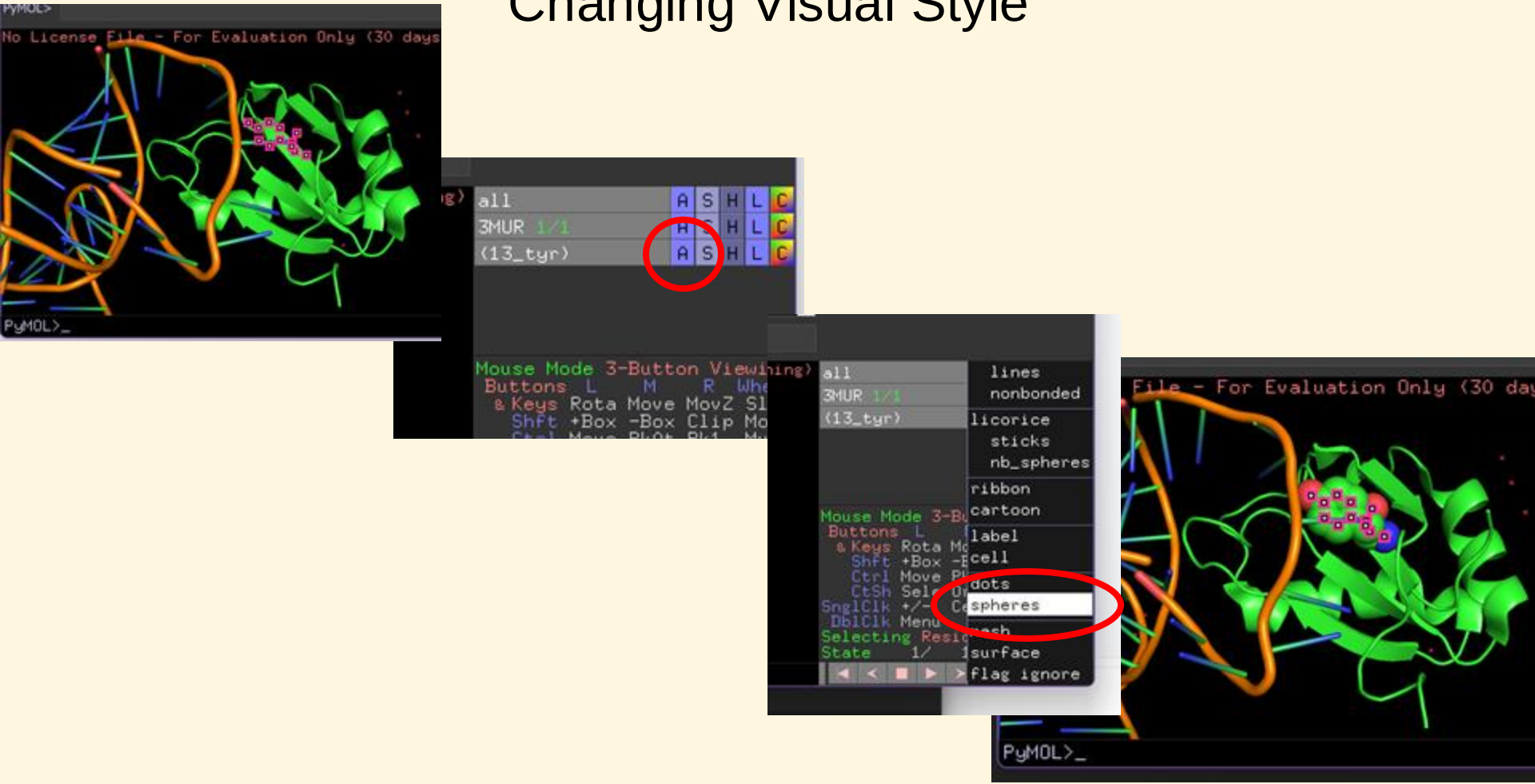
select 13_tyr, /3MUR/A/P/TYR`13

What is included in the selection

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

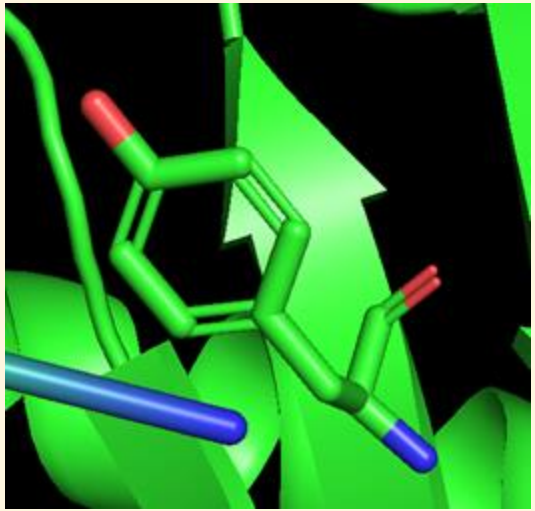
```
fetch 3MUR
set_view (\
     0.180662021,   -0.292291969,   -0.939110339,\
     0.779552281,   -0.539647043,    0.317926973,\
    -0.599715769,   -0.789522171,    0.130363941,\
    -0.000028327,   -0.000032730, -103.635612488,\
    -2.681248903,   15.582657814,  -37.988914490,\
   -43.961441040,  251.230438232,  -20.000000000 )
select 13_tyr, /3MUR/A/P/ILE`12
```

Changing Visual Style

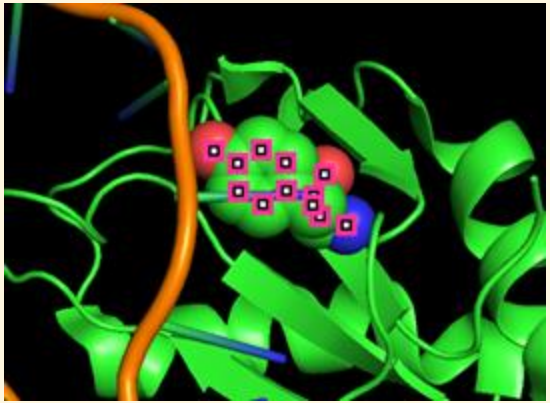


Many Visual Styles Exist

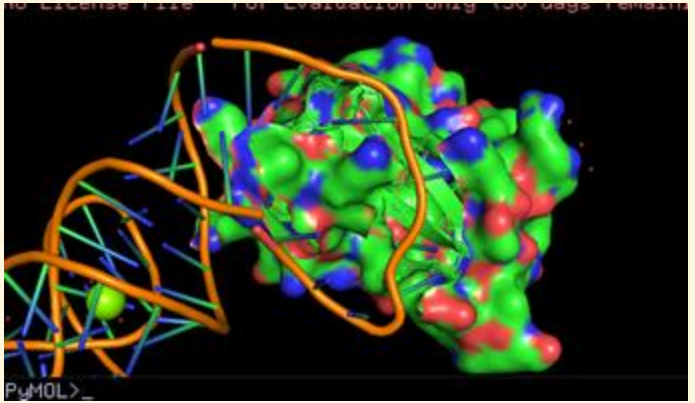
Sticks



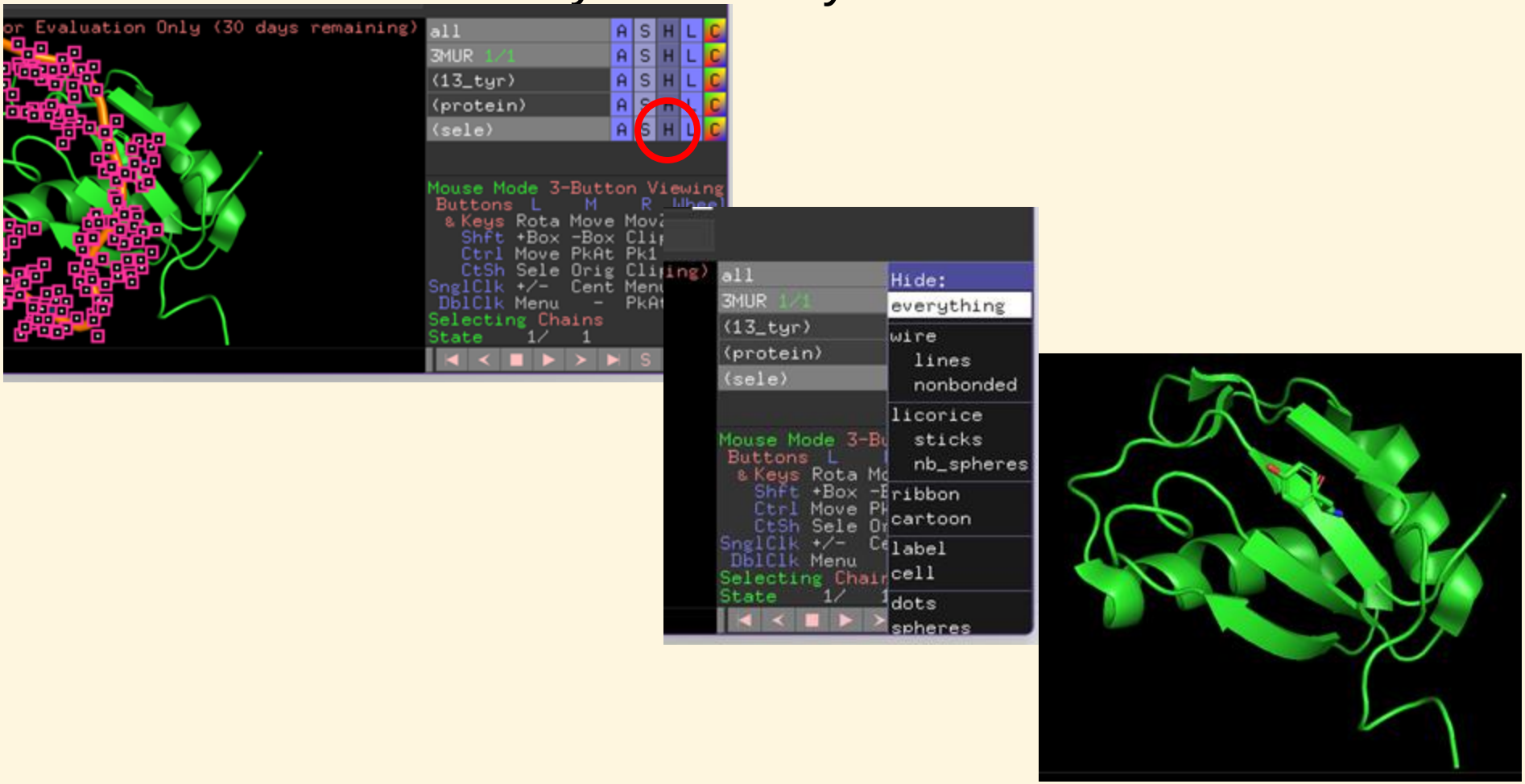
Spheres



Surface

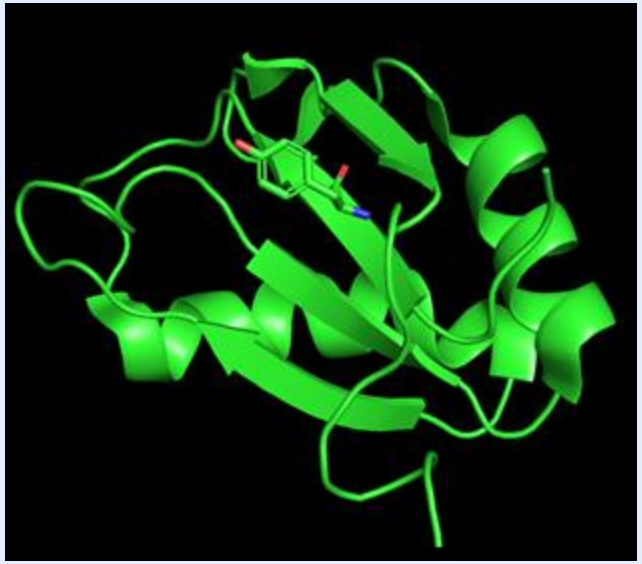


Many Visual Styles Exist



You can do all this via the command line

```
fetch 3MUR
set_view (\
     0.180662021,   -0.292291969,   -0.939110339,\
     0.779552281,   -0.539647043,    0.317926973,\
    -0.599715769,   -0.789522171,    0.130363941,\
    -0.000028327,   -0.000032730, -103.635612488,\
    -2.681248903,   15.582657814,  -37.988914490,\
   -43.961441040,  251.230438232,  -20.000000000 )
select 13_tyr, /3MUR/A/P/ILE`12
select protein, /3MUR/A/P
hide everything
show_as cartoon, protein
show sticks, 13_tyr
```



You can do all this via the command line

hide everything

hide everything

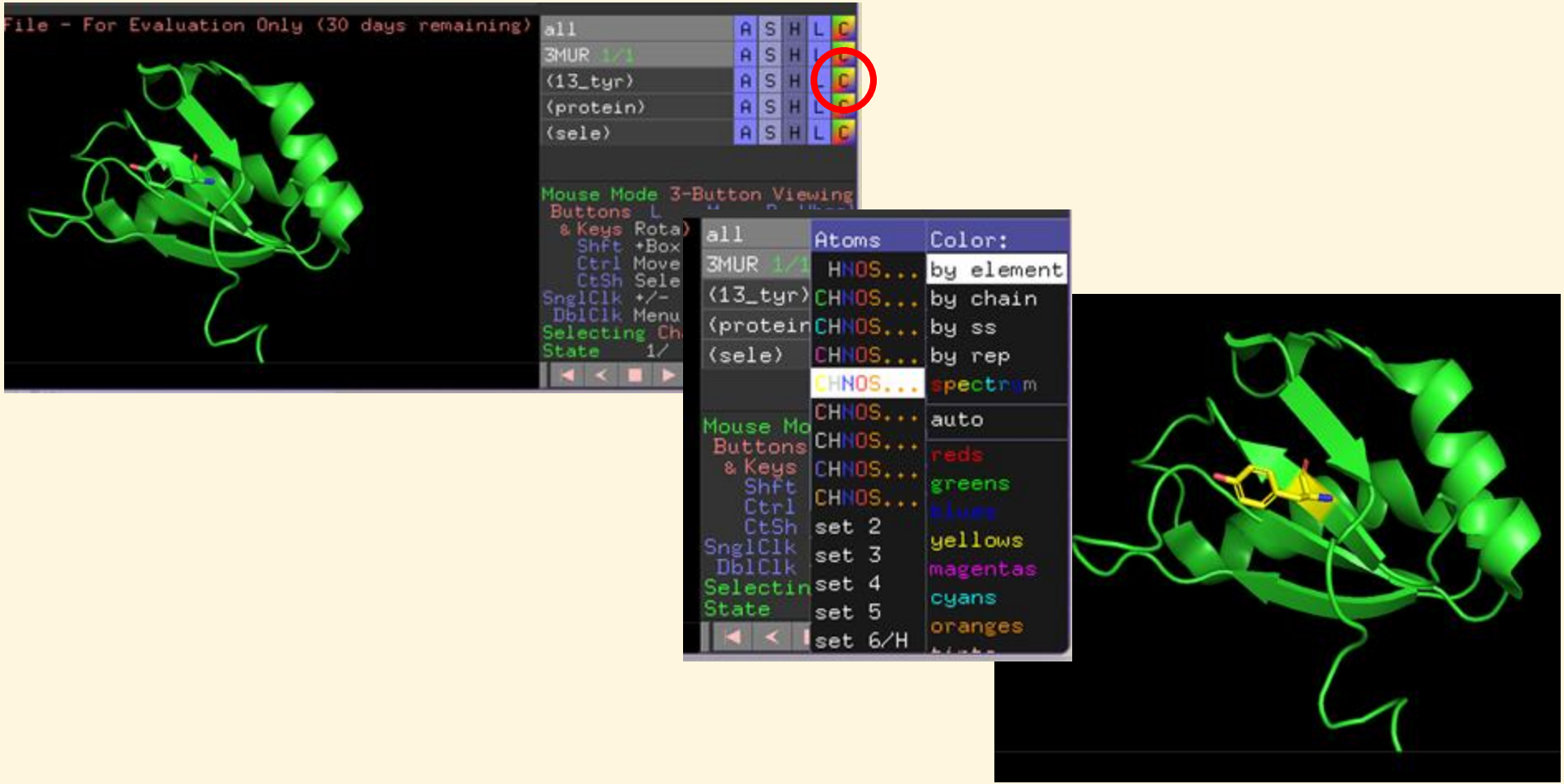
show_as cartoon, protein

Replace all current representations of protein with cartoon

show sticks, 13_tyr

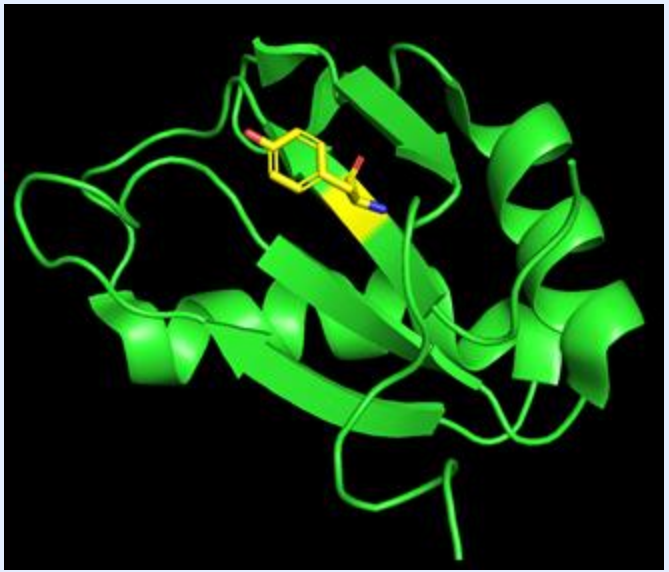
Shows sticks representation for 13_tyr on top all all other representations

Changing Color



You can do all this via the command line

```
fetch 3MUR
set_view (\
     0.180662021,   -0.292291969,   -0.939110339,\
     0.779552281,   -0.539647043,    0.317926973,\
    -0.599715769,   -0.789522171,    0.130363941,\
    -0.000028327,   -0.000032730, -103.635612488,\
    -2.681248903,   15.582657814,  -37.988914490,\
   -43.961441040,  251.230438232,  -20.000000000 )
select 13_tyr, /3MUR/A/P/TYR`13
select protein, /3MUR/A/P
hide everything
show_as cartoon, protein
show sticks, 13_tyr
color yellow, 13_tyr
color atomic, (not elem C)
```



You can do all this via the command line

color yellow, 13_tyr

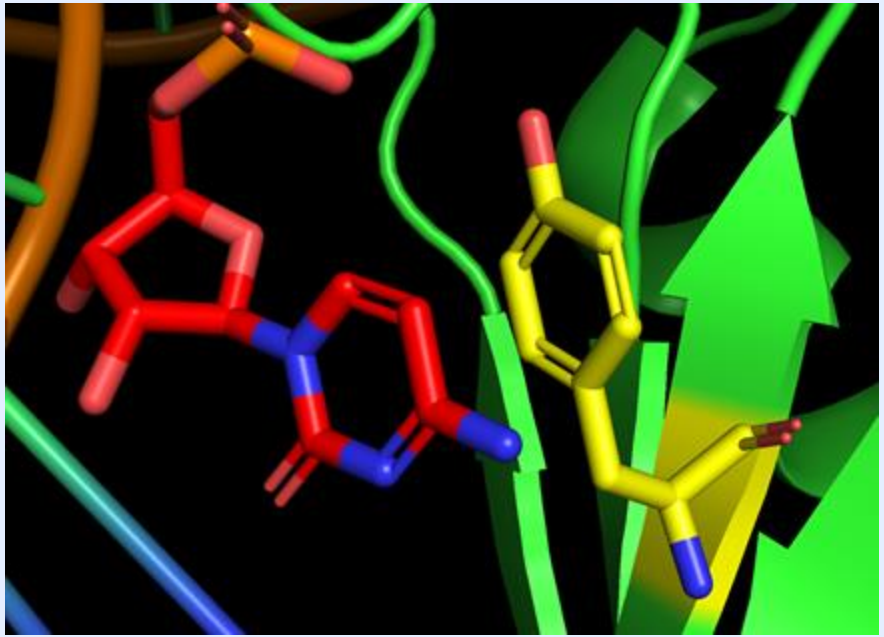
Color all of 13_tyr yellow

color atomic, (not elem C)

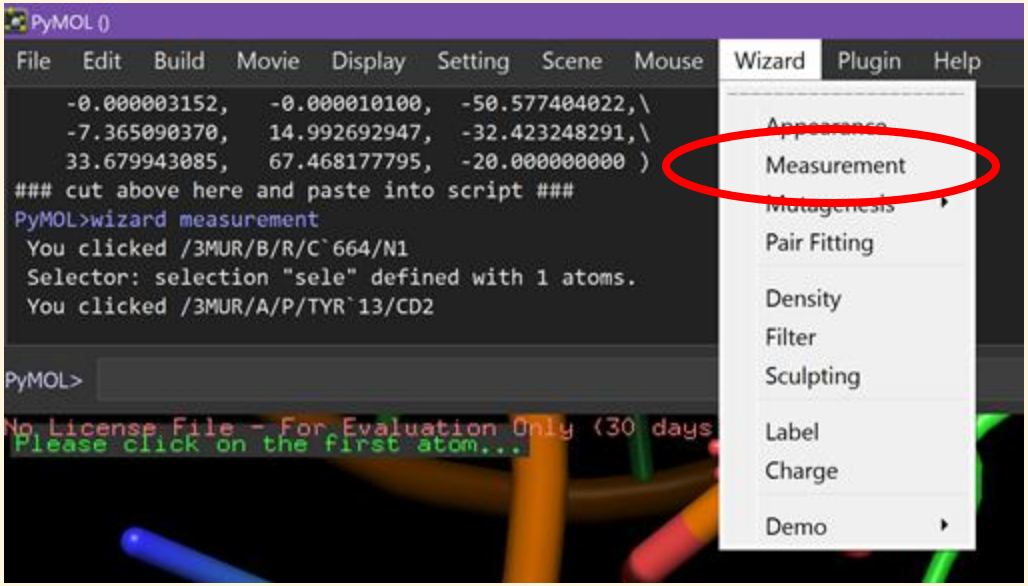
Color all non-carbon (not elem C) atoms by their element

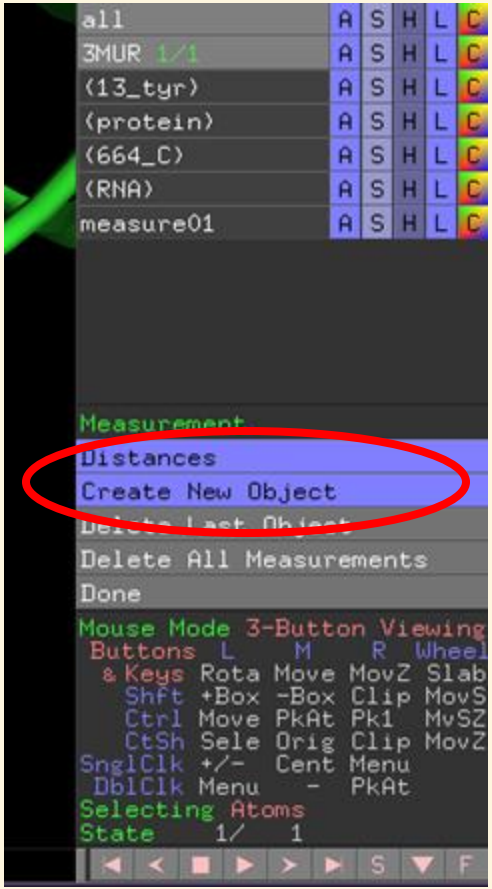
I added a similar representation of C 664 on the RNA to check for pi-pi interactions

```
fetch 3MUR
set_view (\
     0.739973485,   -0.202702120,   -0.641366601,\
    -0.156248644,   -0.979226887,    0.129209325,\
    -0.654235482,    0.004602869,   -0.756276071,\
     0.000002563,    0.000000541,  -40.599575043,\
    -8.614984512,   15.429700851,  -31.411344528,\
    25.389310837,   55.798702240,  -20.000000000 )
select 13_tyr, /3MUR/A/P/TYR`13
select protein, /3MUR/A/P
hide everything
show_as cartoon, protein
show sticks, 13_tyr
color yellow, 13_tyr
select 664_C, /3MUR/B/R/C`664
select RNA./3MUR/B/R
show_as cartoon, RNA
show_as stick, 664_C
color red, 664_C
color atomic, (not elem C)
```

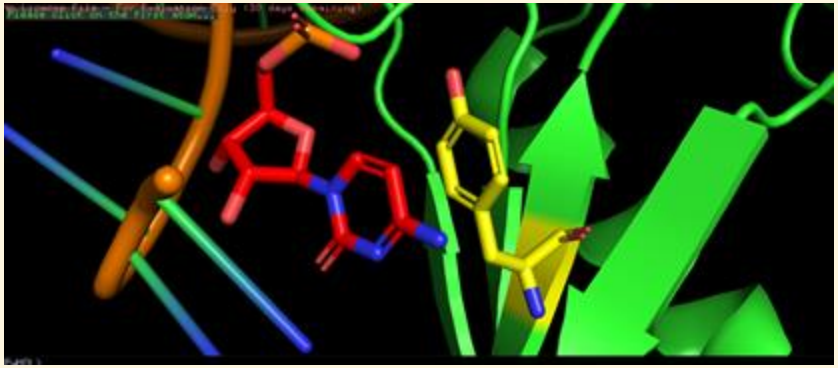


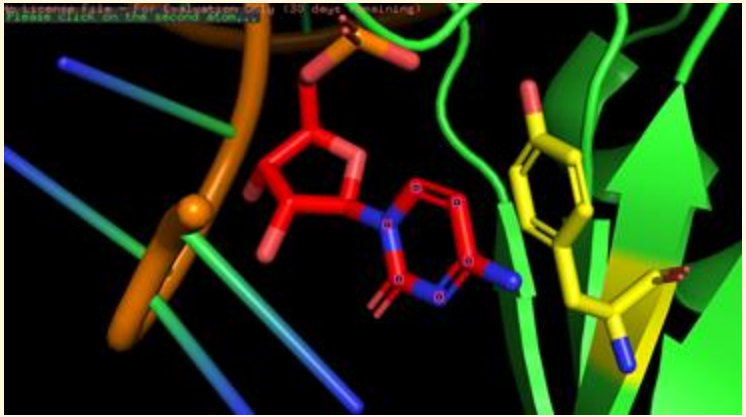
Opening the measurement wizard

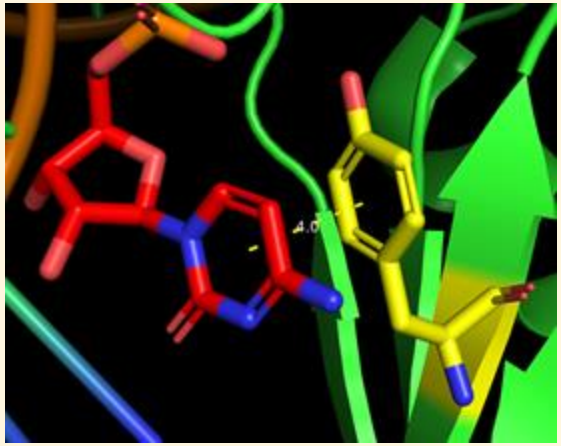




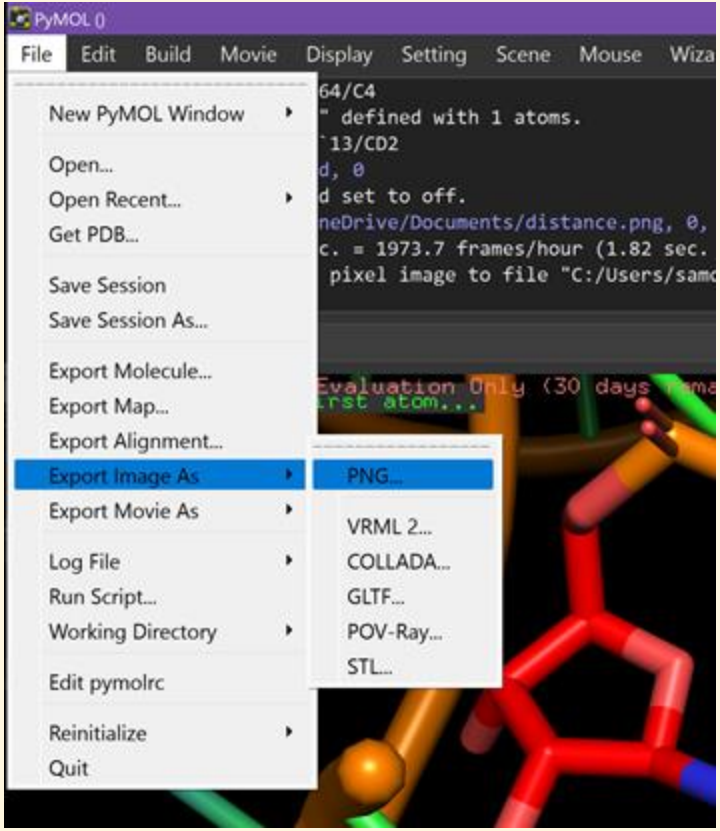
Showing distance

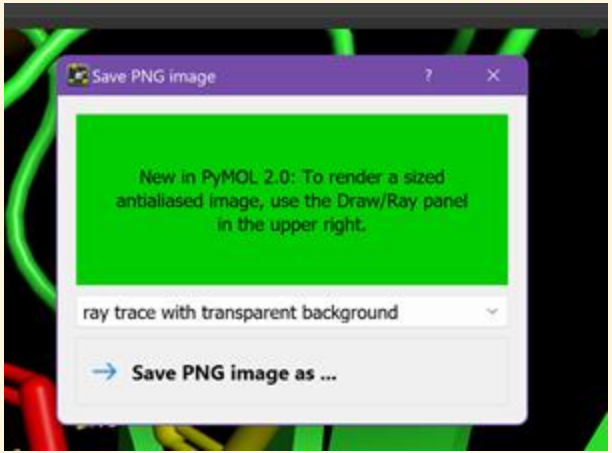


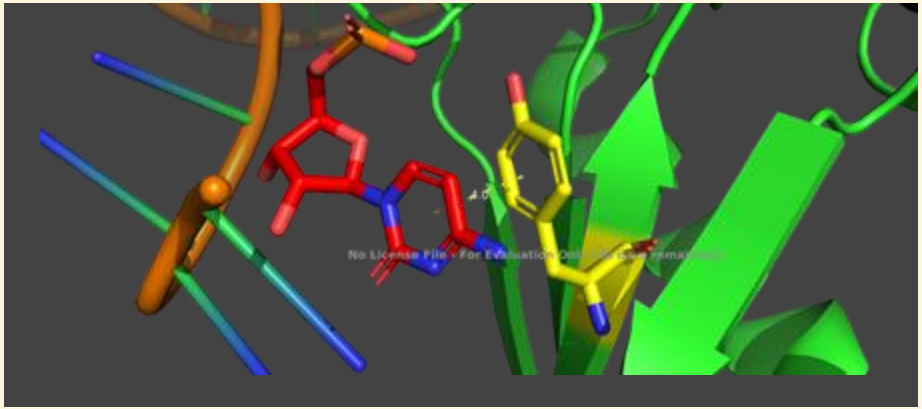




Exporting Image







Script for making a random NT at a random angle

```
import pymol
import random
import time

cmd.reinitialize()

questions = { "Thymine": ['T'], "Adenine": ['A'], "Cytosine": ['C'], "Guanine": ['G']}

answer=random.choice(list(questions.keys()))
pym_frag=questions.get(answer)

flip_it=random.randint(0,1)
x_rotate=random.randint(-45,45)
y_rotate=random.randint(-45,45)
z_rotate=random.randint(0,360)

if flip_it == 1:
    x_rotate=x_rotate + 180

pymol.cmd.fnab(input=pym_frag, name="myDNA", dbl_helix=0)
pymol.cmd.show(representation="sticks")
pymol.cmd.rotate(axis='x',angle=x_rotate)
pymol.cmd.rotate(axis='y',angle=y_rotate)
pymol.cmd.rotate(axis='z',angle=z_rotate)
pymol.cmd.center(selection="myDNA")
```