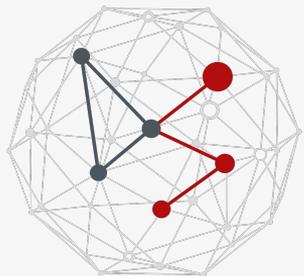


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ANNI



UNIVERSITÀ
DEGLI STUDI
DI PADOVA

  **DIPARTIMENTO
MATEMATICA**



DATA SCIENCE
UNIVERSITY OF PADOVA

PyMOL

Master of Science in Data Science

Damiano Piovesan



PDB

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

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

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

PyMOL by Schrödinger (recommended) <https://www.pymol.org/>

```
# Linux
conda create -n pymol
conda activate pymol
conda install -c conda-forge -c schrodinger pymol-bundle
```



Tutorials

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](#)



Selection

Select amino acids <https://pymolwiki.org/index.php/Select>

```
select resn ARG
```

```
select resn ARG+PHE
```

```
select resi 25+30
```

```
select resi 25-30      (range)
```

Select a particular **protein chain**

```
select chain A
```

Select 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)
```



Useful commands

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

Download the PDB

```
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
```

Select atoms around the ligand (need to define “ligand” selection before)

```
sele nb2, ligand around 3.0
```

Expand the selection to complete residues in the “nb2” selection

```
sele nb3, byres nb2
```

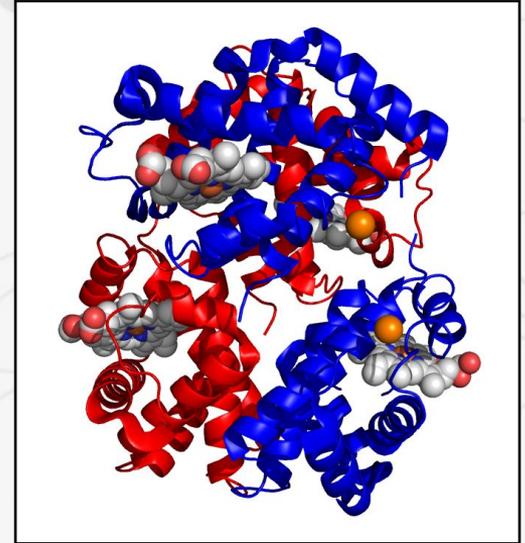


Exercise 1

PDB code: 2HHB, haemoglobin

Consider the following elements: heme groups, alpha & beta chains, phosphate groups

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



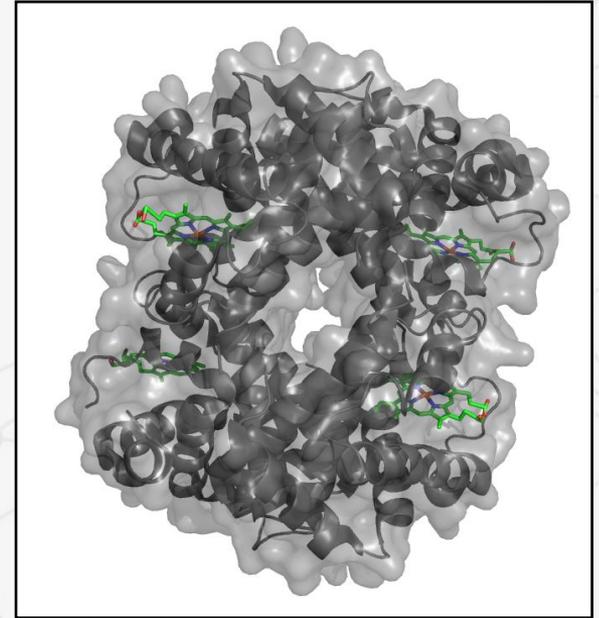
Exercise 1

```
sele alpha_sub, chain A+C  
sele beta_sub, chain B+D  
bg_color white  
sele hem_groups, resn HEM  
set transparency, 0.5, obj01
```



Exercise 2

- Hide phosphate groups
- Show the heme groups as sticks and change the color
- Show the molecule as cartoon in gray color
- Show the protein surface in gray and with transparency (*set transparency, 0.5, element*)
 - Note: you need to duplicate the object to add the surface representation



Scripting

How to run scripts

<https://pymol.org/tutorials/scripting/howtorunscripts.html>

Use command line options from a script

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



Compiled graphics objects (CGO)

<https://pymolwiki.org/index.php/Category:CGO>

Three-dimensional geometries and animations displayed at high-speed via OpenGL

