A Library of Shortcuts For Faster Image Making with PyMOL

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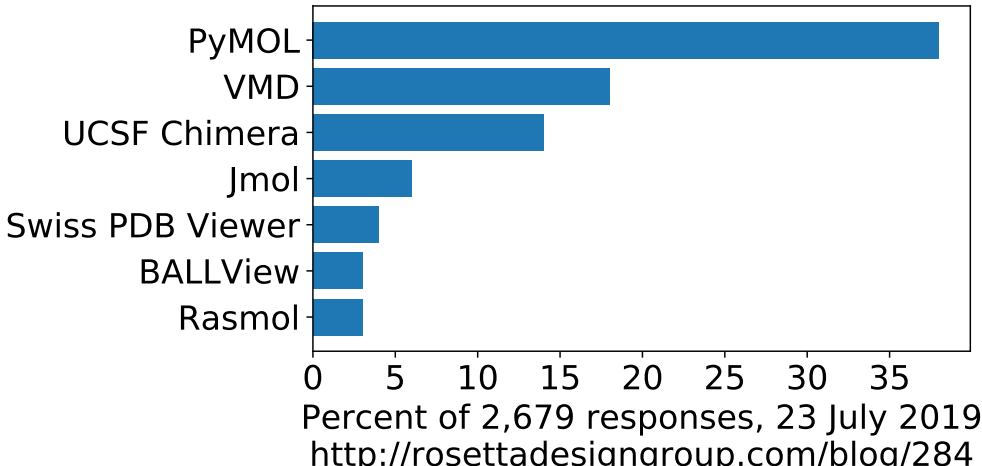
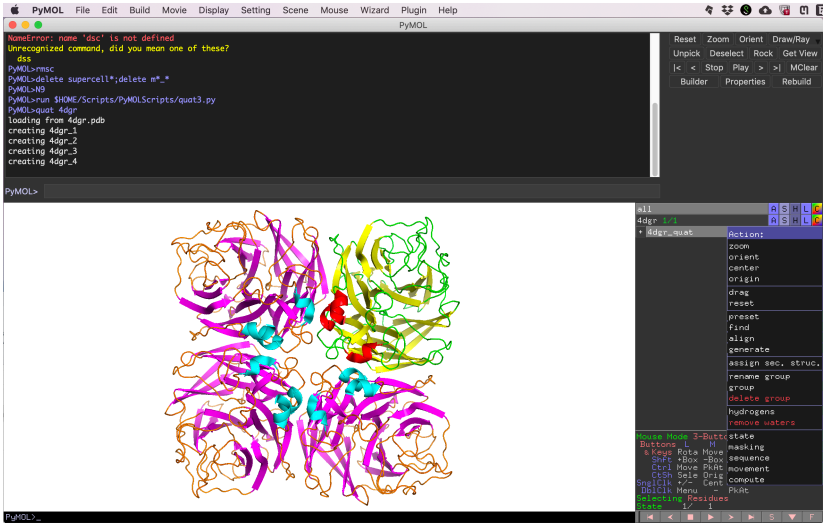
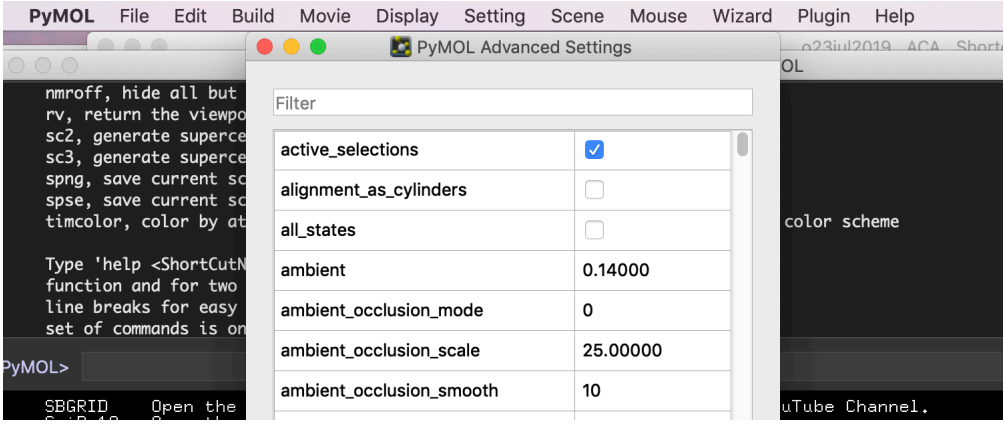
What is your favorite molecular viewer?



PyMOL GUI


PyMOL File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help
PyMOL
NameError: name 'dsc' is not defined
Unrecognized command, did you mean one of these?
dss
PyMOL>rmsc
PyMOL>delete supercell*;delete m*_*
PyMOL>N9
PyMOL>run $HOME/Scripts/PyMOLScripts/quat3.py
PyMOL>quat 4dgr
loading from 4dgr.pdb
creating 4dgr_1
creating 4dgr_2
creating 4dgr_3
creating 4dgr_4
PyMOL>
Reset Zoom Orient Draw/Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear
Builder Properties Rebuild
all
4dgr 1/1
4dgr_quat
Action:
zoom
orient
center
origin
drag
reset
preset
find
align
generate
assign sec. struc.
rename group
group
delete group
hydrogens
remove waters
state
masking
sequence
movement
compute
PkAt
Mouse Mode 3-Butto
Buttons L M
& Keys Rota Move
Shft +Box -Box
Ctrl Move PkAt
CtSh Sele Orig
SnglClk */- Cent
DblClk Menu -
Selecting Residues
State 1/ 1
PyMOL>

Over 600 settings



Use of computer mouse is almost essential!

But, overuse of the mouse leads to repetitive stress injuries.

Tools to reduce use of the mouse

- Interactive quizzes to improve recall

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- Snippet library to recycle useful code
- Shortcuts to save time

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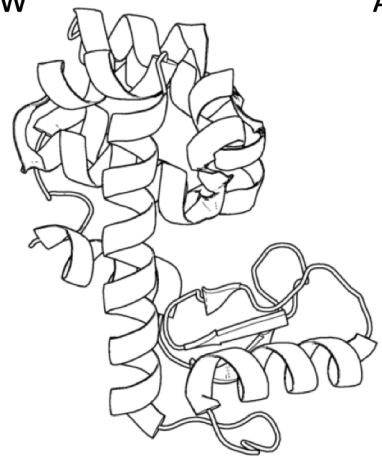
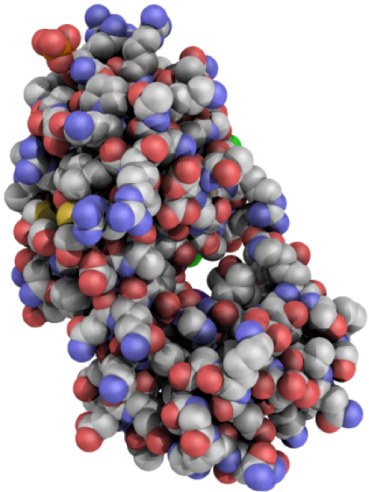
- Address missing features of PyMOL
  (e.g., version control)
- Open external programs
  (e.g., text editors, image editors, MS Word)
- Utilize other Python modules
  (e.g. webbrowser, beautifulSoup4)

Shortcuts missing styles of molecular representation

BW

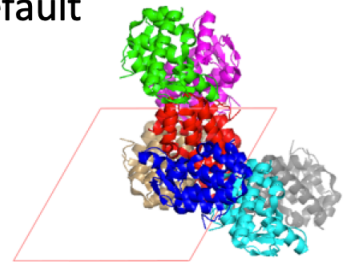


AO

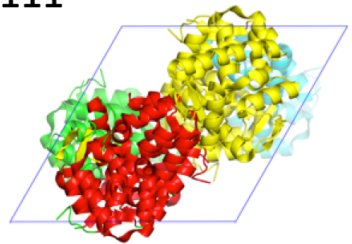


Shortcuts for unit cell arrays

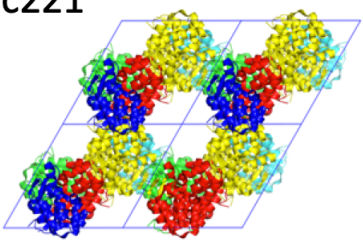
default



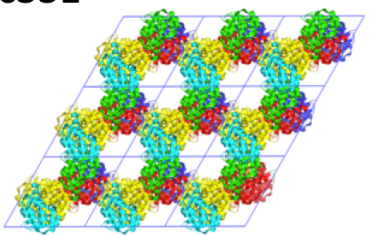
sc111



sc221



sc331



Show many models (NMR and crystal packing)

Shortcuts	Description
nmr	Show all of the models in nmr structure.
nmroff	Hide all but first model in a nmr structure.
rmsc	Remove supercell and the symmetry mates.
sc111	Make a lattice of 1 x 1 x 1 unit cells.
sc221	Make a lattice of 2 x 2 x 1 unit cells.
sc112	Make a lattice of 1 x 1 x 2 unit cells.
sc222	Make a lattice of 2 x 2 x 2 unit cells.
sc331	Make a lattice of 3 x 3 x 1 unit cells.
sc313	Make a lattice of 3 x 1 x 3 unit cells.
sc133	Make a lattice of 1 x 3 x 3 unit cells.
sc333	Make a lattice of 3 x 3 x 3 unit cells.

Saving file with time stamp

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

Saving file with time stamp

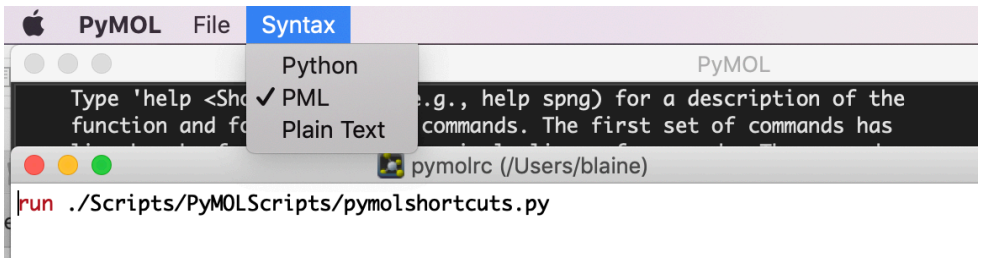
```
spse 3fao
ls 3fao*
3faoy2019m07d18h08m33s30.pse
```

Shortcuts for all other file types:

```
spng
spdb
```

PyMOL's pymolrc editor

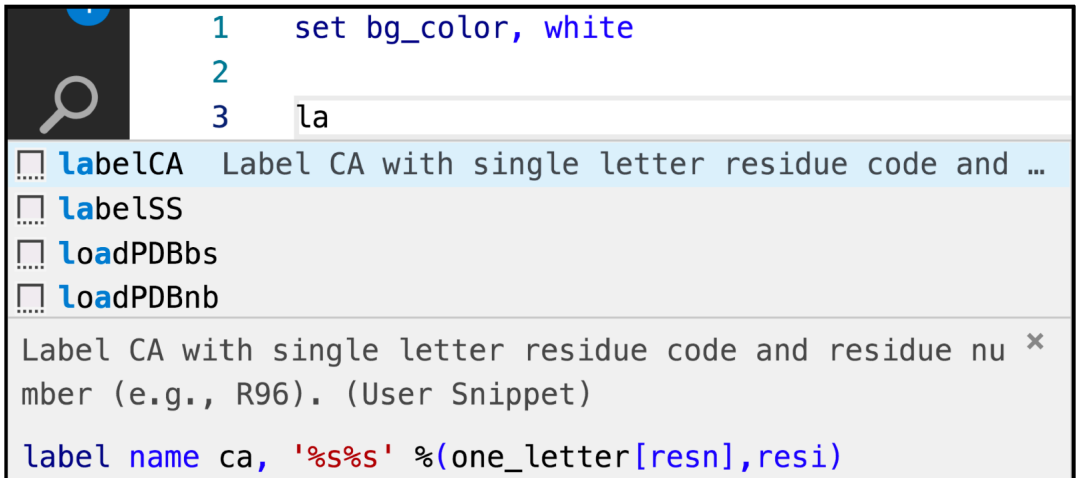
File → edit pymolrc



Open external text editor

Table: Shortcuts to text editors outside of PyMOL.

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


1 set bg_color, white
2
3 la
labelCA Label CA with single letter residue code and …
labelSS
loadPDBbs
loadPDBnb
Label CA with single letter residue code and residue nu
mber (e.g., R96). (User Snippet)
label name ca, '%s%s' %(one_letter[resn],resi)

Tab stops sites are highlighted

```
1   set bg_color, white
2
3   label name ca, '%s%s' %(one_letter[resn],resi)
4
```

Tab stops sites are highlighted

```
1   set bg_color, white
2
3   label name ca, '%s%s' %(one_letter[resn],resi)
4
```

First tab stop replaced with ‘R’

```
1   set bg_color, white
2
3   label name ca, '%s%s' %(one_letter[R],resi)
4
```

Tab stops sites are highlighted

```
1   set bg_color, white
2
3   label name ca, '%s%s' %(one_letter[resn],resi)
4
```

First tab stop replaced with ‘R’

```
1   set bg_color, white
2
3   label name ca, '%s%s' %(one_letter[R],resi)
4
```

Second tab stop replaced with ‘96’

```
1   set bg_color, white
2
3   label name ca, '%s%s' %(one_letter[R],96)
4
```

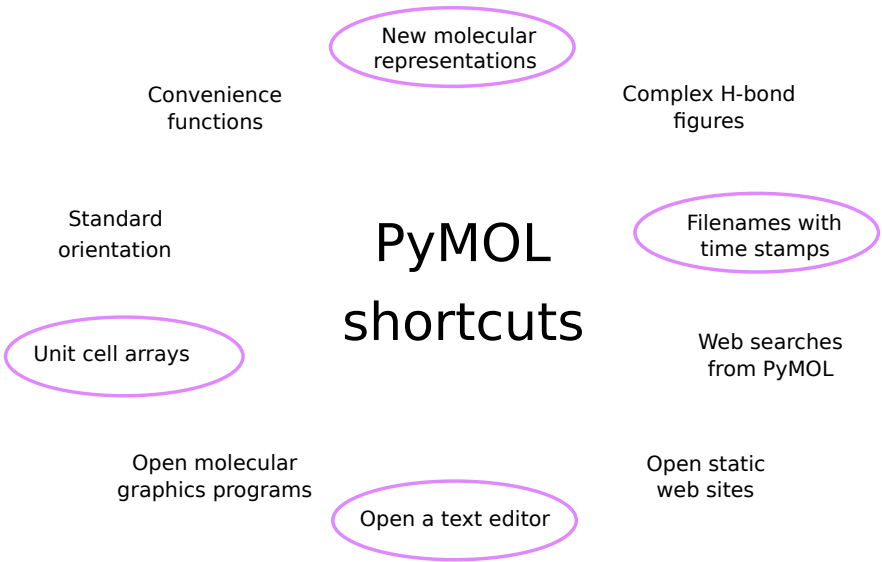
help CBSS

```
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;\
color cb_red, ss H;color cb_yellow,ss S;color cb_green, ss L+;
```

Installation

1. Download from github
   `https://github.com/MooersLab/pymolshortcuts`
   (as raw with ‘py’ file extension)
2. Add `run ~/scripts/pymolshortcuts.py` to pymolrc
3. Download supercell.py and quant.py from PyMOL Wiki
4. Run on the command line in PyMOL
   `conda install requests beautifulsoup4 datetime`

Summary


New molecular representations
Convenience functions
Complex H-bond figures
Standard orientation
PyMOL shortcuts
Filenames with time stamps
Unit cell arrays
Web searches from PyMOL
Open molecular graphics programs
Open a text editor
Open static web sites

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