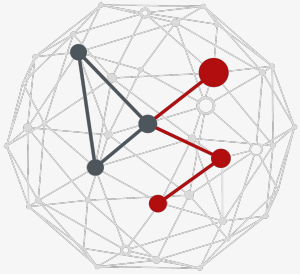
DIPARTIMENTO
MATEMATICA



DATA SCIENCE
UNIVERSITY OF PADOVA

PYMOL

Master of Science in Data Science

Alexander Monzon

PDB

DIPARTIMENTO MATEMATICA

Videos
https://pdb101.rcsb.org/learn/videos

Biological assemblies
https://pdb101.rcsb.org/learn/guide-to-understanding-pdb-data/biological-assemblies

Methods for Determining Atomic Structures
https://pdb101.rcsb.org/learn/guide-to-understanding-pdb-data/methods-for-determining-structure

Resolution
https://pdb101.rcsb.org/learn/guide-to-understanding-pdb-data/resolution

Primary Sequences and the PDB Format
https://pdb101.rcsb.org/learn/guide-to-understanding-pdb-data/primary-sequences-and-the-pdb-format

Install Pymol

Wiki home
https://pymolwiki.org/index.php/Main_Page

Linux install
https://pymolwiki.org/index.php/Linux_Install

Windows install
https://pymolwiki.org/index.php/Windows_Install

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Tutorial

Annemarie Honegger - Intro/Intermediate/Advanced
pymol_AHonegger_1.pdf
pymol_AHonegger_2.pdf
pymol_AHonegger_3.pdf

Short but useful
pymol_cheatsheet.pdf

From De Lano
pymol_delano.pdf

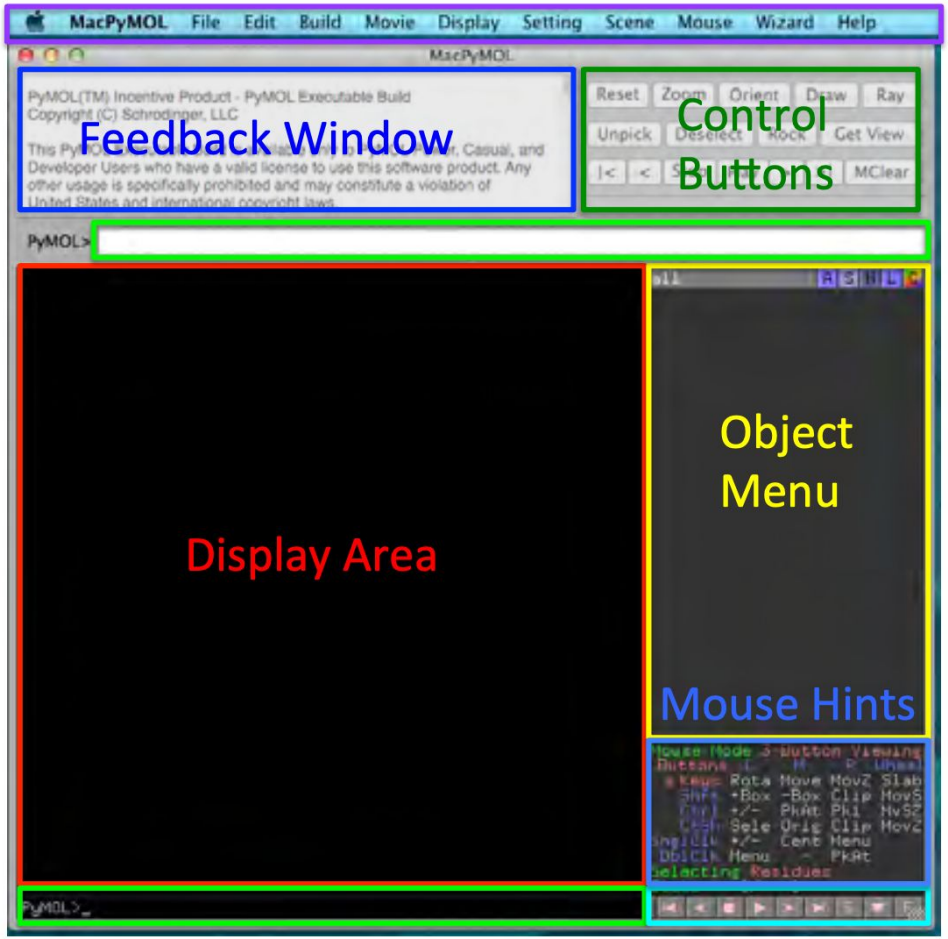
Win/Linux: 2 windows

Control window

- Pull-down menus
- Command line
- Control Buttons
- Feedback window

Viewing Window

- Display area
- Object menu
- Mouse hints
- Movie controls
- Command Line



DEMO, play along

Selection

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Selecting a particular type of **secondary structure** elements:

```
select ss s (will select all beta folded sheets)
select ss h (will select all alpha helices)
select ss '' (will select all connecting regions)
```

Selecting a particular **protein chain:**

```
select chain A
```

Selecting **amino acids:**

```
select resn ARG
select resn ARG+PHE
select resi 25+30
```

Tricky commands

https://pymolwiki.org/index.php/Selection_Algebra

fetch 1ctq

Select the ligand, exclude water from hetero atoms
sele ligand, het and not name o

Select atoms within 3.0 Angstroms from the ligand
sele nb, all within 3.0 of ligand

Sele atoms around the ligand
sele nb2, ligand around 3.0

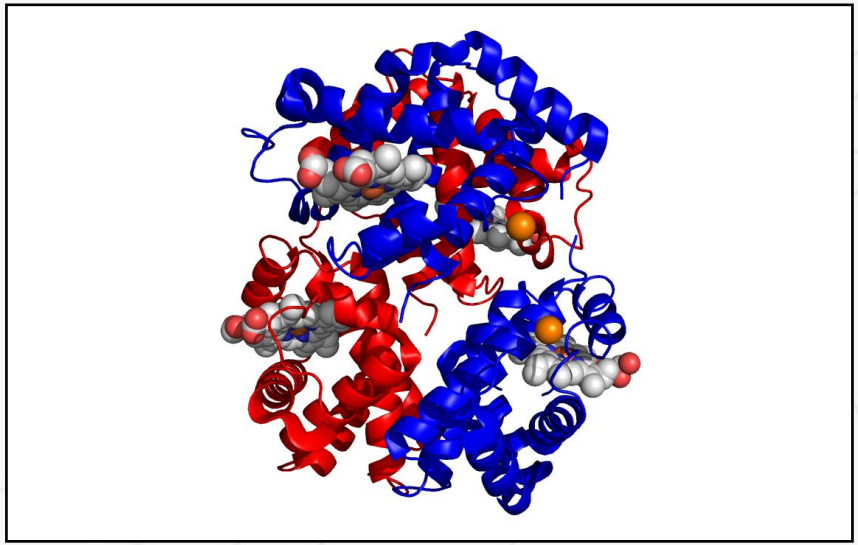
Extend the selection to entire residues involved in the “nb2” selection
sele nb3, byres nb2

Exercise 1:

PDB code: 2HHB, haemoglobin

Consider the following elements: heme groups, chains corresponding to the alpha or beta subunits and the phosphate groups.

- Heme and phosphate groups in sphere representation.
- Protein in cartoon representation, alpha subunit colored in red and beta in blue.
- Render with the *ray* command.



Exercise 2:

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Note: a duplication of the element must be generated to represent it on the surface

- Hide the phosphate groups.
- Represent the heme groups in sticks and change the coloration.
- The surface must be in gray color and with transparency (*set transparency, 0.5, element*) and the representation of the molecule is in cartoon gray color.