

PyMOL is a user-sponsored molecular visualization system on an **open-source foundation**, maintained and distributed by **Schrödinger**.

We are happy to introduce
PyMOL 2.5!!

DOWNLOAD NOW

BUY LICENSE

RELEASE HIGHLIGHTS

<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

The screenshot shows the RCSB PDB website homepage. At the top, there is a navigation bar with links for Deposit, Search, Visualize, Analyze, Download, Learn, More, Documentation, and Careers. On the right side of this bar are buttons for MyPDB and Contact us. Below the navigation bar, the RCSB PDB logo is displayed on the left, followed by statistics: 195,565 Structures from the PDB and 1,000,361 Computed Structure Models (CSM). A search bar is located in the center, with a dropdown menu for '3D Structures' and a search icon. To the right of the search bar is a toggle for 'Include CSM' and a 'Help' link. Below the search bar, there are logos for PDB-101, PDB, EMDataResource, Nucleic Acid Database, and wwPDB Foundation. A teal banner across the middle of the page reads 'NEW! Computed Structure Models (CSM)' with a 'Learn more' button. On the left side, there is a vertical navigation menu with links for Welcome, Deposit, Search, Visualize, Analyze, Download, and Learn. The main content area features a section titled 'RCSB Protein Data Bank (RCSB PDB) enables breakthroughs in science and education by providing access and tools for exploration, visualization, and analysis of:' followed by two bullet points: 'Experimentally-determined 3D structures from the Protein Data Bank (PDB) archive' and 'Computed Structure Models (CSM) from AlphaFold DB and ModelArchive'. Below this text is a paragraph: 'These data can be explored in context of external annotations providing a structural view of biology.' At the bottom of the main content area, there are two promotional banners: one for 'COVID-19 CORONAVIRUS Resources' and another for 'Join the RCSB PDB Team'. On the right side of the main content area, there is a section titled 'September Molecule of the Month' featuring a 3D molecular model of a protein structure with different domains colored in yellow, blue, purple, and red.

RCSB PDB Deposit ▾ Search ▾ Visualize ▾ Analyze ▾ Download ▾ Learn ▾ More ▾ Documentation ▾ Careers MyPDB ▾ Contact us

RCSB PDB 195,565 Structures from the PDB
1,000,361 Computed Structure Models (CSM)

3D Structures Enter search term(s), Entry ID(s), or sequence Include CSM

Advanced Search | Browse Annotations Help

PDB-101 PDB EMDataResource NUCLEIC ACID DATABASE wwPDB Foundation

NEW! Computed Structure Models (CSM) [Learn more](#)

Welcome

Deposit

Search

Visualize

Analyze

Download

Learn

RCSB Protein Data Bank (RCSB PDB) enables breakthroughs in science and education by providing access and tools for exploration, visualization, and analysis of:

- Experimentally-determined 3D structures from the Protein Data Bank (PDB) archive
- Computed Structure Models (CSM) from AlphaFold DB and ModelArchive

These data can be explored in context of external annotations providing a structural view of biology.

COVID-19 CORONAVIRUS Resources

Join the RCSB PDB Team

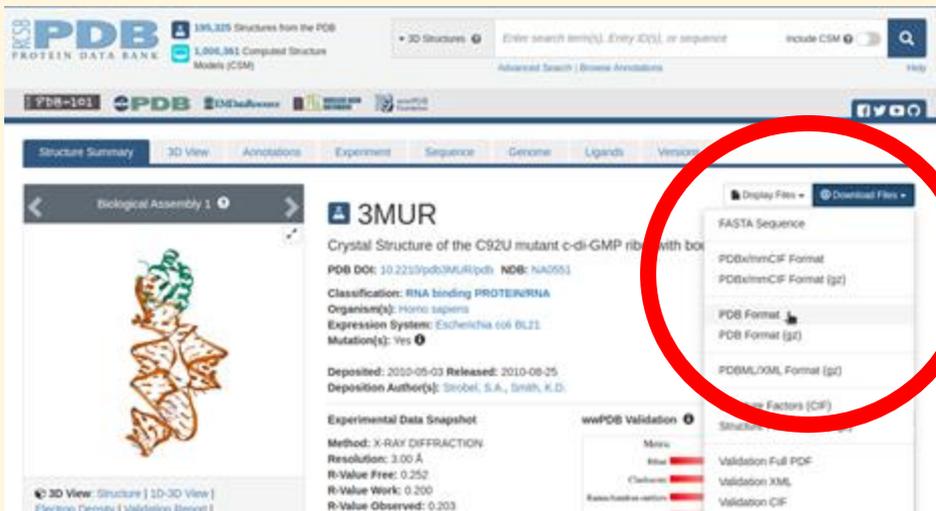
September Molecule of the Month

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

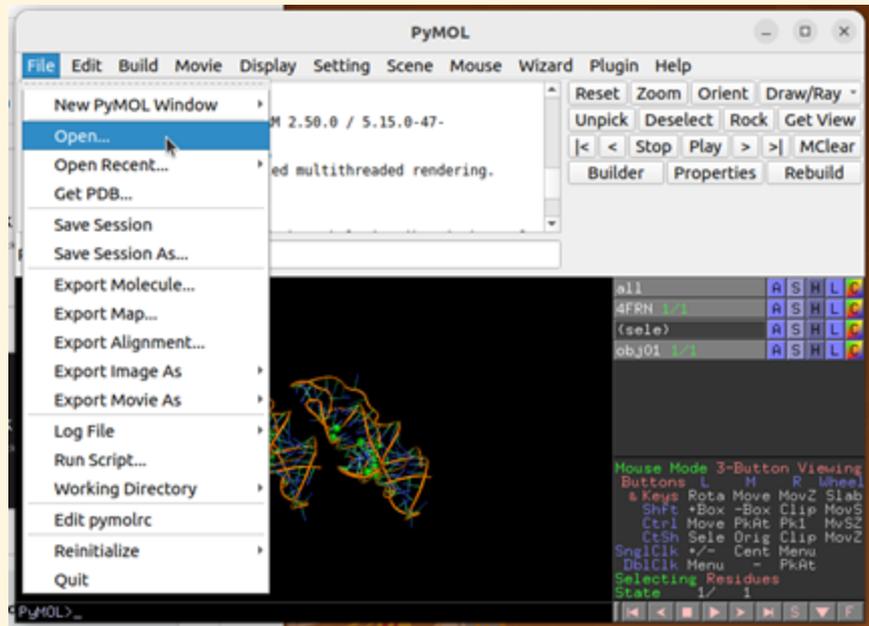
Download PDB file

File → Open...



The screenshot shows the PDB website interface for the 3MUR structure. The 'Download Files' button is circled in red. A dropdown menu is open, showing various file formats for download:

- FASTA Sequence
- PDB/mmCIF Format
- PDB/mmCIF Format (gz)
- PDB Format
- PDB Format (gz)
- PDB/LOXAL Format (gz)



The screenshot shows the PyMOL software interface. The 'File' menu is open, and the 'Open...' option is highlighted. The interface includes a menu bar (File, Edit, Build, Movie, Display, Setting, Scene, Mouse, Wizard, Plugin, Help), a toolbar with buttons like Reset, Zoom, Orient, Draw/Ray, Unpick, Deselect, Rock, Get View, and a 3D molecular model of a protein structure.

PyMol Wiki



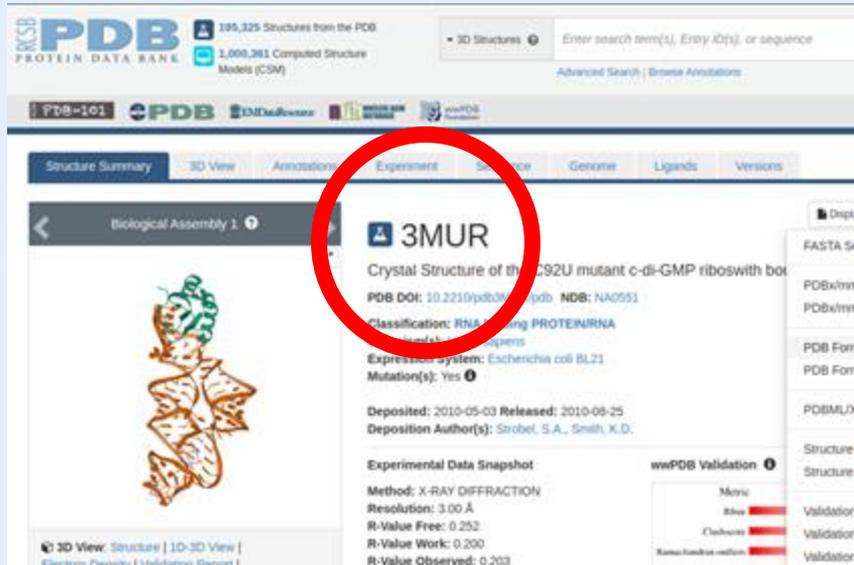
The image shows a screenshot of the PyMol Wiki Main Page. On the left side, there is a vertical sidebar with a purple header image containing the text 'PyMOLWiki'. Below the header, the sidebar contains a list of navigation links: 'Main page', 'Recent changes', 'Random page', 'Help', 'SBGrid Resources', and 'SBGrid Consortium'. The main content area on the right has a top navigation bar with 'Main page' and 'Discussion' buttons. Below this, the title 'Main Page' is displayed in a large serif font. Underneath the title is a large, solid red rectangular area, which appears to be a placeholder or a redaction.

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

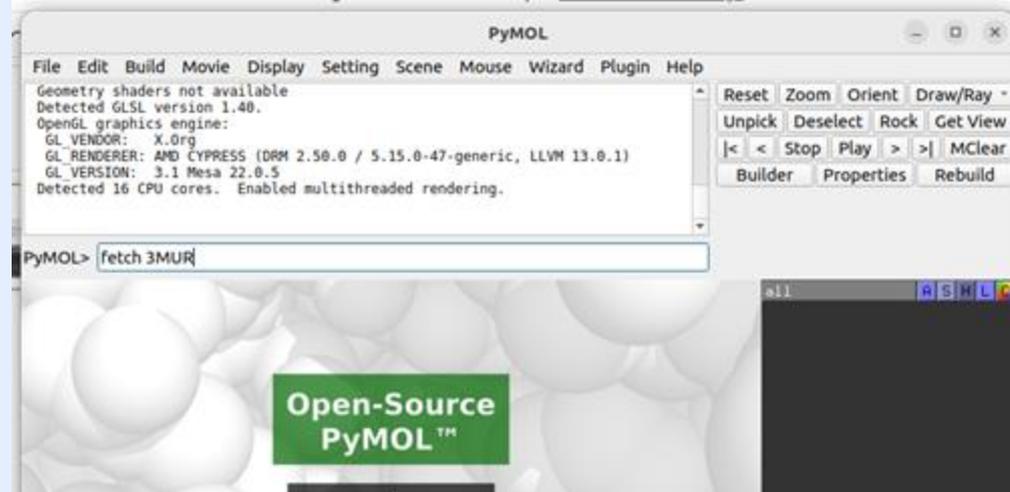
Opening a structure

Find PDB Number

> fetch *PDB Number*

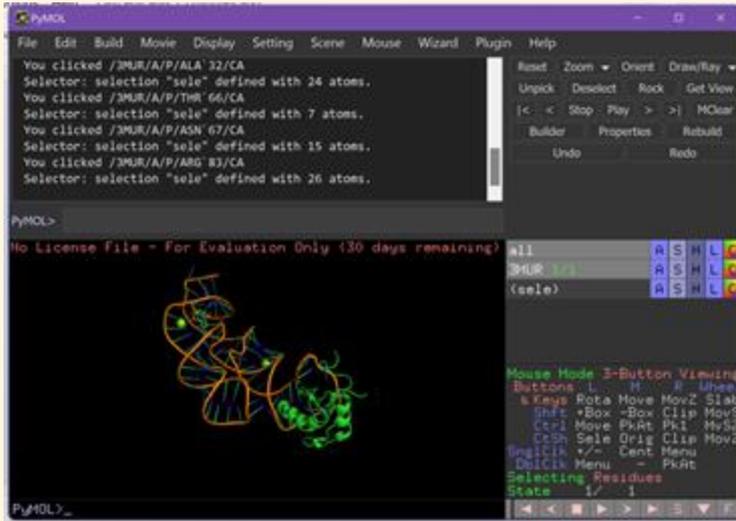


The screenshot shows the PDB website interface. The search bar at the top contains the text "3MUR", which is circled in red. Below the search bar, the entry for "3MUR" is displayed. The title is "Crystal Structure of the C92U mutant c-di-GMP riboswitch bound to c-di-GMP". The PDB ID is 3MUR, and the DOI is 10.2201/pdb3MUR/pdb3MUR. The classification is RNA binding PROTEIN/RNA. The expression system is Escherichia coli BL21. The deposition date is 2010-05-03, and the release date is 2010-08-25. The authors are Strobel, S.A., and Smith, K.D. The experimental data snapshot shows the method as X-RAY DIFFRACTION, resolution as 3.00 Å, R-Value Free as 0.252, R-Value Work as 0.200, and R-Value Observed as 0.203. The wwPDB Validation section shows metrics for Missing, Clashes, and Ramachandran outliers, all with red bars indicating validation status.

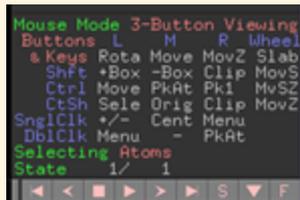


The screenshot shows the PyMOL software interface. The command line at the bottom contains the text "fetch 3MUR". The main window displays a 3D model of a protein structure, which is currently blank. The PyMOL logo and the text "Open-Source PyMOL™" are visible in the bottom right corner. The top menu bar includes File, Edit, Build, Movie, Display, Setting, Scene, Mouse, Wizard, Plugin, and Help. The right sidebar contains various controls such as Reset, Zoom, Orient, Draw/Ray, Unpick, Deselect, Rock, Get View, and MClear.

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: @1-may-2019  
Detected 8 CPU cores. Enabled multithreaded rendering.
```

```
PyMOL> fetch 4QK8
```

```
please wait ...
```

```
TITLE: Thermoanaerobacter pseudethanolicus c-di-AMP-riboswitch
```

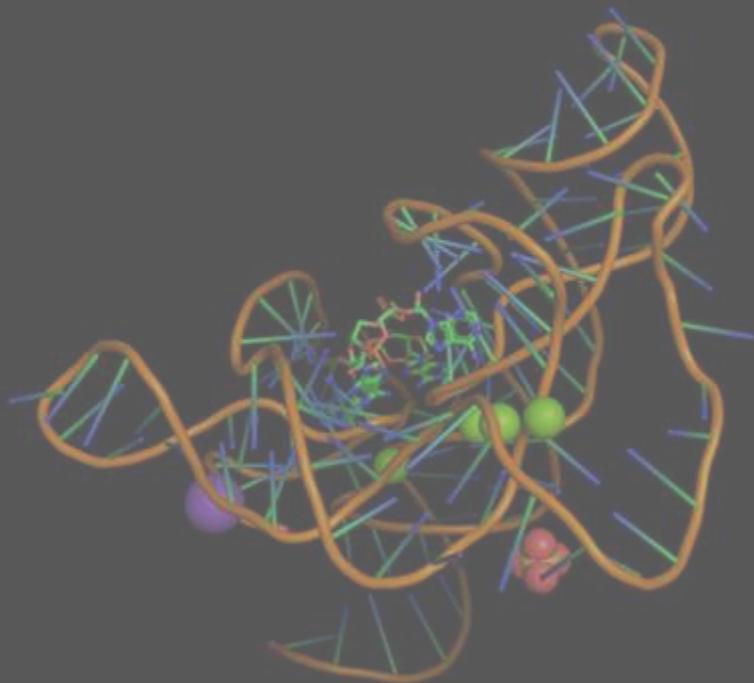
```
ExecutiveLoad-Detail: Detected mmCIF
```

```
CmdLoad: loaded as "4QK8".
```

```
PyMOL>
```

```
for EDUCATIONAL USE ONLY
```

Display Area



```
PyMOL>
```

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

```
All  
4QK8 1/1
```

```
Mouse Mode 3-Button Viewing  
Buttons L H R Wheel  
4 Keys Rotate Move MoveZ Slab  
Shift+Box +Box Clip Move5  
Ctrl+Mouse Pick Pick MoveZ  
Ctrl+Shift+Mouse Pick Clip MoveZ  
SingleClick *??: Cent Menu  
DoubleClick Menu = Pick  
Selecting Residue  
State 1/1
```

```
GL_VENDOR: ATI Technologies Inc.  
GL_RENDERER: AMD Radeon Pro 455 OpenGL Engine  
GL_VERSION: 2.1 ATI-2.4.9  
License Expiry date: @1-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

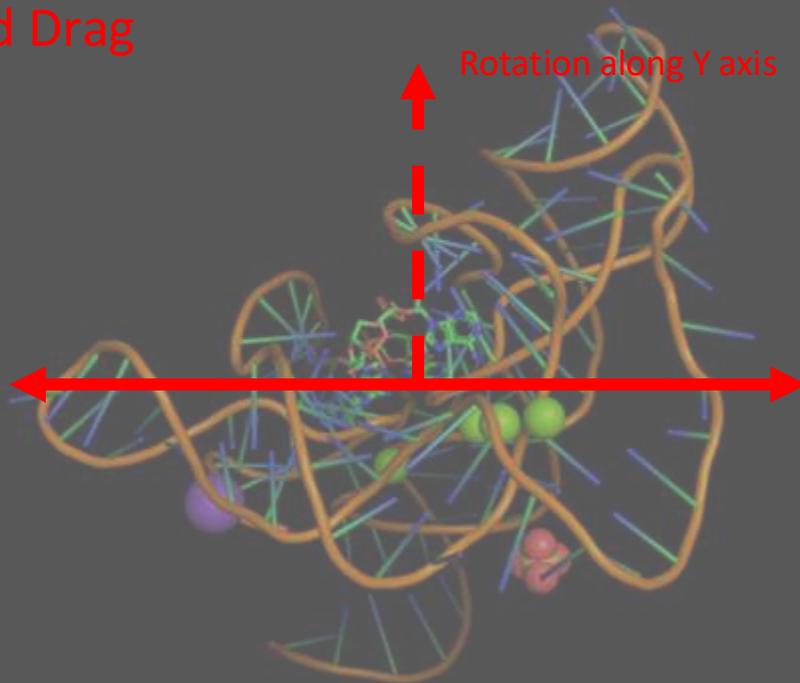
CmdLoad: loaded as "4QK8".

PyMOL>

For Educational Use Only

Left Click and Drag

Rotation along Y axis



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

All
4QK8

Mouse Mode 3-Button Viewing
Buttons L H R Wheel
4 Keys Rotate Move MoveZ Slab
Shift+Box +Box Clip Move5
Ctrl+Mouse Pick Pick MoveZ
Ctrl+Shift+Mouse Pick Clip MoveZ
SingleClick *??: Cent Menu
DoubleClick Menu = PickRt
Selecting Residues
State 1/ 1

PyMOL>

```
GL_VENDOR: ATI Technologies Inc.  
GL_RENDERER: AMD Radeon Pro 455 OpenGL Engine  
GL_VERSION: 2.1 ATI-2.4.9  
License Expiry date: @1-may-2019  
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PyMOL>fetch 4QK8

please wait ...

TITLE Thermoanaerobacter pseudethanolicus c-di-AMP-riboswitch

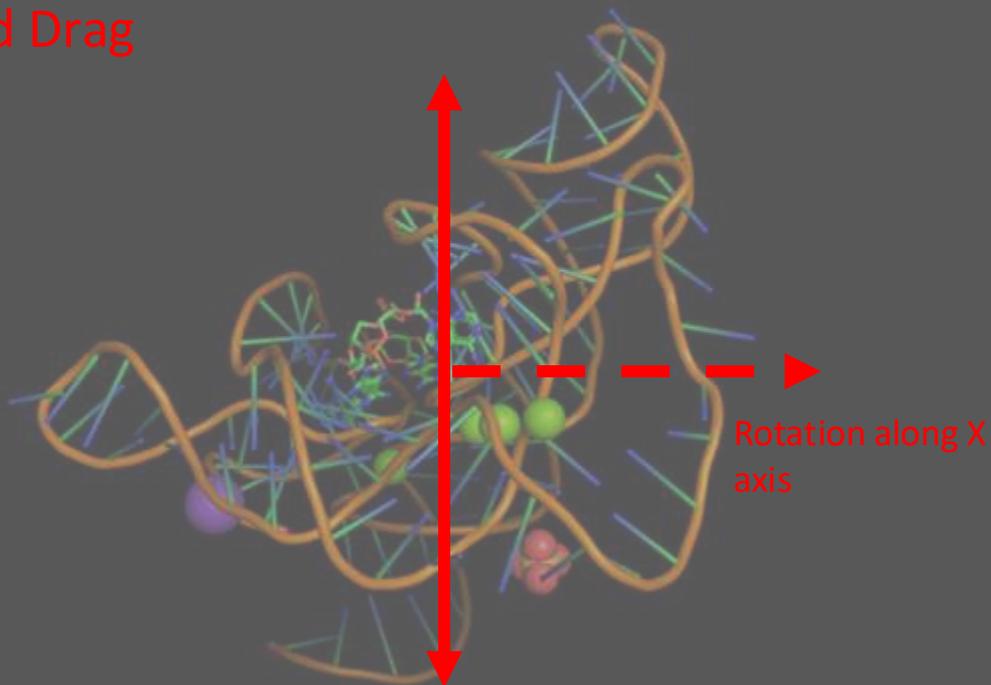
ExecutiveLoad-Detail: Detected mmCIF

CmdLoad: loaded as "4QK8".

PyMOL>

For Educational Use Only

Left Click and Drag



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

4QK8
4QK8

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
4 Keys Rotate Move MoveZ Slab
Shift+Box +Box Clip Move5
Ctrl+Mouse Pick Pick MoveZ
Ctrl+Shift+Mouse Drag Clip MoveZ
SingleClick *??: Cent Menu
DoubleClick Menu = PickRt
Selecting Residue
State 1/ 1

PyMOL>

```
GL_VENDOR: ATI Technologies Inc.  
GL_RENDERER: AMD Radeon Pro 455 OpenGL Engine  
GL_VERSION: 2.1 ATI-2.4.9  
License Expiry date: @1-may-2019  
Detected 8 CPU cores. Enabled multithreaded rendering.
```

PyMOL>fetch 4QK8

please wait ...

TITLE: Thermoanaerobacter pseudethanolicus c-di-AMP-riboswitch

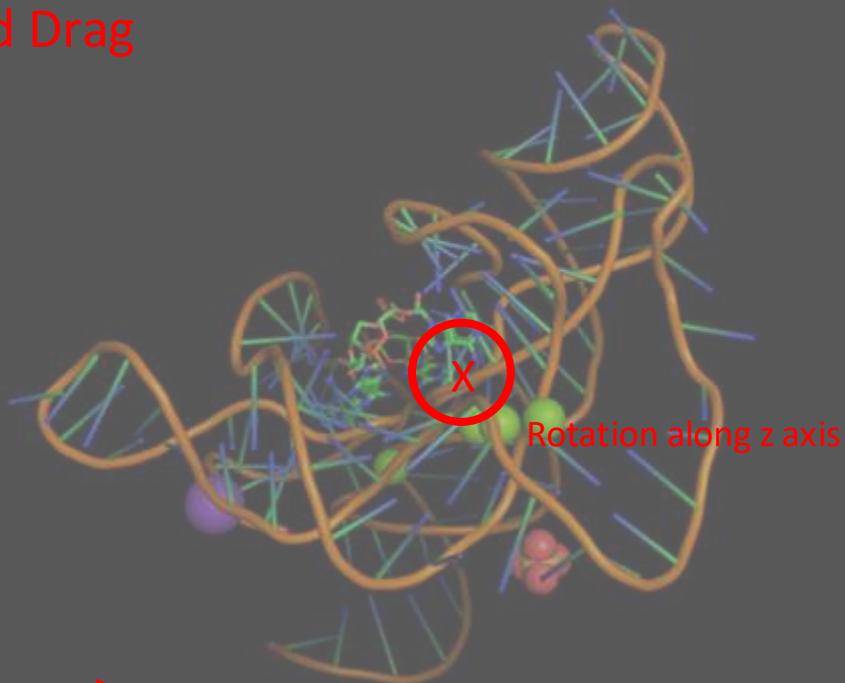
ExecutiveLoad-Detail: Detected mmCIF

EndLoad: loaded as "4QK8".

PyMOL>

For Educational Use Only

Left Click and Drag



PyMOL>

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

All
4QK8

Mouse Mode 3-Button Viewing
Buttons L H R Wheel
4 Keys Rotate Move MoveZ Slab
Shift+Box +Box Clip Move5
Ctrl+Move Pick Pick MoveZ
Ctrl+Shift+Move Orig Clip MoveZ
SingleClick *??: Cent Menu
DoubleClick Menu = PickRt
Selecting Residue
State 1/ 1

```
GL_VENDOR: ATI Technologies Inc.  
GL_RENDERER: AMD Radeon Pro 455 OpenGL Engine  
GL_VERSION: 2.1 ATI-2.4.9  
License Expiry date: @1-may-2019  
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```

```
PyMOL> fetch 4QK8
```

```
please wait ...
```

```
TITLE: Thermoanaerobacter pseudethanolicus c-di-AMP-riboswitch
```

```
ExecutiveLoad-Detail: Detected mmCIF
```

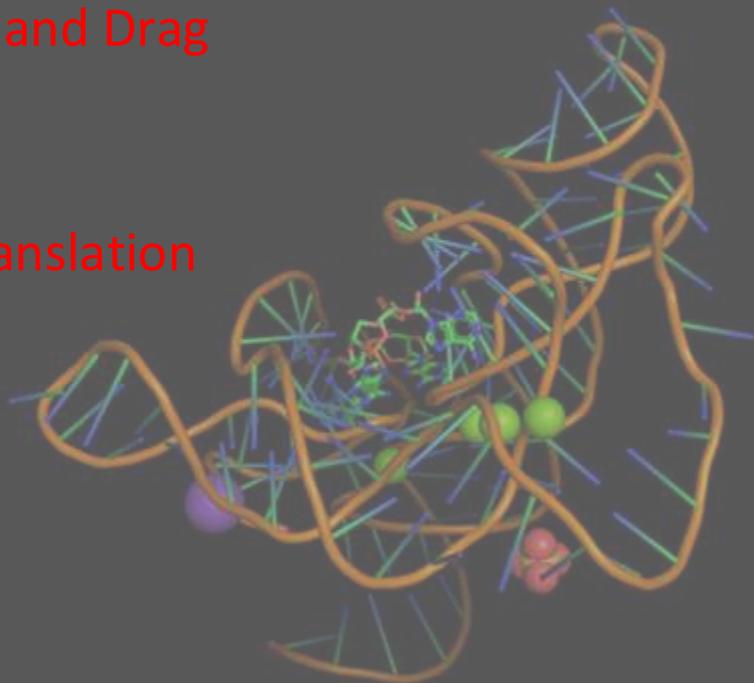
```
CmdLoad: loaded as "4QK8".
```

```
PyMOL>
```

```
For Educational Use Only
```

Middle Click and Drag

XY translation



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

```
All  
4QK8 1/1
```

```
Mouse Mode 3-Button Viewing  
Buttons L M R Wheel  
4 Keys Rotate Move MoveZ Slab  
Shift+Box +Box Clip Move5  
Ctrl+Mouse Pick Pick MoveZ  
Ctrl+Shift+Mouse Drag Clip MoveZ  
SingleClick *??: Cent Menu  
DoubleClick Menu = PickRt  
Selecting Residue  
State 1/1
```

```
PyMOL>
```

```
GL_VENDOR: ATI Technologies Inc.  
GL_RENDERER: AMD Radeon Pro 455 OpenGL Engine  
GL_VERSION: 2.1 ATI-2.4.9  
License Expiry date: @1-may-2019  
Detected 8 CPU cores. Enabled multithreaded rendering.
```

```
PyMOL> fetch 4QK8
```

```
please wait ...
```

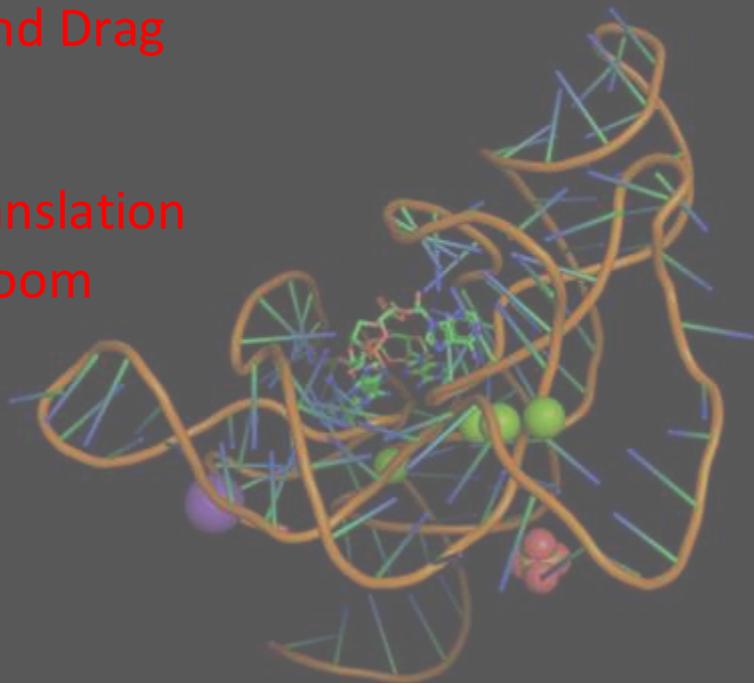
```
TITLE: Thermoanaerobacter pseudethanolicus c-di-AMP-riboswitch  
ExecutiveLoad-Detail: Detected mmCIF  
CndLoad: loaded as "4QK8".
```

```
PyMOL>
```

```
3D EDITOR: 3D VIEW ONLY
```

Right Click and Drag

Z translation
or Zoom



```
PyMOL>
```

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

```
All  
4QK8 1-1
```

```
Mouse Mode 3-Button Viewing  
Buttons L H R Wheel  
4 Keys Rotate Move MoveZ Slab  
Shift+Box +Box Clip Move5  
Ctrl+Mouse Pick Pkl MoveZ  
Ctrl+Shift+Mouse Pick Clip MoveZ  
SingleClick *??: Cent Menu  
DoubleClick Menu = PickRt  
Selecting Residue  
State 1/ 1
```

```
3D EDITOR: 3D VIEW ONLY
```

```
GL_VENDOR: ATI Technologies Inc.  
GL_RENDERER: AMD Radeon Pro 455 OpenGL Engine  
GL_VERSION: 2.1 ATI-2.4.9  
License Expiry date: @1-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>

For EDUCATIONAL USE ONLY

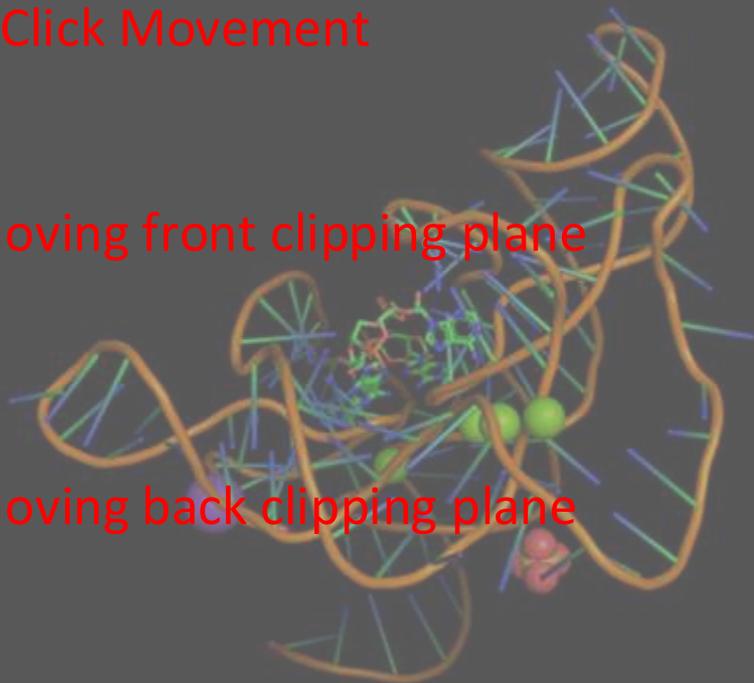
Shift + Right Click Movement



Moving front clipping plane



Moving back clipping plane

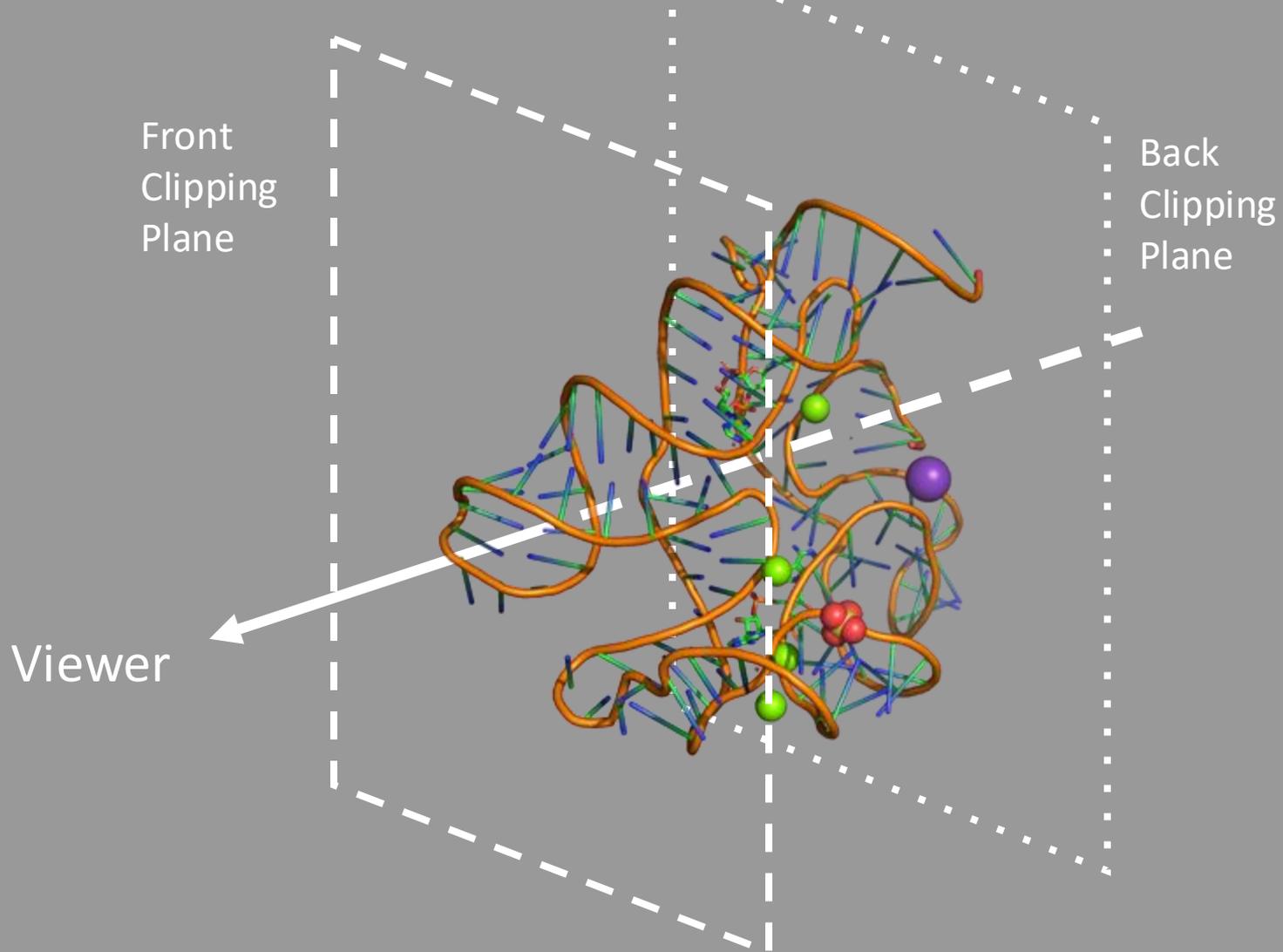


Reset Zoom Orient Draw/Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear
Builder Properties Rebuild

All
4QK8

```
Mouse Mode 3-Button Viewing  
Buttons L M R Wheel  
4 Keys Rotate Move MoveZ Slab  
Shift+Box +Box Clip Move5  
Ctrl+Mouse Pick Pick MoveZ  
Ctrl+Shift+Mouse Drag Clip MoveZ  
SingleClick *??: Cent Menu  
DoubleClick Menu = PickRt  
Selecting Residue  
State 1/ 1
```

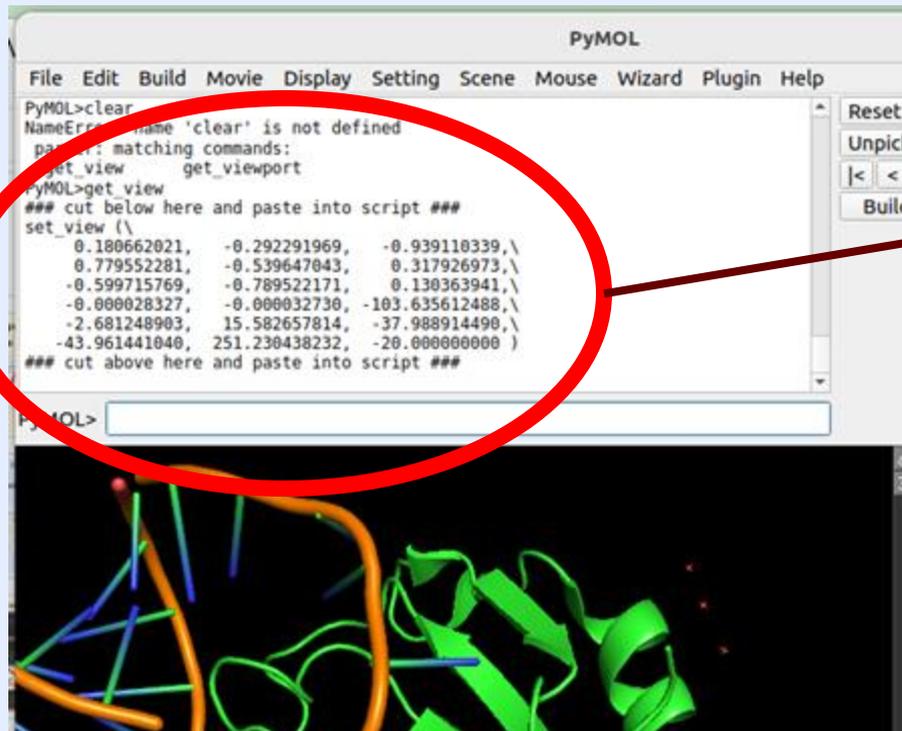
PyMOL>



Moving the Structure

Move structure where you want and run:

> get_view



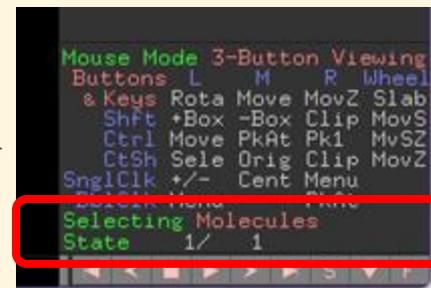
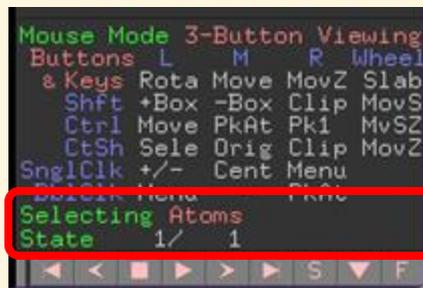
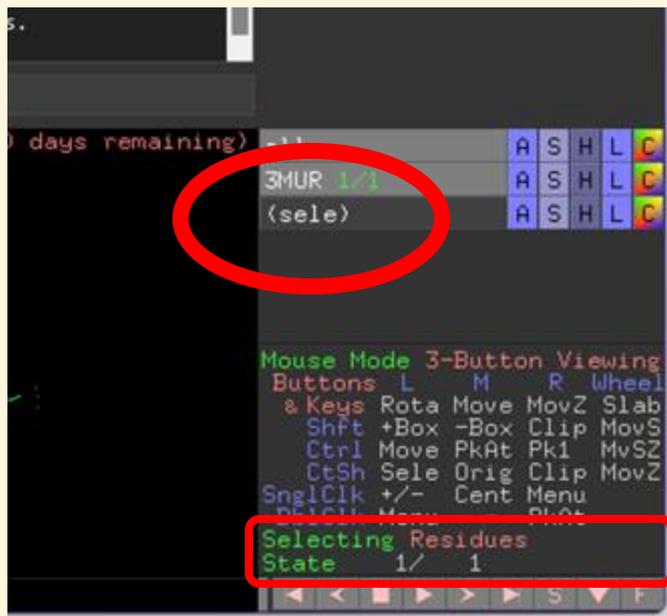
fetch *PDB Number*

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)

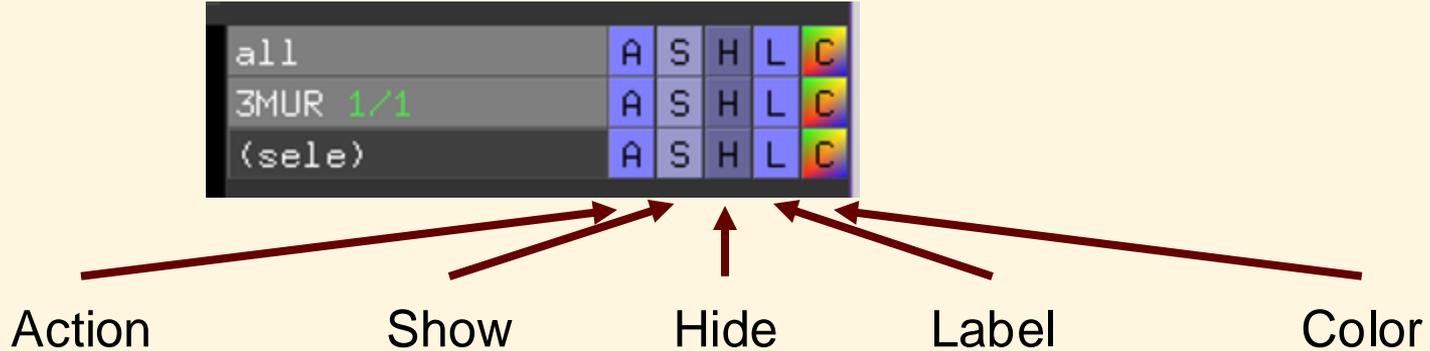
Selecting parts of the structure

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

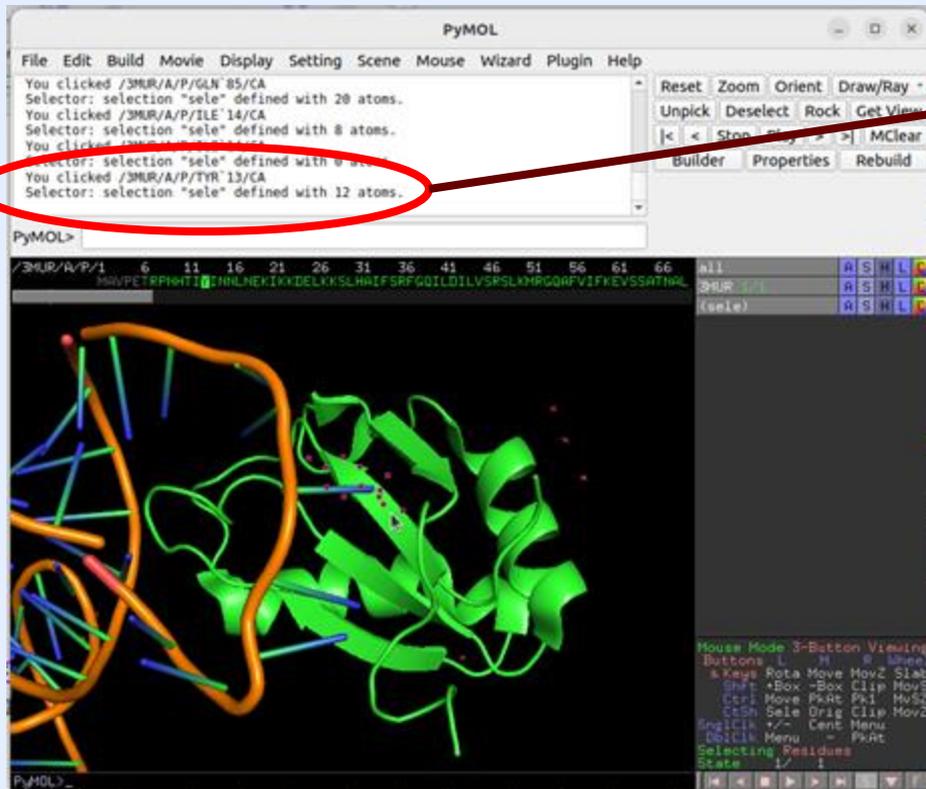
When you select a residue it tells you what the name of that residue is

The name of the object

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

What is included in the selection

/object-name/seg-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,\
```

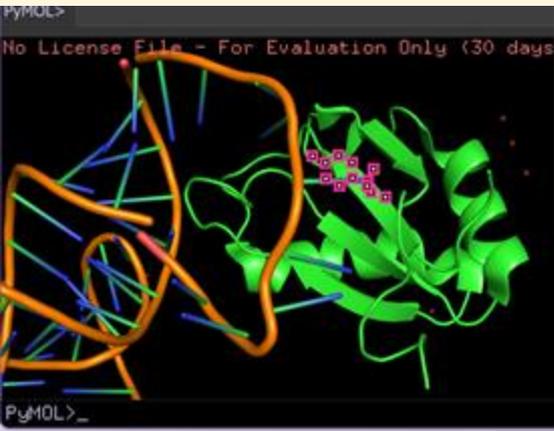
```
-0.000028327, -0.000032730, -103.635612488,\
```

```
-2.681248903, 15.582657814, -37.988914490,\
```

```
-43.961441040, 251.230438232, -20.000000000 )
```

```
select 13_tyr, /3MUR/A/P/ILE`12
```

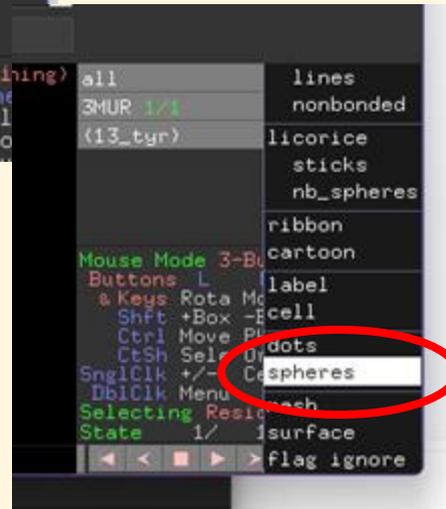
Changing Visual Style



```
PyMOL> style
```

all	A	S	H	L	C
3MUR 1/1	A	S	H	L	C
(13_tyr)	A	S	H	L	C

Mouse Mode 3-Button Viewing)
Buttons L M R Wht
& Keys Rota Move MovZ Sl
Shft +Box -Box Clip Mo
Ctrl Move Pl
CtSh Selc
SnglClk +/-
DbtClk Menu
Selecting Resid
State 1/
flag ignore



```
PyMOL> style
```

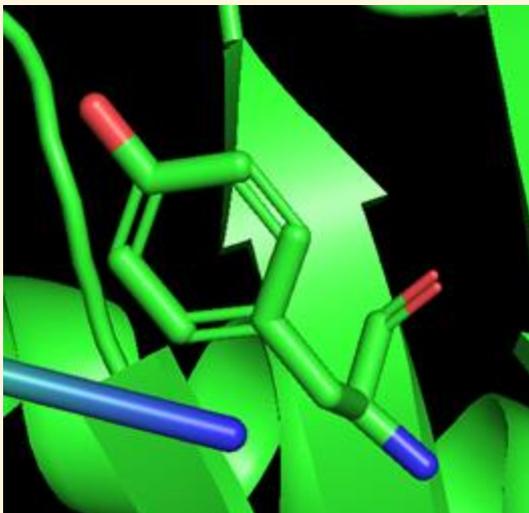
all	lines
3MUR 1/1	nonbonded
(13_tyr)	licorice
	sticks
	nb_spheres
	ribbon
	cartoon
	label
	cell
	dots
	spheres
	mesh
	surface
	flag ignore

Mouse Mode 3-Button Viewing)
Buttons L M R Wht
& Keys Rota Move MovZ Sl
Shft +Box -Box Clip Mo
Ctrl Move Pl
CtSh Selc
SnglClk +/-
DbtClk Menu
Selecting Resid
State 1/
flag ignore

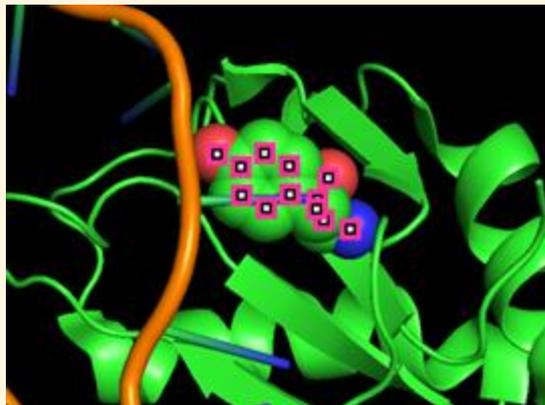


Many Visual Styles Exist

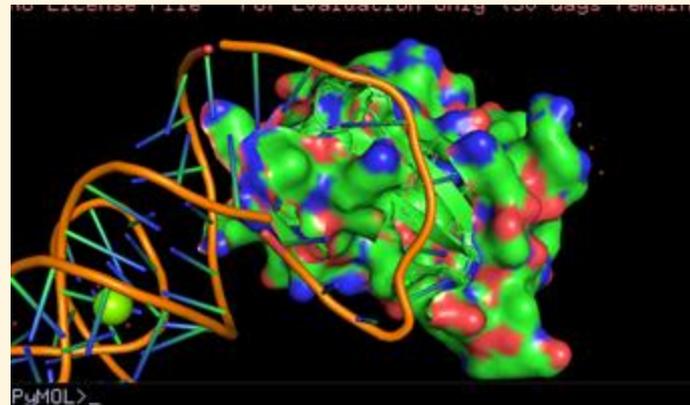
Sticks



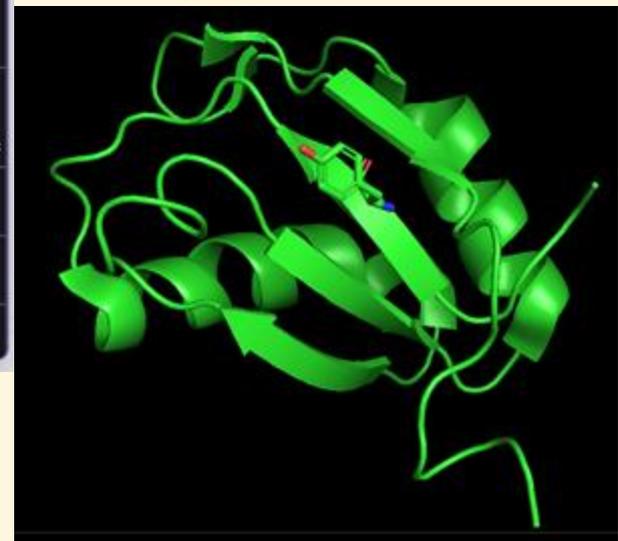
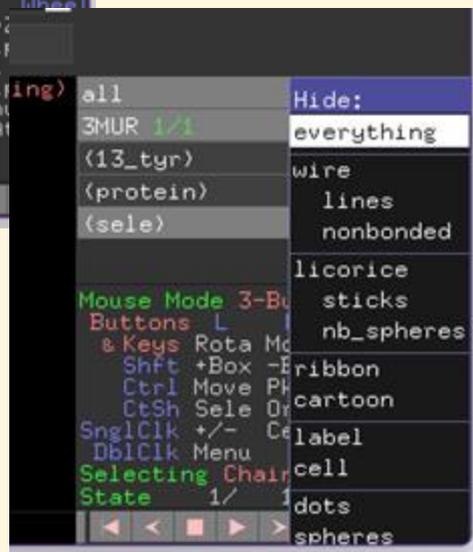
Spheres



Surface

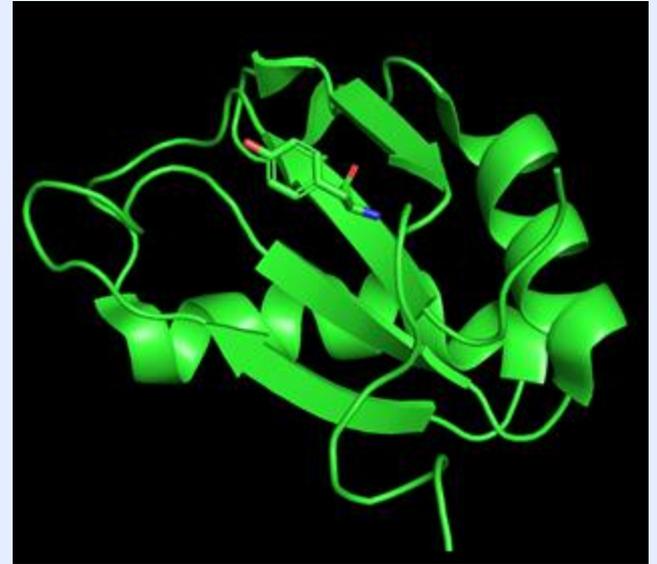


Many Visual Styles Exist



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

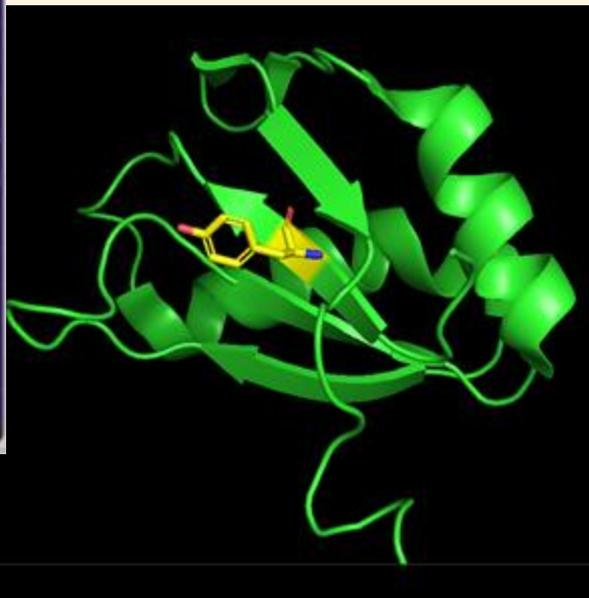
show_as **cartoon**, **protein**

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
```

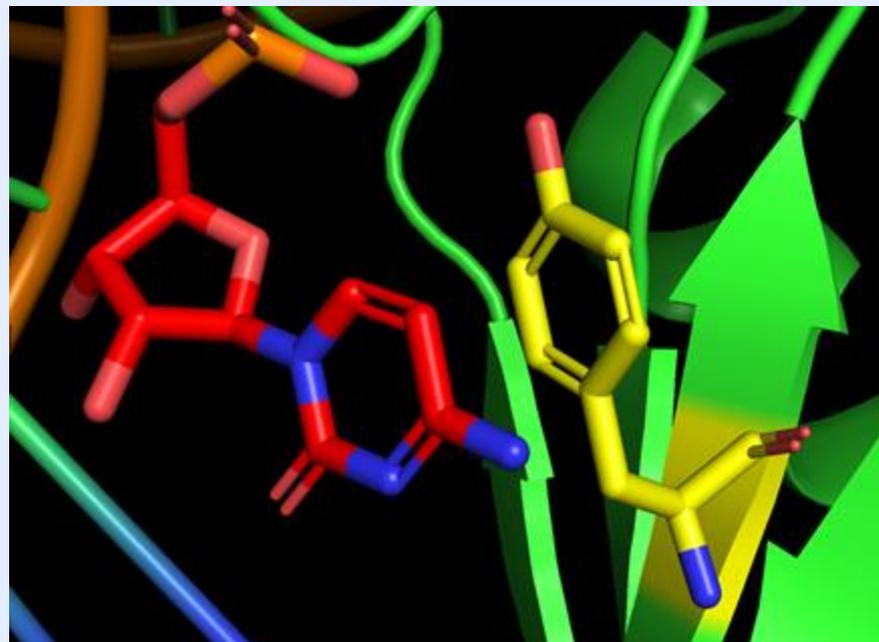
```
select RNA, /3MUR/B/R
```

```
show_as cartoon, RNA
```

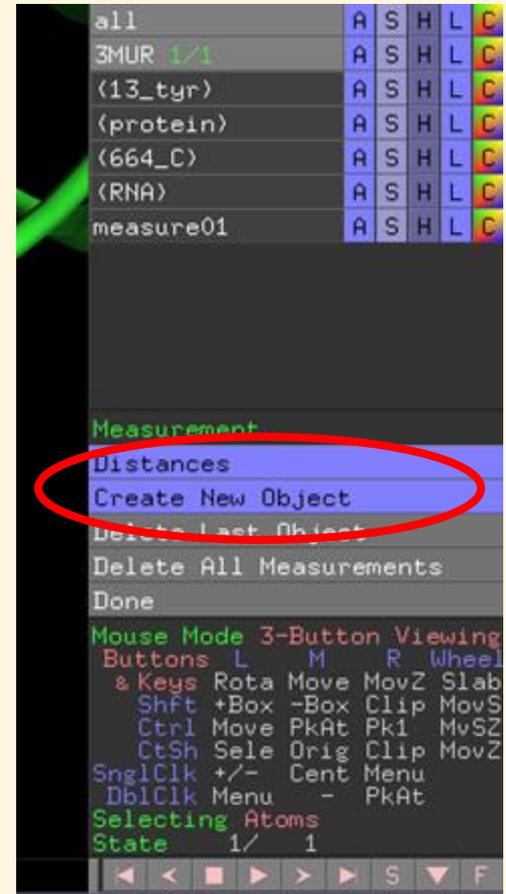
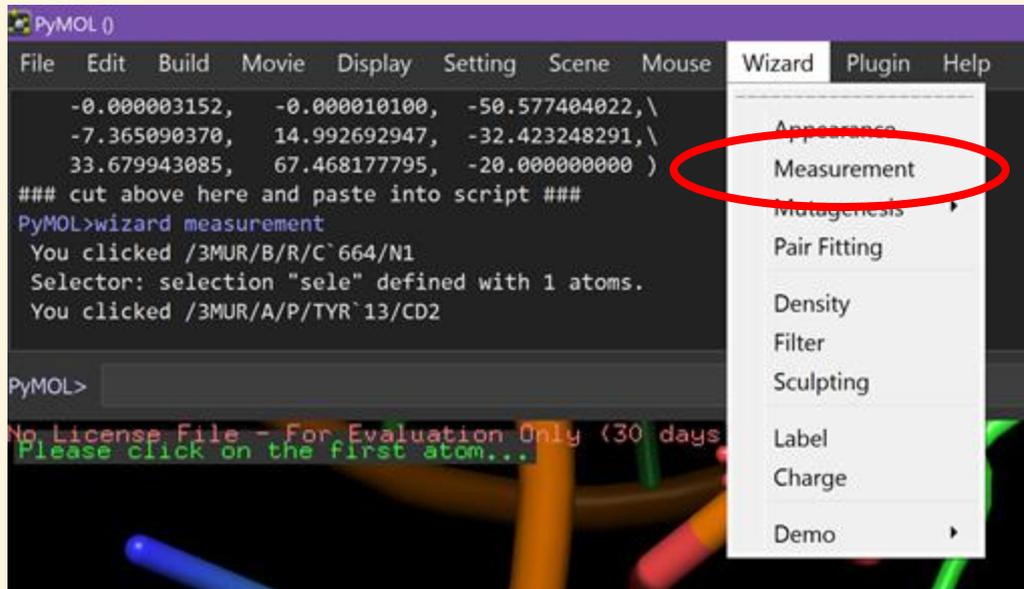
```
show_as stick, 664_C
```

```
color red, 664_C
```

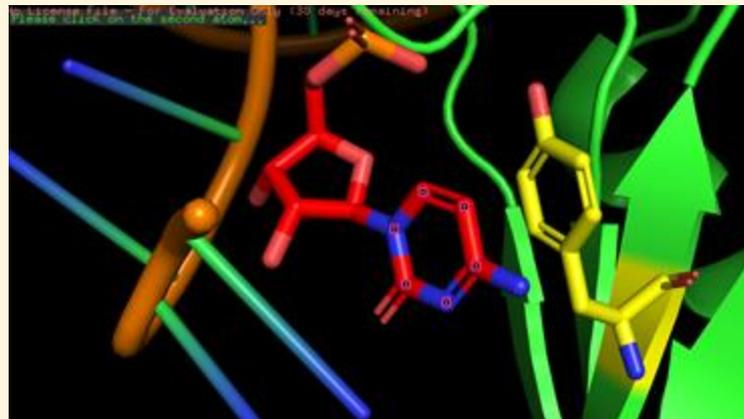
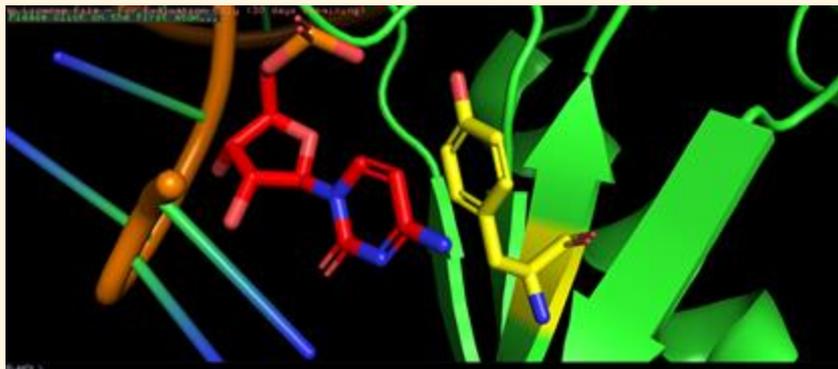
```
color atomic, (not elem C)
```



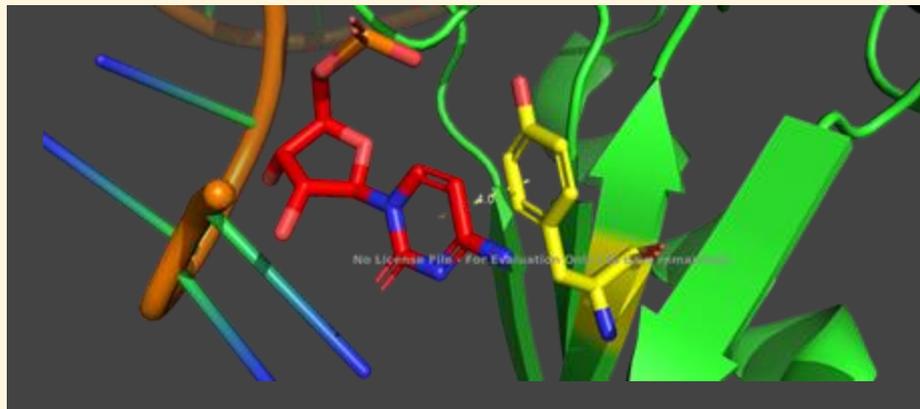
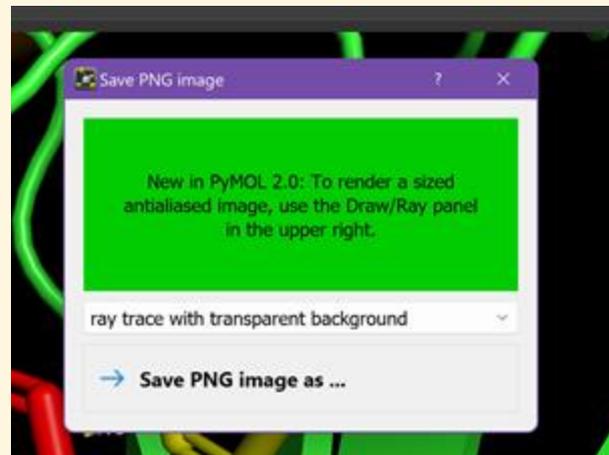
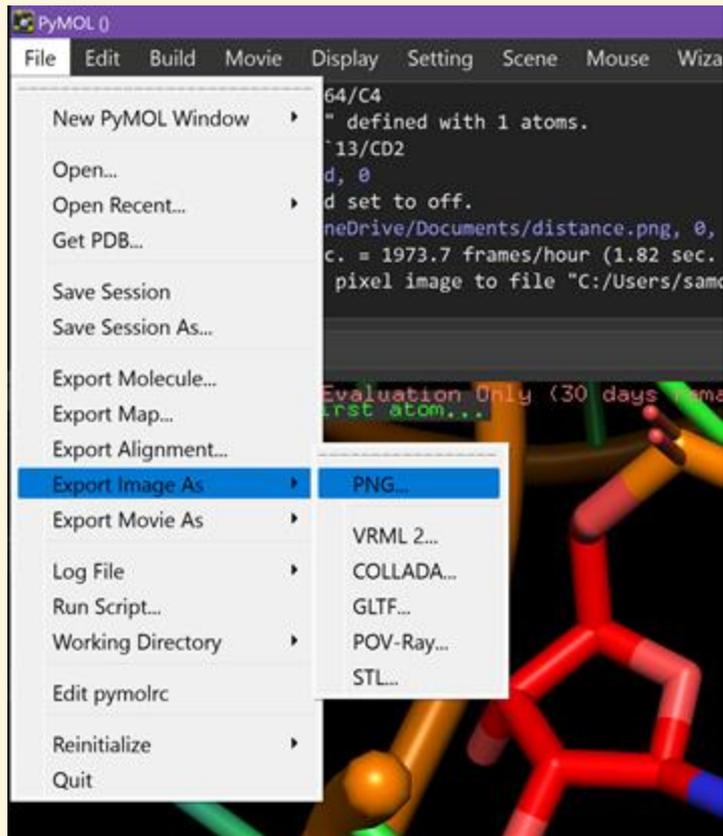
Opening the measurement wizard



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")
```