Vizualization of structures by PyMol

Disclaimer: any structure is just a model!

Get the pdb: pdb.org or pdbe.org

Documentation about pdb file format: http://www.wwpdb.org/documentation/file-format

Example:
- go to pdb.org -> type in search 'Nrd1'-> download entries 2LO6 and 3CLJ
- open with text reader

Download Pymol: http://www.pymol.org/
Manuals and hints: http://pymolwiki.org or type `help`

To load pdb-file:
- open Pymol -> File -> Open

or
- type `fetch PDBID`

Save pymol session:
- Pymol -> File -> Save session as …

or
- `save folder/folder/…/thisSession.pse`

To save logs for the session and use later as a script:
- File -> Log or `log_open log1.pml`

To see sequence:
- button S in the right bottom corner

or
- type `set seq_view, 1`

Pymol panels:
A - action
S - show
H - hide
L - label
C - color

Vizualization modes:

lines (e.g. `show lines`)
sticks
cartoon (use `dss`, dss defines secondary structure based on backbone geometry and hydrogen bonding patterns)
ribbon
surfase
spheres

Color:

by element
by secondary structure
by chain

Selection: http://pymol.sourceforge.net/newman/user/S0220commands.html

```
select name, (selection)
```

atom type: `name` or `n.`,

```
select carbons, name ca+cb+cg+cd
```

residue type: `resn` or `r.`,

```
select aas, resn asp+glu+asn+gln ; select bases, resn a+g
```

residue number: `resi` or `i.`,

```
select nterm, resi 1-10
```

chain: `chain` or `c.`,

```
select firstch, chain a
```

NMR structures (try on 2LO6):

- to see the whole bundle `set all_states, on`
- to align states `intra_fit PDBID`
- to split all states as separate objects `split_states PDBID`
- hide hydrogens `hide (hydro)`/`show (hydro)`

X-ray structures (try on 3CLJ, 2GQW)

Lamb, A.L., Kappock, T.J., and Silvaggi, N.R. (2015). You are lost without a map: Navigating the sea of protein structures. Biochimica et Biophysica Acta (BBA) - Proteins and Proteomics 1854, 258–268.

- color by chain
- split chains: `split_chains`
- hide water `hide (solvent)`
- add hydrogens: action -> hydrogen -> add
- select water `select water, resn hoh`
- color by B-factor:

```
spectrum b, blue_white_red, minimum=20, maximum=50
as cartoon
cartoon putty
```

- generation of symmetry and electron density maps (http://pymol.sourceforge.net/newman/user/S0400xtal.html)

Electrostatics (to see positive, negative, neutral areas)

Action -> generate -> vacuum electrostatics -> protein contact potential

Distance measurements

Wizard -> measurement

```
distance test, 10/CA, 50/CA
select around10, i. 12 a. 10
```

Hydrogen-bonds: http://www.protein.osaka-u.ac.jp/rcsfp/supracryst/suzuki/jpxtal/Katsutani/en/hydrogenbond.php

Action -> find-> polar contacts -> select from menu

Get surface : http://www.pymolwiki.org/index.php/Get_Area

1. select area of interest -> Action -> duplicate
2. Action -> compute -> select from menu

Alignment

1. Load structures of interest
2. Action -> align -> to molecule

several alternatives: http://pymolwiki.org/index.php/Cealign#Multiple_Structure_Alignments

Interface residues: http://www.pymolwiki.org/index.php/InterfaceResidues

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Vizualization for publication: http://www.pymolwiki.org/index.php/Publication_Quality_Images

```
bg_color white
ray 1000, 1000
save test_image.png
```

Scripting: http://pymolwiki.org/index.php/Simple_Scripting

Multiple sequence alignment visualisation: ConSurf server http://consurf.tau.ac.il/

LigPlot: Automatically generates schematic diagrams of protein-ligand interactions for a given PDB file. http://www.ebi.ac.uk/thornton-srv/software/LIGPLOT/

UCSF Chimera - more sophisticated then PyMol : https://www.cgl.ucsf.edu/chimera/