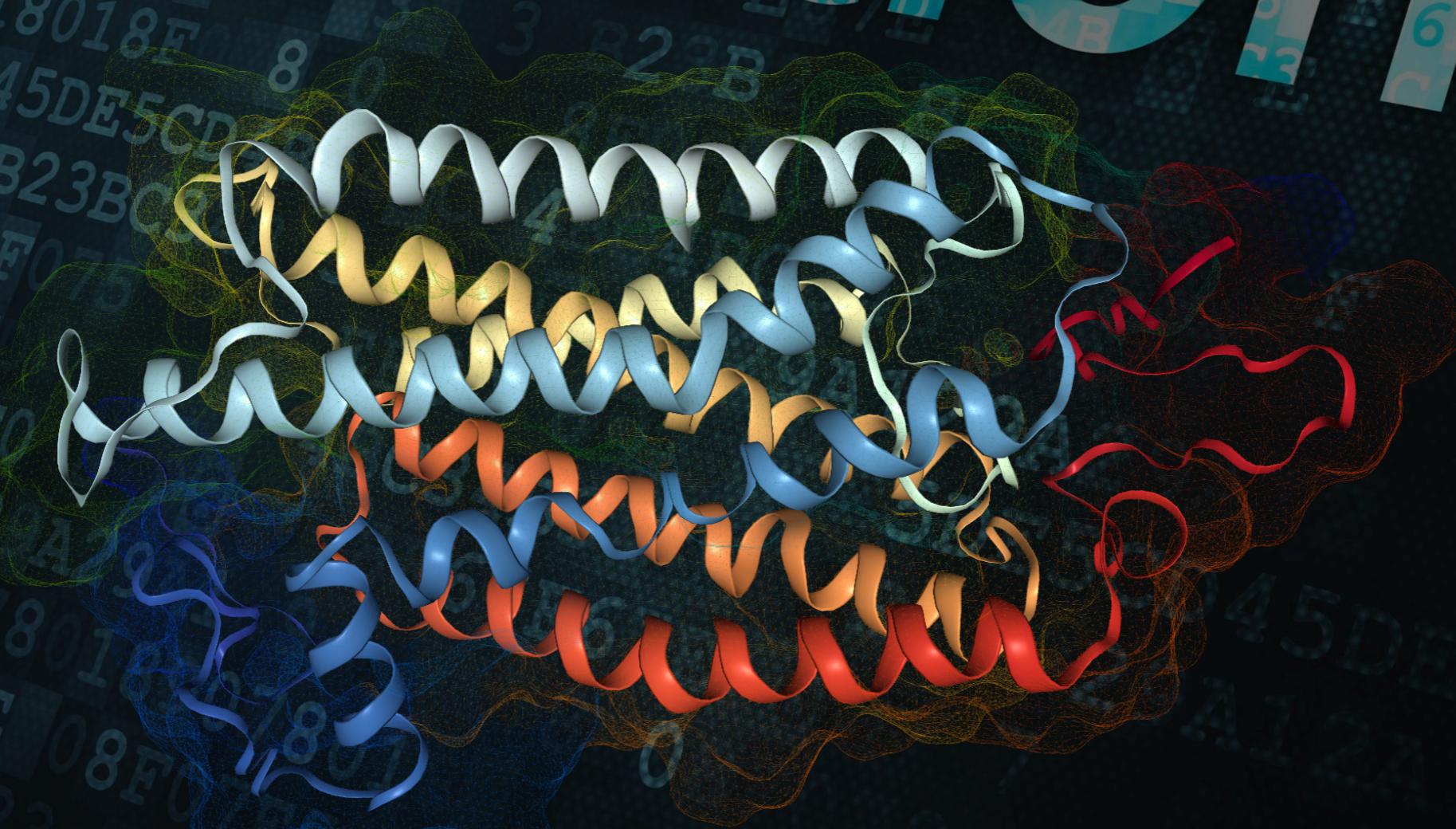


AmberTools

Integration



- **nglview: trajectory visualization in Jupyter notebook**
- **pytraj: cpptraj Python binding**
- **pdb4amber: Rewrite + more functions**
- **amber-jupyterhub for teaching**
- **AmberTools binary distribution**

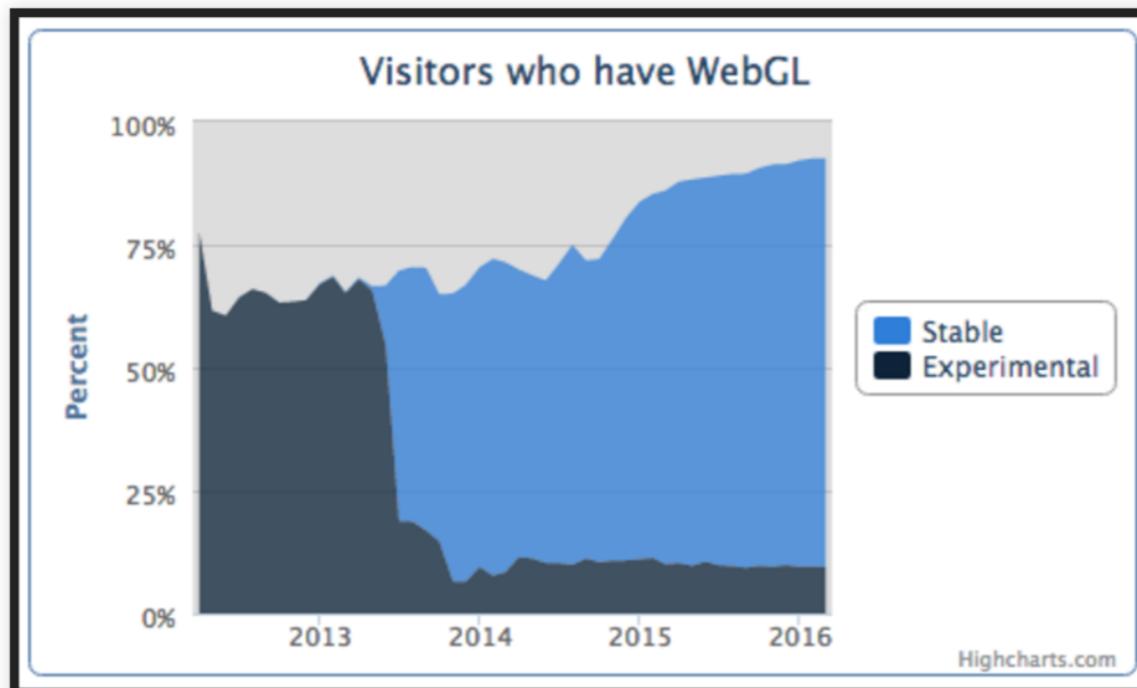
NGL Viewer

BROWSER ADVANCES

- JavaScript approaches native speed
- WebGL offers plugin-free access to the graphics card

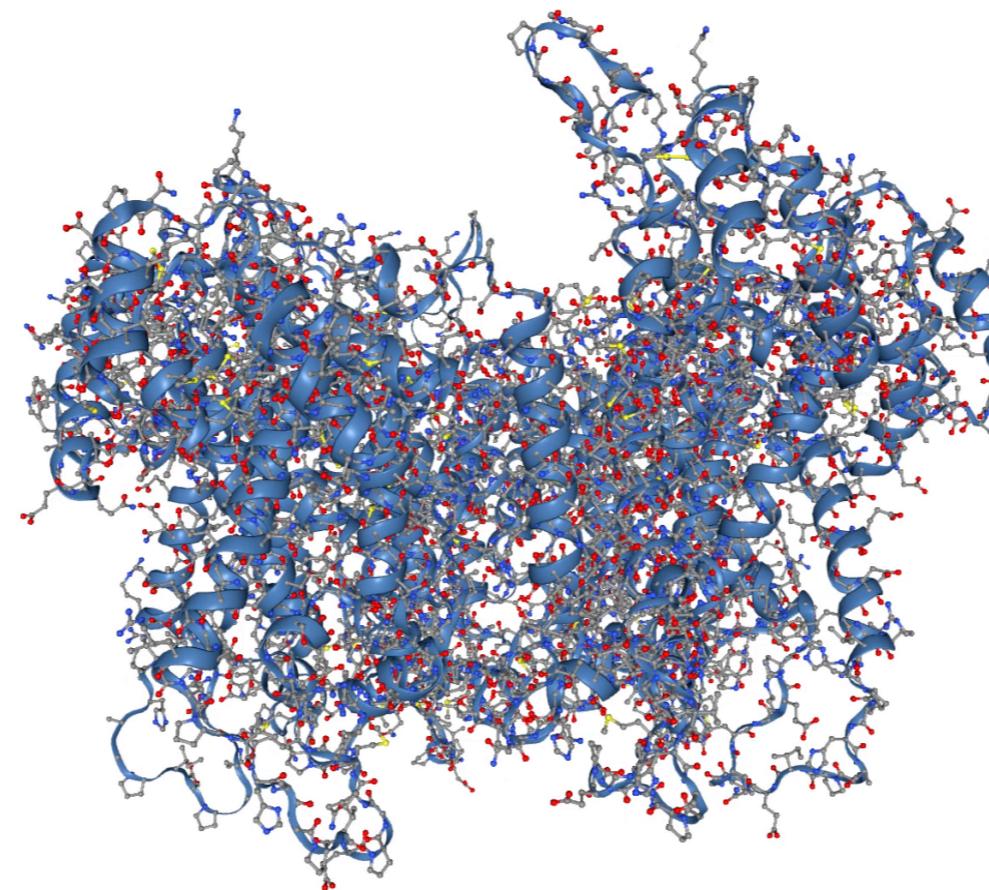


JavaScript



webglstats.com

HIV-1 capsid- 216 hexameric and 12 pentameric subunit, ~2.4M unique atoms



SDSC
SAN DIEGO SUPERCOMPUTER CENTER

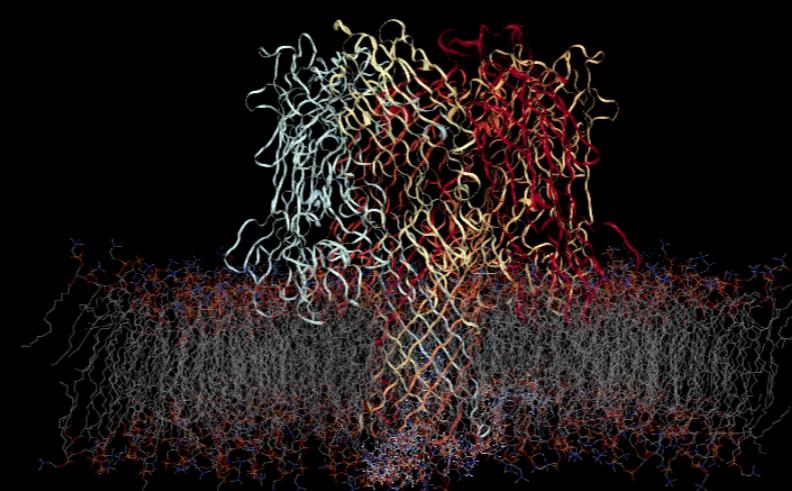
nglview: Trajectory viewer for Jupyter notebook

File Edit View Insert Cell Kernel Widgets Help | Python [conda root] ●

```
In [4]: import pytraj as pt
traj = pt.iterload('./grid.dcd', top='./ahl+dna_DNA.pdb')
traj
```

```
pytraj.TrajectoryIterator, 9 frames:
Size: 0.066826 (GB)
<Topology: 332192 atoms, 80812 residues, 0 mols, non-PBC>
```

```
In [5]: view = traj.visualize()
view.clear()
view.add_cartoon()
view.background = 'black'
view
```



pause

nglview: Jupyterlab

File Notebook Editor Terminal Console Help

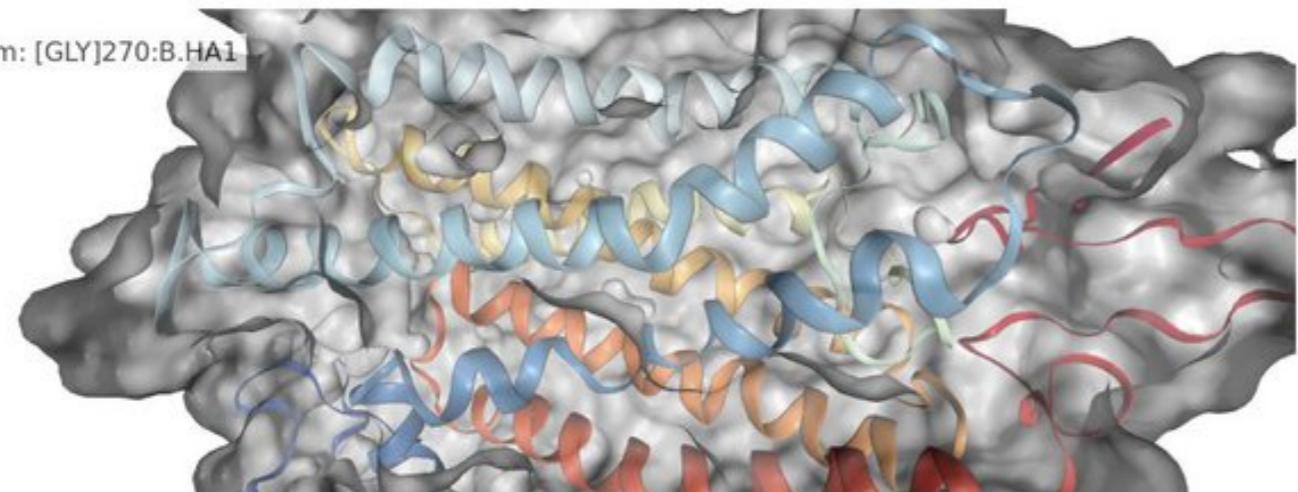
Launcher Untitled1.ipynb Untitled.ipynb

Python [default] O

In [15]:

```
import nglview
representations = [
    dict(type='cartoon', color='residueindex')
]
view = nglview.demo()
view.clear()
view.add_cartoon(color='atomindex')
view
```

Atom: [GLY]270:B.HA1



In [17]:

```
view.clear()
view.add_cartoon(color='residueindex')
view.add_surface(opacity=0.4)
```

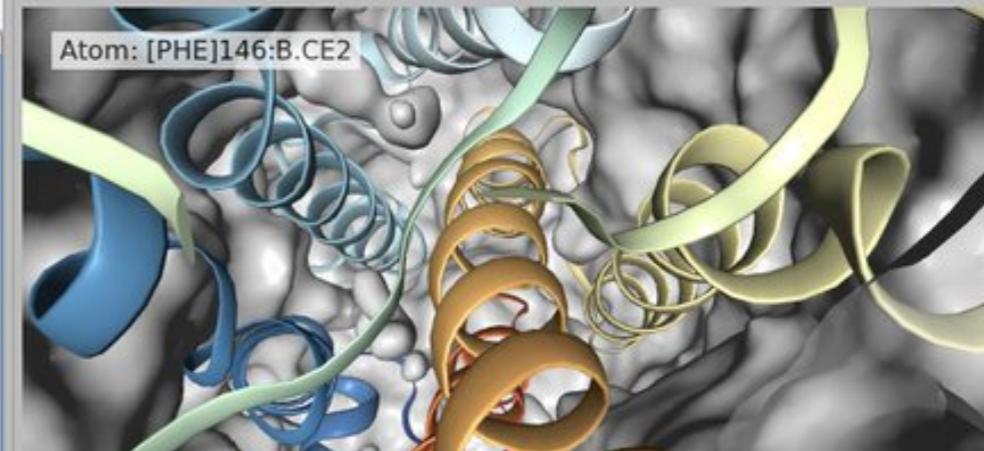
In [7]:

```
from jamber.builder import build_protein
seq = 'ALA '*10
build_protein(seq, ['alpha:1-10']).visualize()
```



Mirrored Output x

Atom: [PHE]146:B.CE2



Mirrored Output x



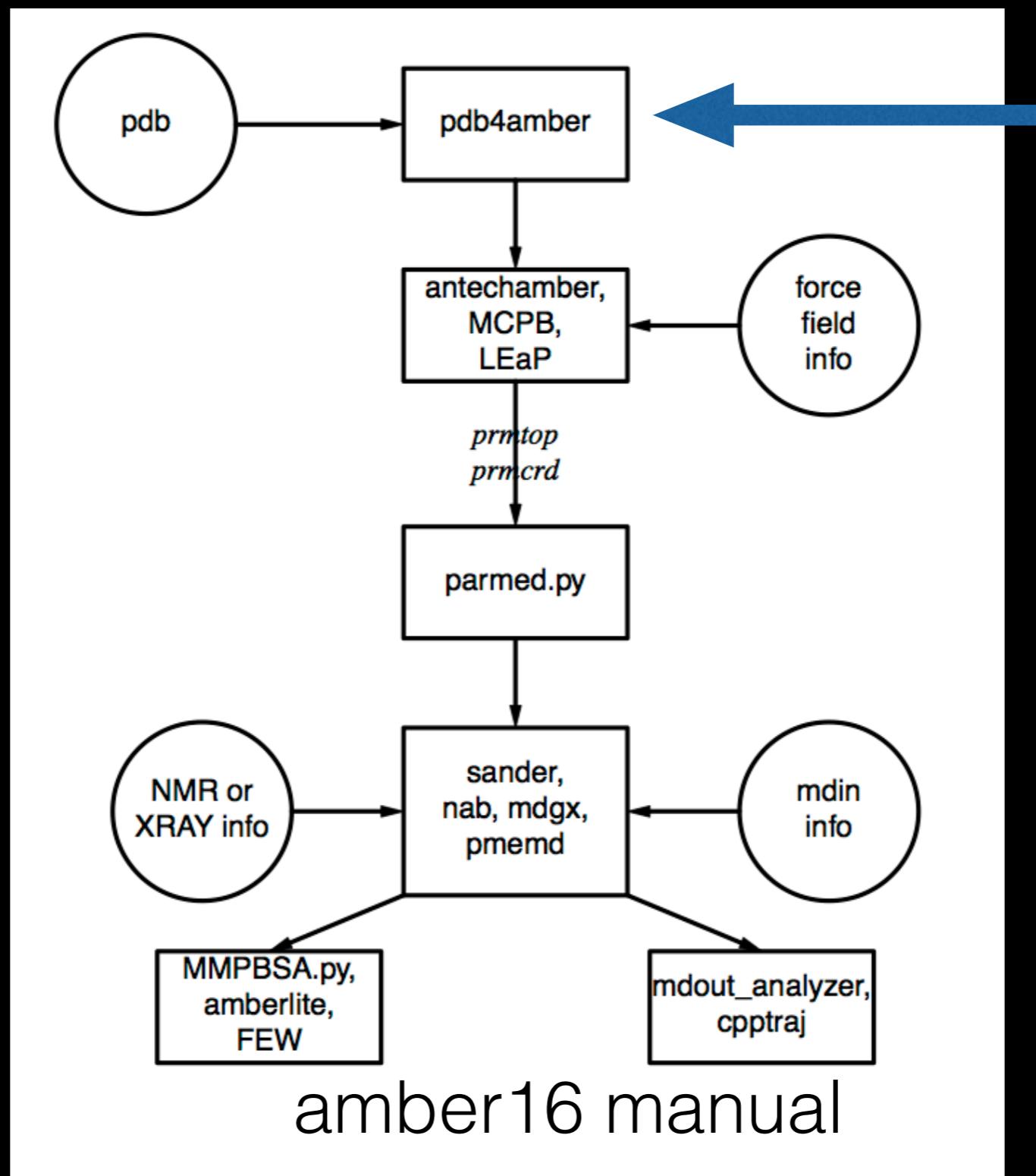
Console 1 x

Python 3.5.2 |Anaconda custom (64-bit)| (default, Jul 2 2016, 17:53:06)
Type "copyright", "credits" or "license" for more information.

IPython 5.1.0 -- An enhanced Interactive Python.
? -> Introduction and overview of IPython's features.
%quickref -> Quick reference.
help -> Python's own help system.
object? -> Details about 'object', use 'object??' for extra details.

In []:

pdb4amber: rewrite + more functions



pdb4amber

File Edit View Insert Cell Kernel Widgets Help | Python [conda root] ●

```
        }},  
        {"type": "licorice", "params": {  
            "sele": "6",  
        }},  
        {"type": "licorice", "params": {  
            "sele": "10-20 and not hydrogen"  
        }}  
    ]
```

In [*]:

```
from pdb4amber.visualizer import ViewerEditor  
import parmed  
  
parm = parmed.load_file('trpcage.pdb')  
parm.box = None  
editor = ViewerEditor(parm)  
view = editor.visualize()  
view.representations = representations  
view.background = 'black'  
view
```

In []:

```
editor.mutate([(5, 'LYS')])  
editor.add_missing_atoms()
```

In []:

```
editor.leapify()
```

In []:

```
editor.minimize(igb=8, maxcyc=200)
```

Amber Jupyterhub

GitHub, Inc. [US] | https://github.com/Amber-MD/amber-jupyterhub

This repository Search Pull requests Issues Gist

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Multi-user server for Jupyter notebooks for AMBER users. Edit

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32 commits 1 branch 0 releases 1 contributor MIT

Branch: master ▾ New pull request Create new file Upload files Find file Clone or download ▾

hainm committed on GitHub Update README.md Latest commit 0500465 on Jan 10

File	Commit Message	Time
images	login	2 months ago
Dockerfile	add hello user with password	2 months ago
LICENSE	Initial commit	2 months ago
README.md	Update README.md	a month ago
install.md	more	2 months ago
run_hub.sh	update Dockerfile and install.md guide	2 months ago
setup_jupyterhub_without_docker.sh	some notes	a month ago

Sign in

Warning: JupyterHub seems to be served over an unsecured HTTP connection. We strongly recommend enabling HTTPS for JupyterHub.

Username:

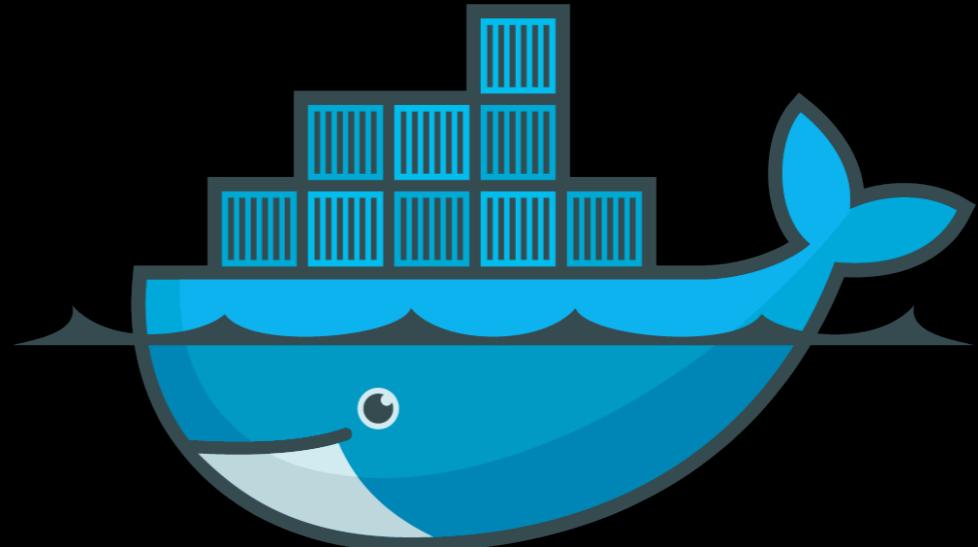
Password:

Sign In

AmberTools binary distribution

`python $AMBERHOME/AmberTools/src/conda-recipe/scripts/build_all.py`
(on Mac OS)

CONDA[®]



docker

`conda install ambertools=17 -c ambermd`

(Or download tar file, untar and source amber.sh)

AmberTools auto build

GitHub, Inc. [US] https://github.com/Amber-MD/ambertools-conda-build

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ambertools-conda-build. EXPERIMENTAL. Edit

ambertools conda ambermd molecular-dynamics-simulation Manage topics

348 commits 4 branches 1 release 1 contributor MIT

Branch: master New pull request Create new file Upload files Find file Clone or download

hainm committed on GitHub [upload] update.21 (#6) ... Latest commit ec8be4c 14 days ago

appveyor-ci	add appveyor	3 months ago
docker-build-amber	Revert "block circleci branch"	2 months ago
docker-build-box	fix	3 months ago
recipe	[upload] update.21 (#6)	14 days ago
scripts	[upload] update.21 (#6)	14 days ago
tests	[ci skip] README.md	2 months ago
.travis.yml	[upload]: Update recipe amber master (#4)	2 months ago
LICENSE	Initial commit	6 months ago
README.md	[upload] update.21 (#6)	14 days ago

Where?

- github.com/Amber-MD/XXX
 - XXX=cpptraj, ParmEd, pytraj, pdb4amber, setup-scripts, ambertools-conda-build, amber-jupyterhub
- github.com/arose/nglview