

Tools to Ease the Use of PyMOL

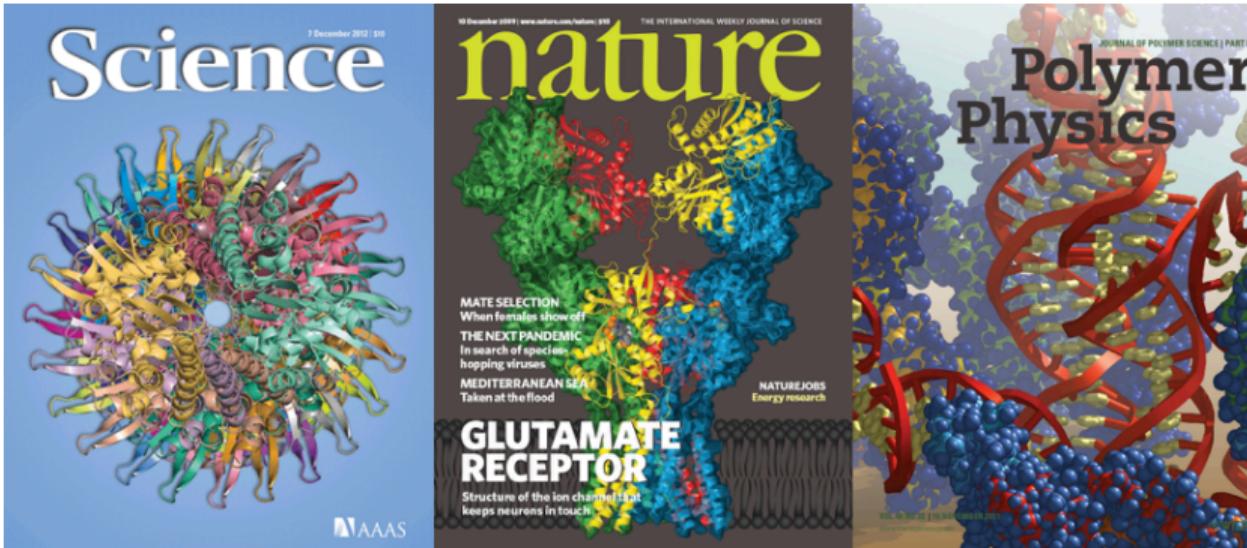
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blaine-mooers@ouhsc.edu
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<http://github.com/MooersLab/user-meeting-workshop-2024>

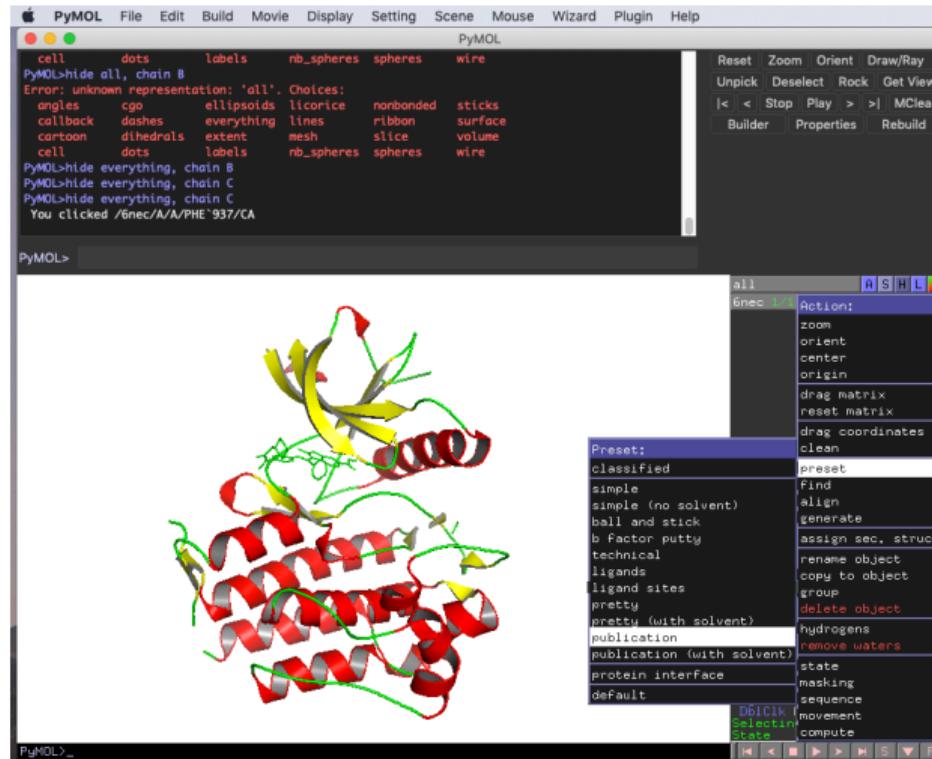
Department of Biochemistry & Physiology
University of Oklahoma Health Sciences, Oklahoma City

Computational Methods in Structural Biology
SSRL/LCLS Users Meeting
September 26, 2024

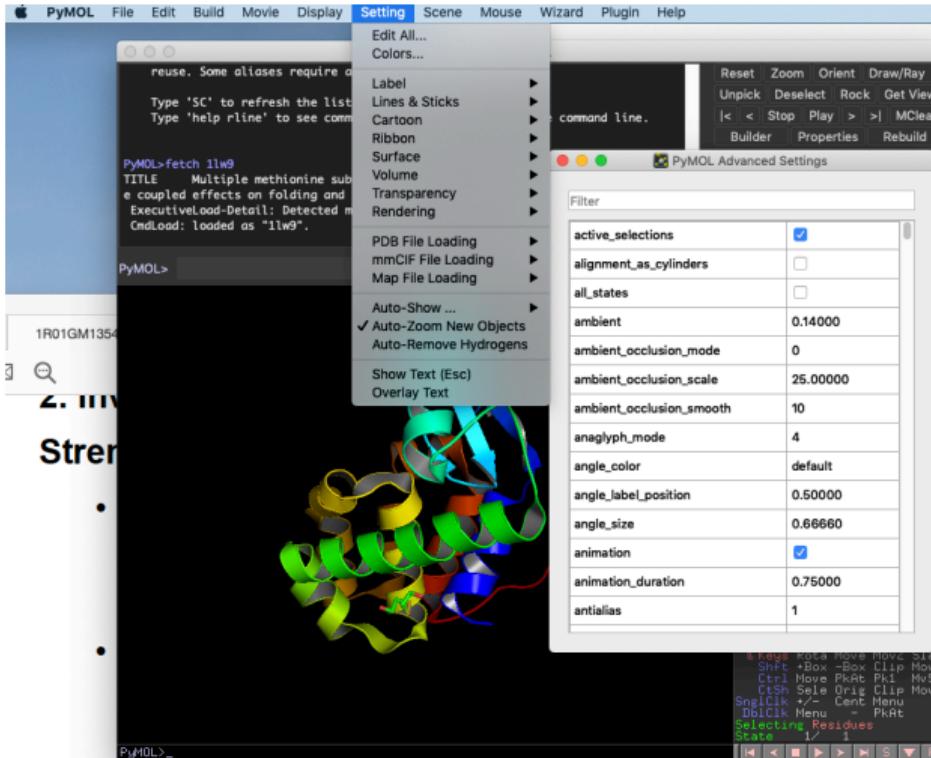
Cover images made with PyMOL



Presets



Settings



Outline

- roundview.py: horizontal scripting
- pymolshortcuts.py: extends PyMOL
- pymolsnips: pml script writing
- pymolpysnips: computational notebooks

The problem

```
PyMOL>get_view
### cut below here and paste into script ####
set_view(\n
    -0.832868993,      0.398498207,      0.383896619,\n
    -0.260102808,      -0.894237876,      0.363985002,\n
    0.488390923,       0.203309149,      0.848513067,\n
    0.000000000,        0.000000000,     -61.396984100,\n
    -46.246913910,     -4.663769245,      42.401920319,\n
    56.260883331,      66.533096313,     -20.000000000 )\n### cut above here and paste into script ####
```

The solution

```
PyMOL>roundview  
set_view(-0.83,0.4,0.38,-0.26,-0.89,0.36,0.49,0.2,0.\  
85,0.0,0.0,-61.4,-46.25,-4.66,42.4,56.26,66.53,-20.0);
```

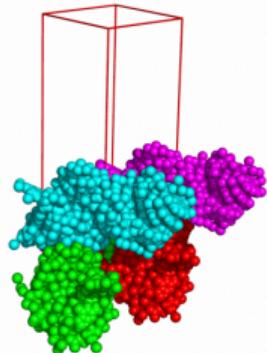
<https://github.com/MooersLab/EasyPyMOL>

Mooers (2016) *Protein Sci.*, 25, 1873-1882.

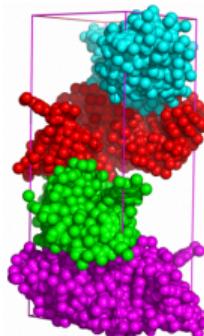
Crystal packing

A -> generate -> symmetry mates

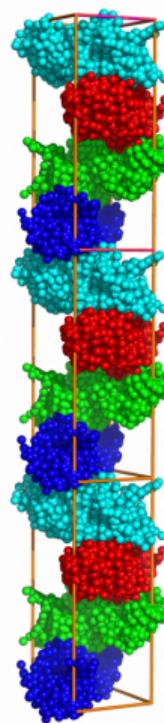
5D99



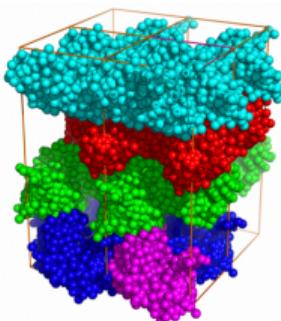
sc111



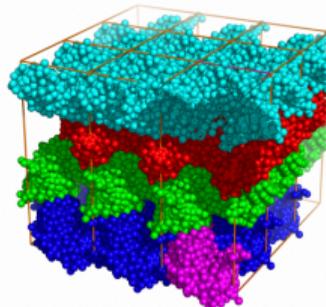
sc113



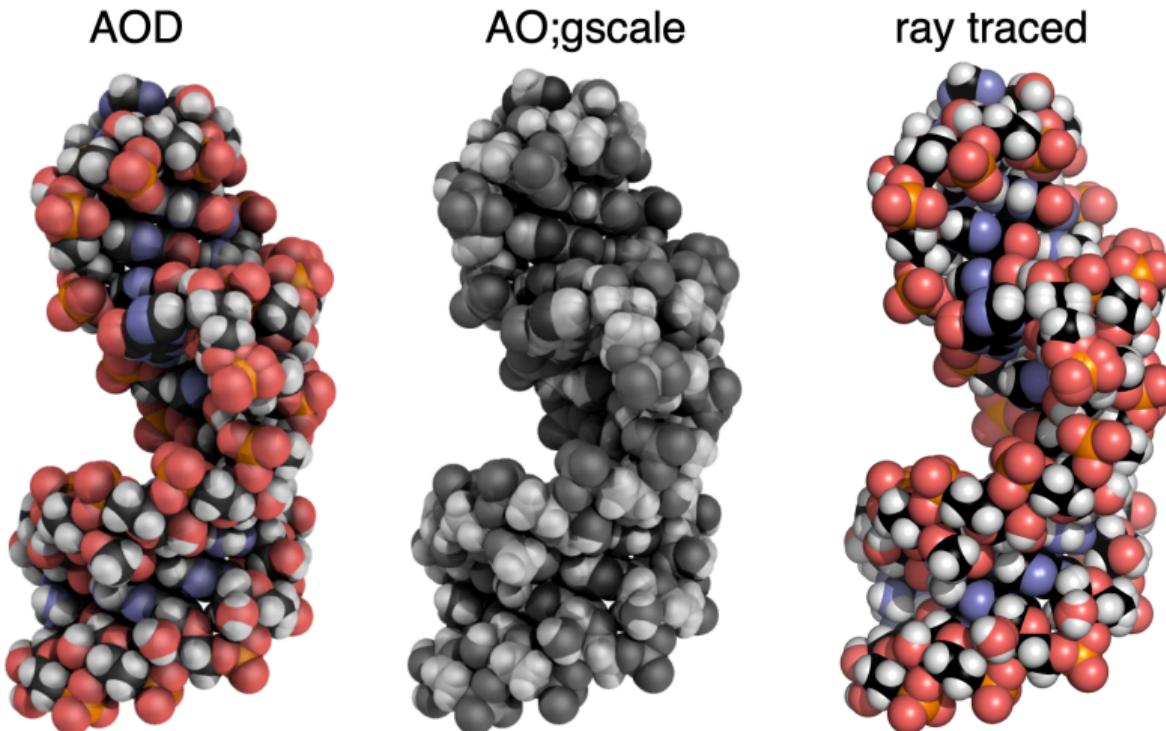
sc221



sc331

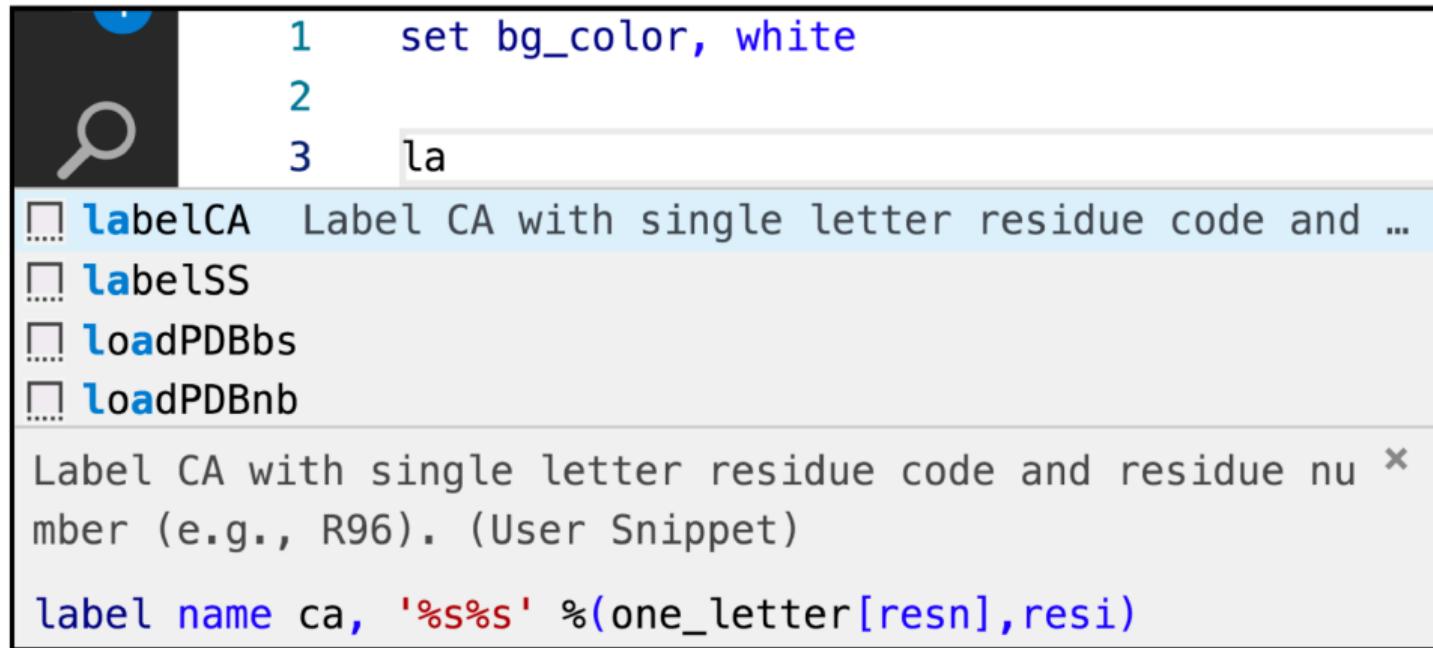


Ambient occlusion



Mooers (2020) *Protein Sci.*, 29, 268-276.

Tab trigger to insert a snippet in VSC



The screenshot shows a VS Code interface with a search icon in the top-left corner. In the code editor, the following code is visible:

```
1 set bg_color, white
2
3 la
```

A dropdown menu is open below the code, listing several snippets:

- labelCA Label CA with single letter residue code and ...
- labelSS
- loadPDBbs
- loadPDBnb

The snippet "labelCA" is selected, and its description is displayed below the list:

Label CA with single letter residue code and residue number (e.g., R96). (User Snippet)

The snippet definition is shown at the bottom:

```
label name ca, '%s%s' %(one_letter[resn],resi)
```

<https://github.com/MooersLab/pymolsnips>

Mooers and Brown (2021) *Protein Sci.*, 30, 262-269.

lsSnips snippet

lsSnips lists available tab triggers

```
4 lsSnips
```

| | |
|---|---|
|  lsSnips | List all snips by tab trigger and description... |
| cspheres | Colored spheres. |
| discreteCartoonColoring | Turn on discrete colors between secondary structure elements. |
| distance | H-bond distances. |
| doubleBond | Valence bond. |
| drawHbonds | Draw H-bonds. |
| duplicateObject | Duplicate object. |
| ellipcol | Set ellipsoid color. |
| extractPartObj | Create a new object from part of an existing object. |
| fasta | Print Fasta from PDB file. |
| fetch2FoFc | Fetch 2FoFc map. |

Supported text editors

| | | |
|----------|-------------|--------------|
| Atom | Geany | Neovim |
| BBedit | Gedit | Sublime Text |
| Brackets | Kate | TextMate |
| CudaText | Komodo Edit | Vim |
| Emacs | Light Table | VS Code |
| Expresso | Micro | |

Rmarkdown “knitted” to a PDF

```
library(reticulate)
use_condaenv("r-reticulate")

from pymol import cmd
cmd.do("reinitialize")

## PyMOL not running, entering library mode (experimental)
cmd.do("fetch 6VXX")
cmd.do("zoom (resi 614 and chain A)")
cmd.label(selection="chain A and resi 614 and name CB", expression="%s-%s' % (resn,resi)")
cmd.set(label_color, black; set label_size, 48")
cmd.set(stick_radius, 0.12")
cmd.hide cartoon; show sticks"
cmd.set ray_shadows, 0")
cmd.draw"
cmd.png /Users/blaine/D614Greticulate.png, 800, 500, dpi=300")
```

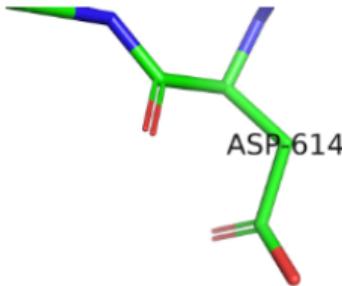
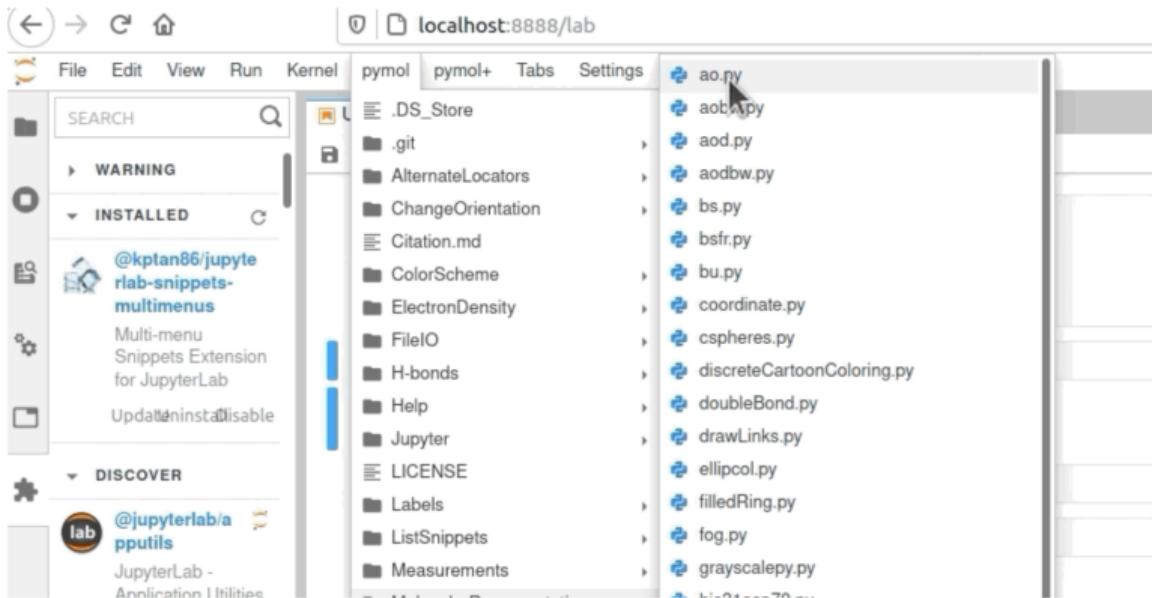


Figure 1: Caronavirus SARS2 Spike Protein site 61.

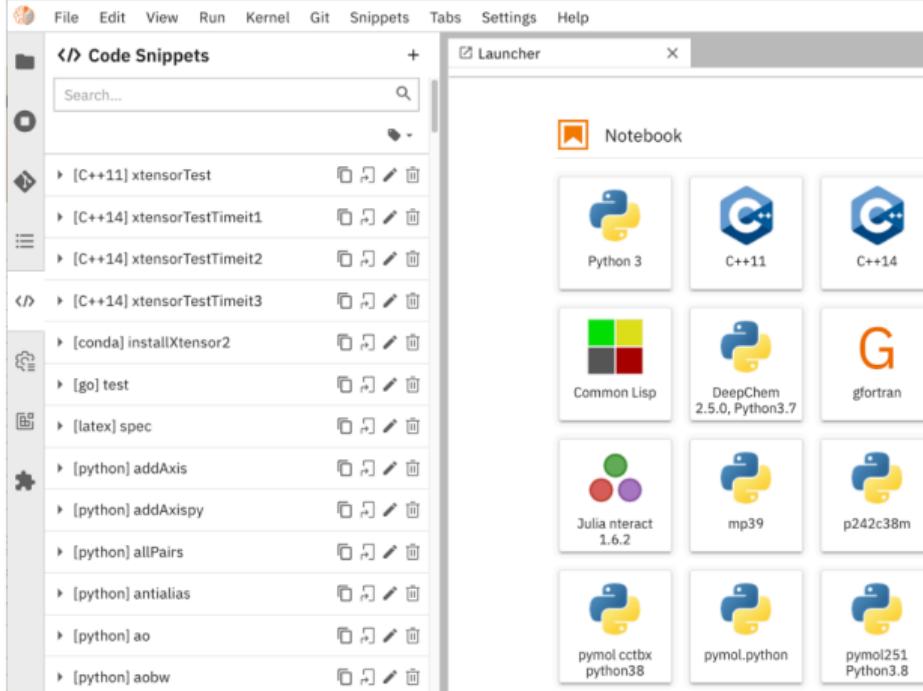
<https://github.com/MooersLab/rstudiopymolpysnips>

Snippets via pull-down menus in Jupyter Lab



<https://github.com/MooersLab/jupyterlabpymolpysnips>
Mooers (2021) Computing in Science & Engineering 23, 47-53.

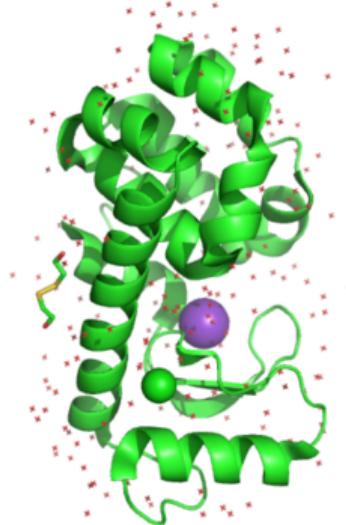
Snippets via tags in Jupyter Lab



Requires the Elyra extension.

<https://github.com/MooersLab/taggedpymolpysnips>

Test snippet in Colab Notebook



```
✓ 2s from pymol import cmd
from IPython.display import Image
cmd.fetch("1lw9")
cmd.orient("1lw9")
cmd.rotate("z","270")
cmd.png("test.png")
Image(filename = "test.png", unconfined=True)
```

<https://github.com/MooersLab/colabOpenSourcePyMOLpySnips>
<https://github.com/MooersLab/colabpymolpysnips>

Source code block in org-mode

```
#+BEGIN_SRC jupyter-python :session pymol :kernel cp38 :exports both :results raw drawer
from pymol import cmd
from IPython.display import Image

cmd.do('fetch 7JU5:A, type=cif, async=0;')
cmd.do('set_view (-0.11,0.47,-0.88,-0.56,0.7,0.44,0.82,0.54,0.19,0.0,0.0,-203.71,20.89,\n
6.7,-25.54,174.56,232.88,-20.0);')
cmd.do("set_color oxygen, [1.0,0.4,0.4];")
cmd.do("set_color nitrogen, [0.5,0.5,1.0];")
cmd.do("remove solvent;")
cmd.do("as spheres;")
cmd.do("util.cbaw;")
cmd.do("bg white;")
```

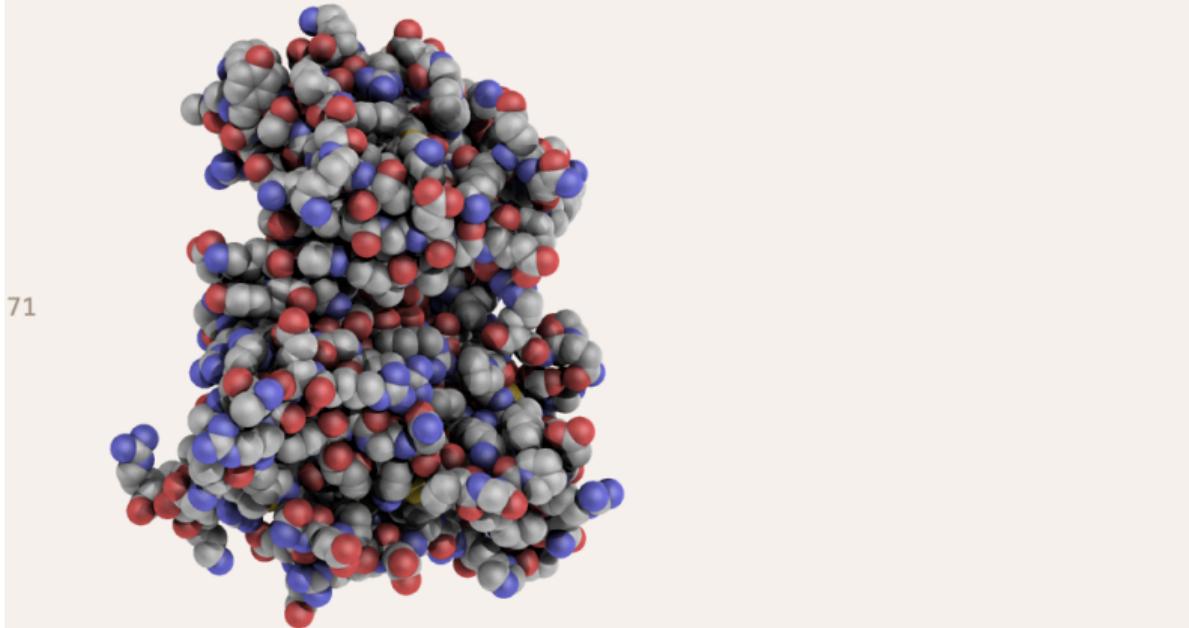
jupyter-python :session pymol :kernel cp38

```
cmd.set specular,0.25,
cmd.do("set ambient,0;")
cmd.do("set direct,0;")
cmd.do("set reflect,1.5;")
cmd.do("set ray_shadow_decay_factor, 0.1;")
cmd.do("set ray_shadow_decay_range, 2;")
cmd.do("set depth_cue, 0;")
cmd.do("ray;")
cmd.do('png /Users/blaine/7JU5A.png, 600, 600, dpi=300;')
PATH = "/Users/blaine/"
Image(filename=_PATH + "7JU5A.png", width=300, height=300, unconfined=True)
#+END_SRC
```

<https://github.com/MooersLab/orgpymolpysnips>

Output from above source block

```
65 Image(filename = PATH + "7JU5A.png", width=300, height=300, unconfined=True)
66 #+END_SRC
67
68 #+RESULTS:
69 :results:
70 # Out[1]:
```



Summary

- roundview.py supports horizontal scripting
- pymolshortcuts.py extends PyMOL
- pymolsnips supports writing pml scripts in text editors
- pymolpysnip libraries support computational narratives in:
 - RStudio
 - Jupyter Lab
 - Google Colab
 - Org Mode

Acknowledgements

- Thomas Holder, Schrödinger LLC
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- Oklahoma Data Science Workshop
- >500 first-year graduate students

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- NIH: P30 GM145423, P30 CA225520, P30 AG050911

Questions?

What is next?

- GUI pull-down access to shortcuts
- Running PyMOL by speech-to-text in Jupyter and Colab
- Running PyMOL by voice commands via Talon Voice

Features important for practical work

| Features | Org Mode | Jupyter |
|------------------------------------|----------|---------|
| Tab triggers | +++ | - |
| Tab stops | +++ | - |
| Snippet groups | +++ | + |
| Parallel sessions in same document | + | - |
| Rendering speed | - | ++ |
| Scrolling speed | - | ++ |
| Ease and speed to PDF | +++++ | + |