

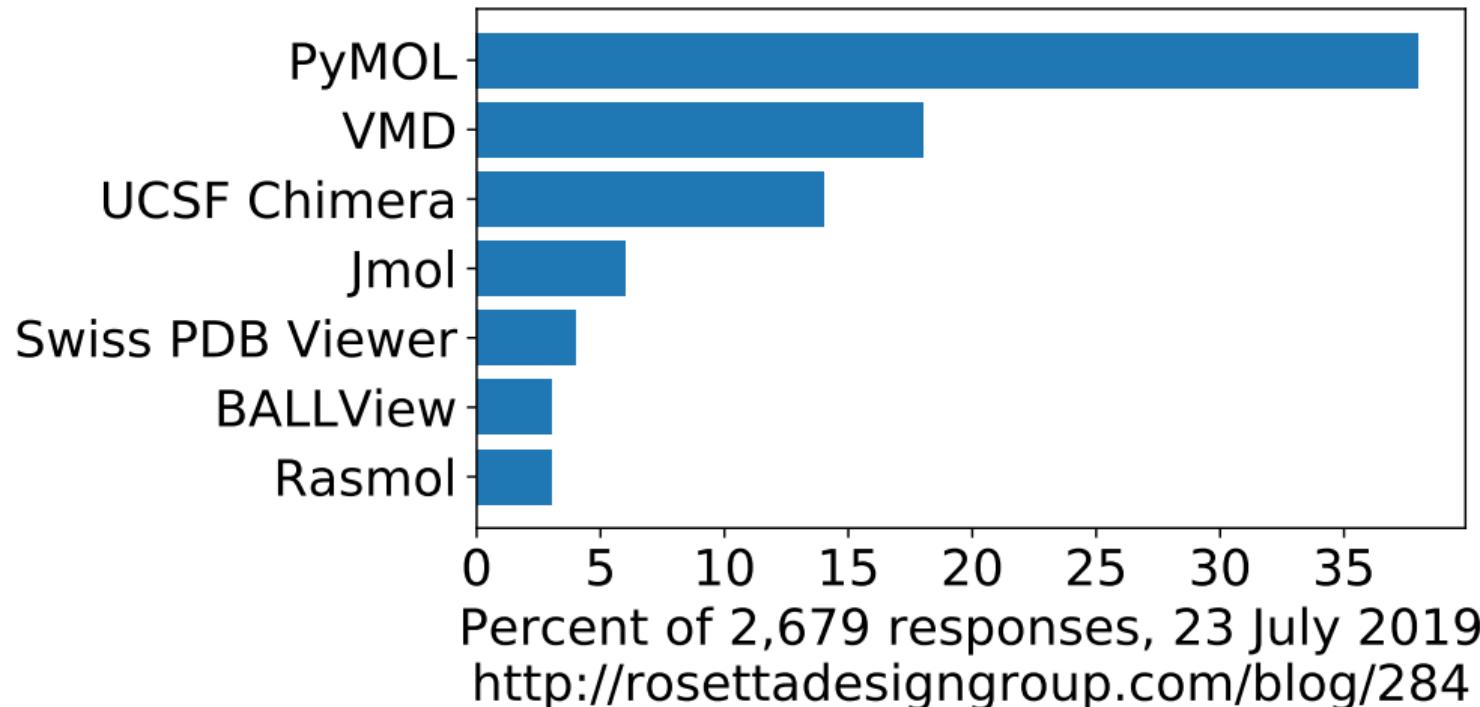
Creation of Exquisite Images of Biomolecular Structures in PyMol with Shortcuts

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Southwest Theoretical and Computational Conference
University of Oklahoma
Norman, Oklahoma
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What is your favorite molecular viewer?



Warren Delano, the genius behind PyMOL

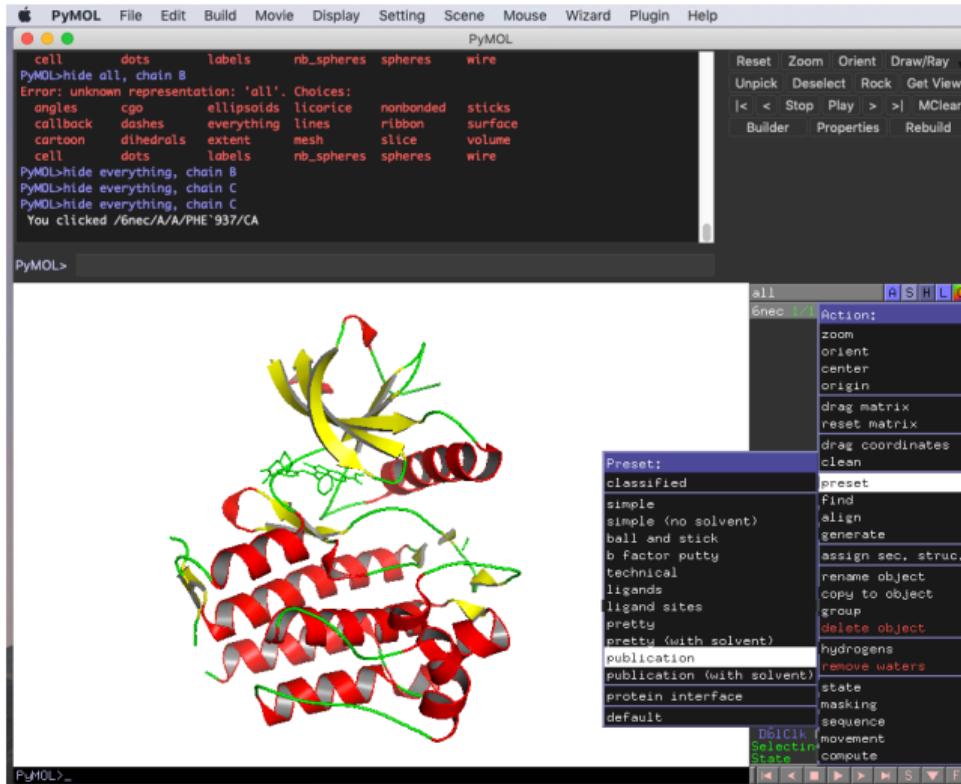
June 21, 1972 – November 3, 2009



pymolsnips, the ao tab trigger in VSC

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

PyMOL's GUI



6NEC, RET Kinase-Nintedanib (Terzyan et al. 2019)

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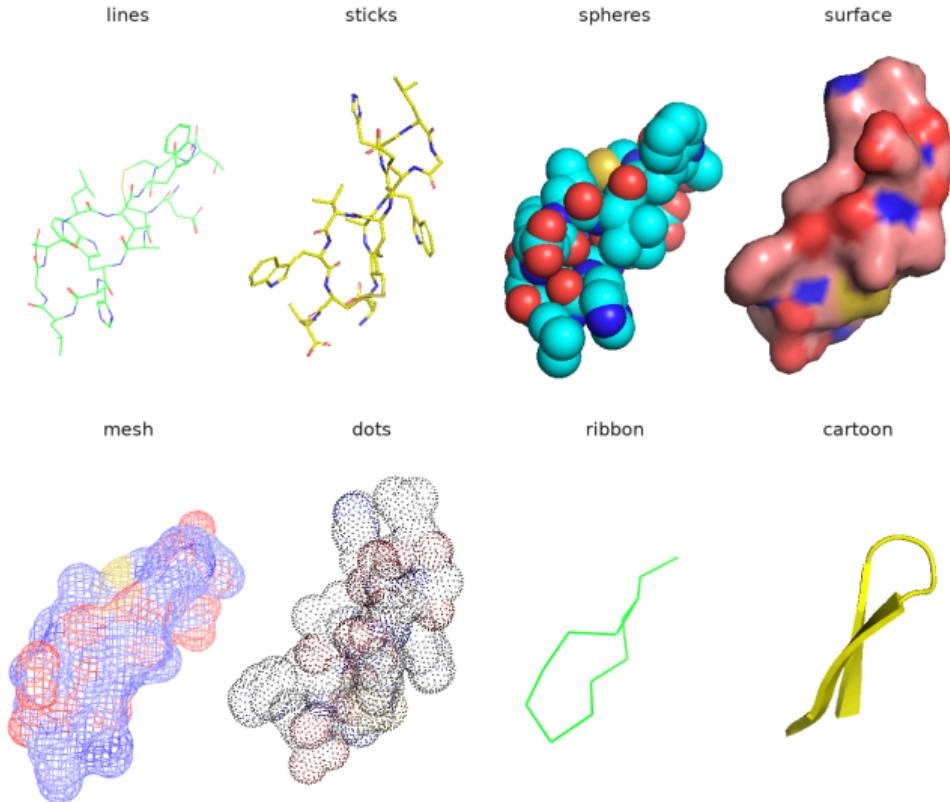
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- ▶ Add styles of molecular representation
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- ▶ Open external programs
(e.g., text editors, image editors, MS Word)

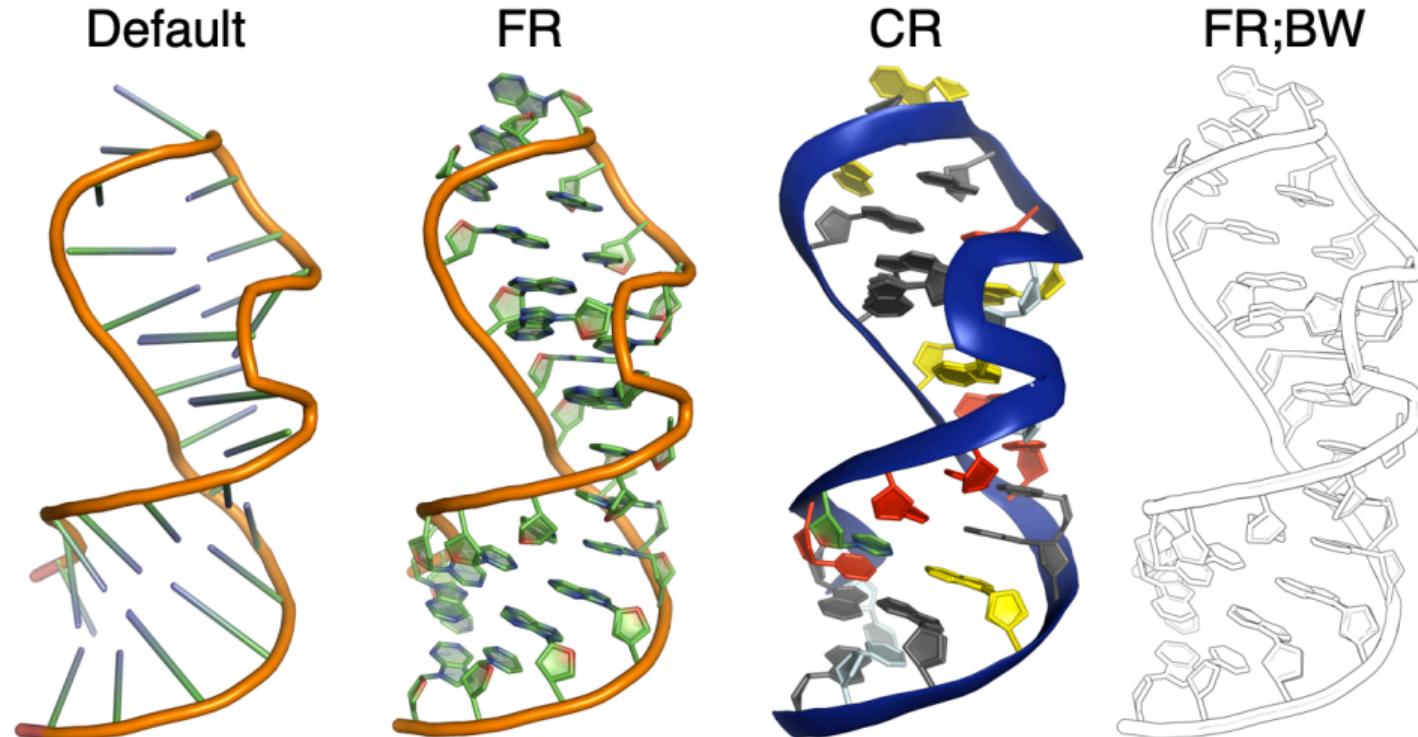
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- ▶ Utilize other Python modules
(e.g., webbrowser)

PyMOL's molecular representations

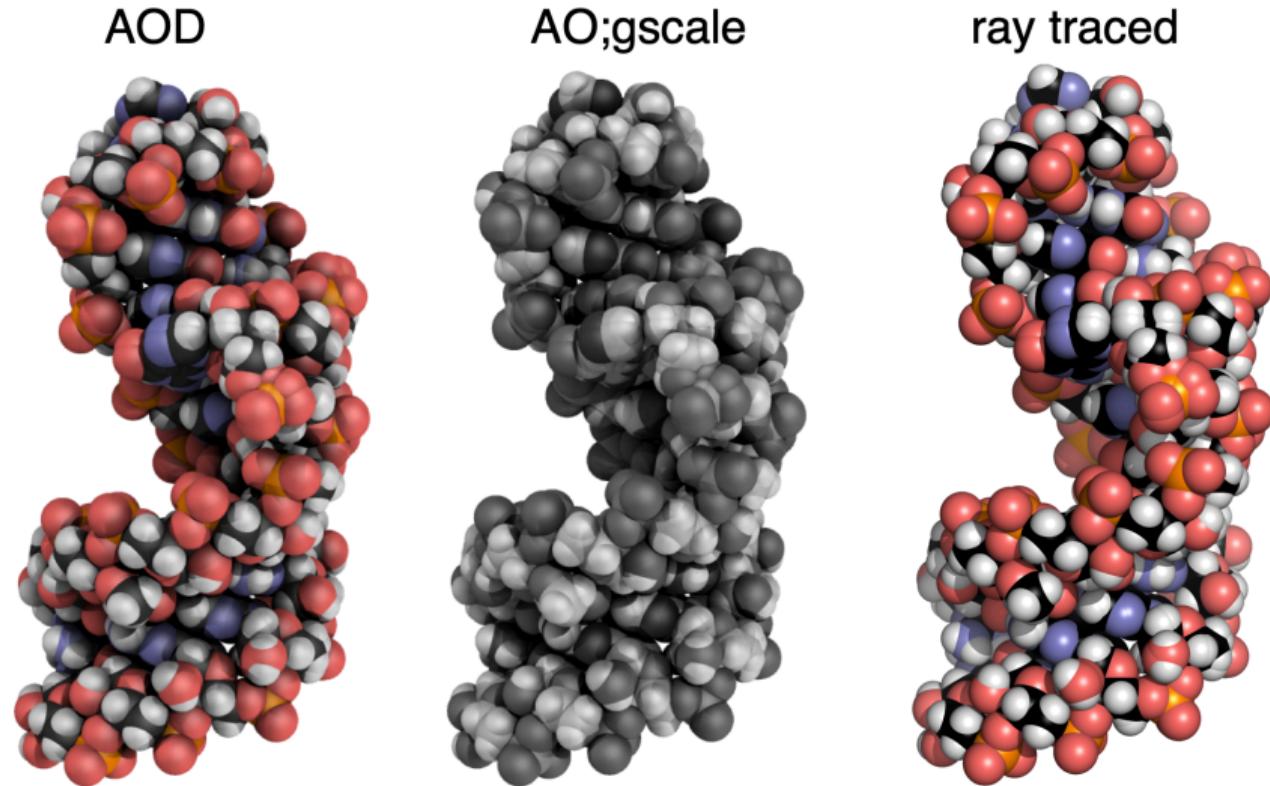


Extending PyMOL's molecular representations



5d99, RNA hairpin (Mooers 2016)

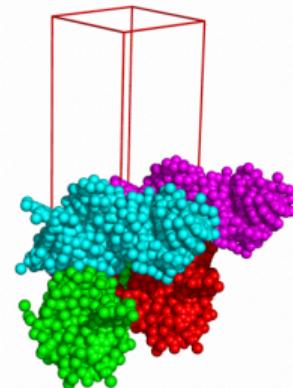
Ambient occlusion (photorealistic) effect



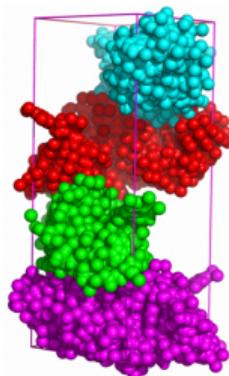
Shortcuts for unit cell arrays

A -> generate -> symmetry mates

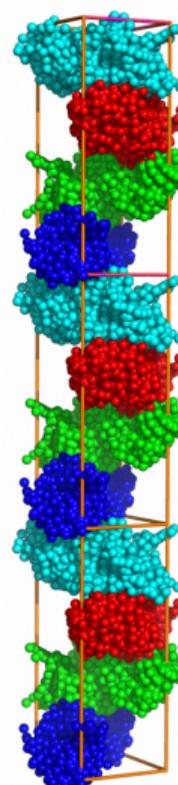
5D99



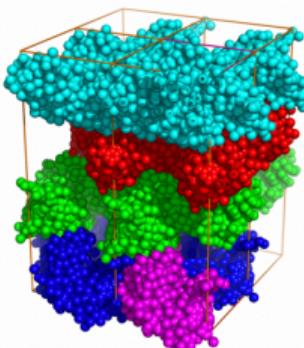
sc111



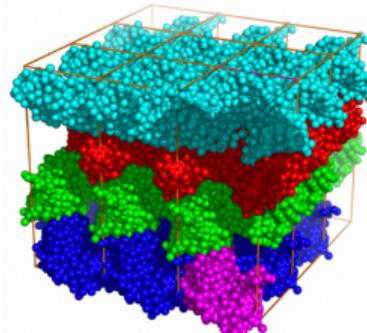
sc113



sc221



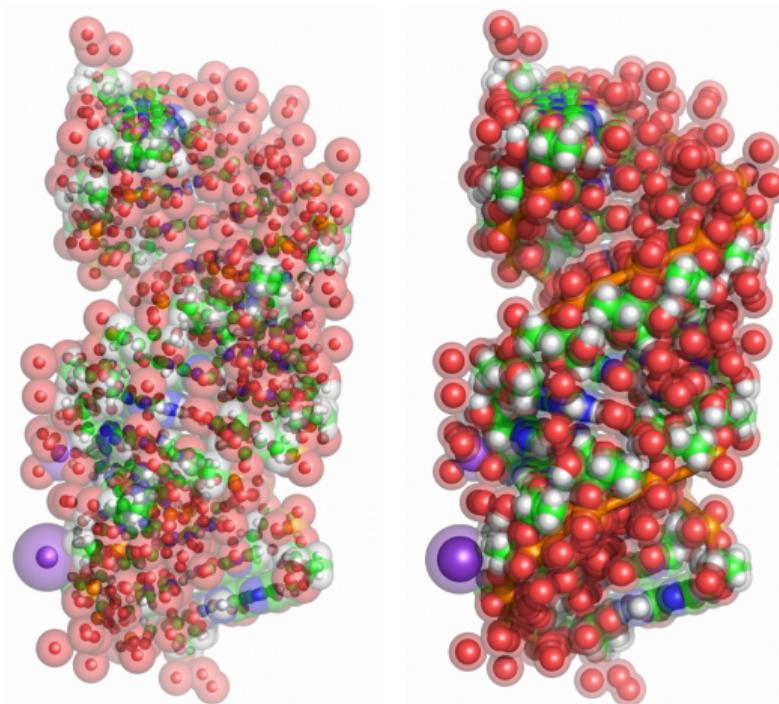
sc331



Pearl effect

PE33

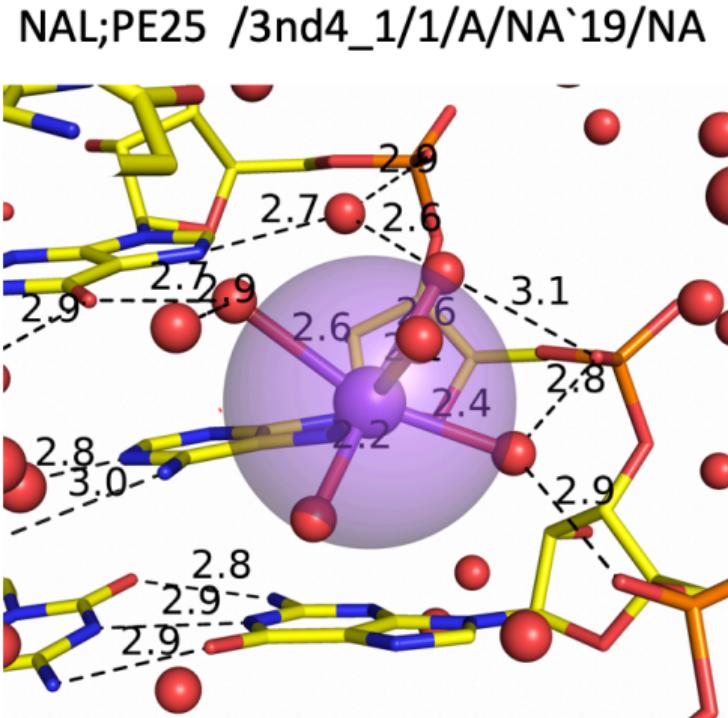
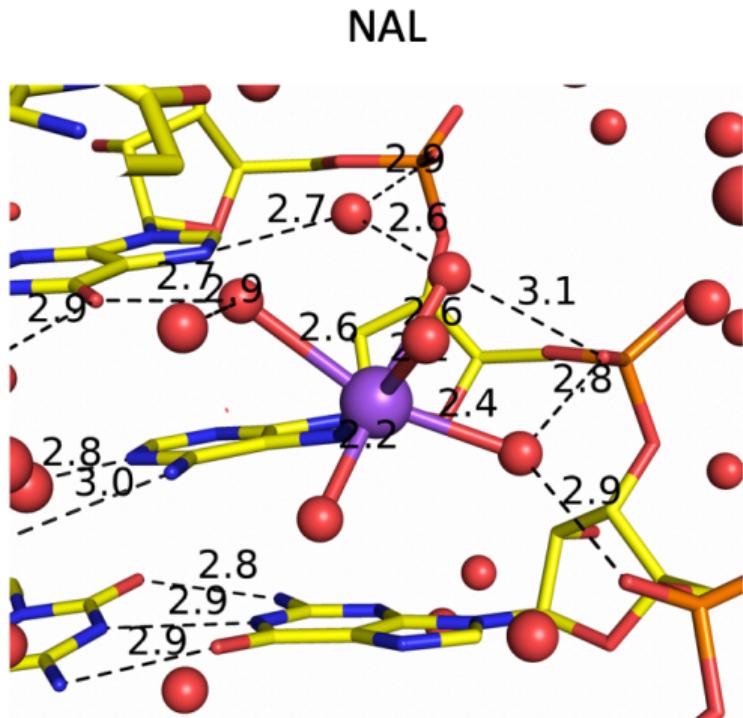
PE85



3nd3, dsRNA with run of 8Us (Mooers and Singh 2011)

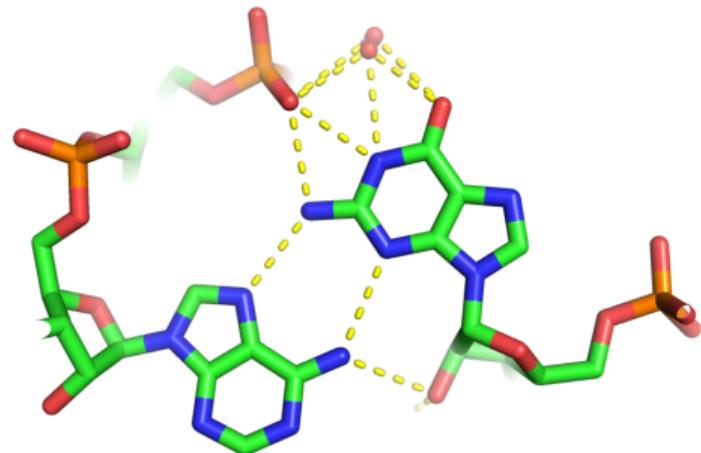
Coordinate covalent bonds

NAL serves as a template.

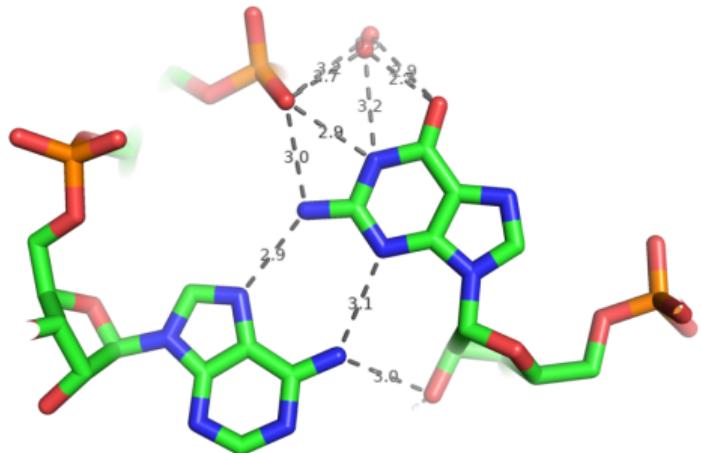


Hydrogen bonds

Default

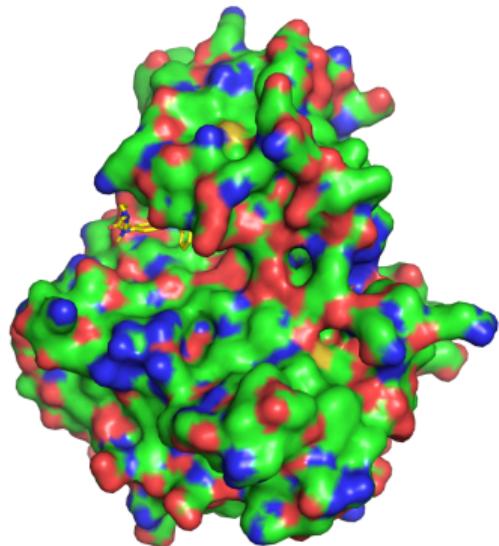


hb

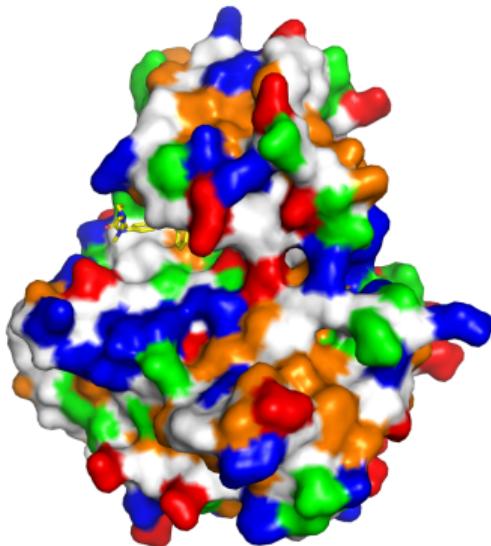


Coloring by biophysical properties

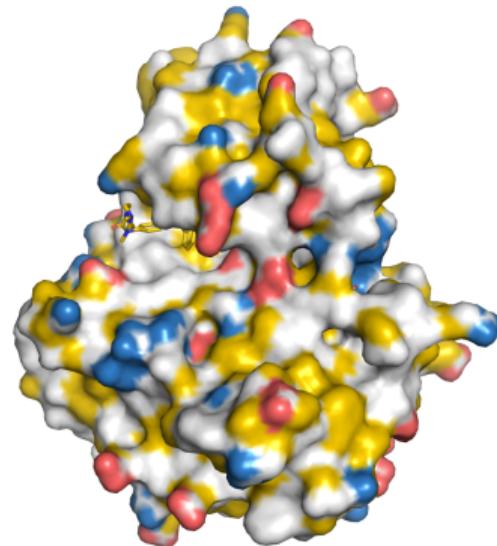
Default



timcolor



yrb



Hagemans et al. 2015

Saving file with time stamp

```
spse 3fao
ls 3fao*
3faoy2019m07d18h08m33s30.pse
```

Saving file with time stamp

```
spse 3fao
ls 3fao*
3faoy2019m07d18h08m33s30.pse
```

Shortcuts for all other file types:

```
spng
spdb
smol
smae
smoe
sout
spqr
```

Open external text editor

Table: Shortcuts to text editors outside of PyMOL.

Shortcut	Editor
atom	Atom
st3	Sublime Text 3
mate	TextMate
vim	vim
emacs	emacs
npp	notepad++
gedit	gedit
code	Visual Studio Code

Submit search terms from command line

Shortcut	Engine
AB	Amazon Books
AX	arXiv
BR	BioRxiv
GH	GitHub
GS	Goolge Scholar
PDB	Protein Databank
PM	PubMed
PML	PyMOL mailing list
RG	Research Gate
SD	Science Direct
SO	Stackoverflow
MA	All searchable sites
MC	10 core sites

Open top N hits in N separate tabs

Shortcut	Engine
GHN	GitHub
GSN	Google Scholar
PDBN	Protein Databank
PMN	PubMed
IPMN	List of searchterms Pubmed
PMLN	PyMOL mailing list
RGN	Research Gate

```
conda install requests beautifulsoup4 datetime
```

help CBSS

DESCRIPTION

Apply colorblind-friendly coloring to ribbon or cartoon representations.
Depends on colorblindfriendly.py.
Script is assumed to be stored in \$HOME/Pymol-script-repo/.....

USAGE

Type 'CBSS' to execute.....

The commands with linebreaks:

```
run ~/Pymol-script-repo/colorblindfriendly.py;  
as cartoon;  
color cb_red, ss H;  
color cb_yellow,ss S;  
color cb_green, ss L+;
```

The commands without linebreaks:

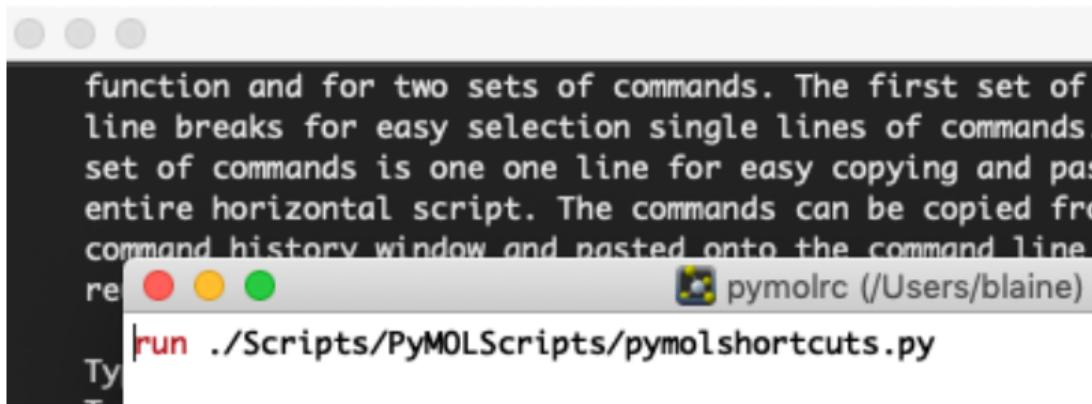
```
run $HOME/Pymol-script-repo/colorBlindFriendly.py;as cartoon;\ncolor cb_red, ss H;color cb_yellow,ss S;color cb_green, ss L+;
```

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

pymolshortcutsNobs4.py → RAW → (left-click)

Save Page As pymolshortcutsNobs4.py.txt

File → edit pymolrc



A screenshot of a terminal window titled "pymolrc (/Users/blaine)". The window contains a block of text describing a function and two sets of commands. Below the text, there is a command prompt with a red, yellow, and green button bar. The command "run ./Scripts/PyMOLScripts/pymolshortcuts.py" is typed into the terminal.

```
function and for two sets of commands. The first set of  
line breaks for easy selection single lines of commands.  
set of commands is one one line for easy copying and pas  
entire horizontal script. The commands can be copied fro  
command history window and pasted onto the command line  
re ● ● ●
```

run ./Scripts/PyMOLScripts/pymolshortcuts.py

Summary

Convenience
functions

Standard
orientation

Unit cell arrays

Open molecular
graphics programs

New molecular
representations

Complex H-bond
figures

Filenames with
time stamps

PyMOL shortcuts

Web searches
from PyMOL

Open static
web sites

Open a text editor

Acknowledgements

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