COBB2035 · RECITATION 2 (but actually 1)

PyMOL

Today

Install	Get open-source PyMOL running in a clean conda environment.
Demo	Follow Along
Basic ✓	Ray-traced figure of profilin 1: wild type vs. the M114T ALS variant.
Extra ✓+	Cryo-EM map of a glycine receptor. Identify evidence of a chloride atom that is not in the pdb.

Installing PyMOL

Open-source PyMOL. No license, no registration.

```
conda create -n pymol python=3.11
conda activate pymol
conda install conda-forge::pymol-open-source
```

Launch it:

```
pymol
```

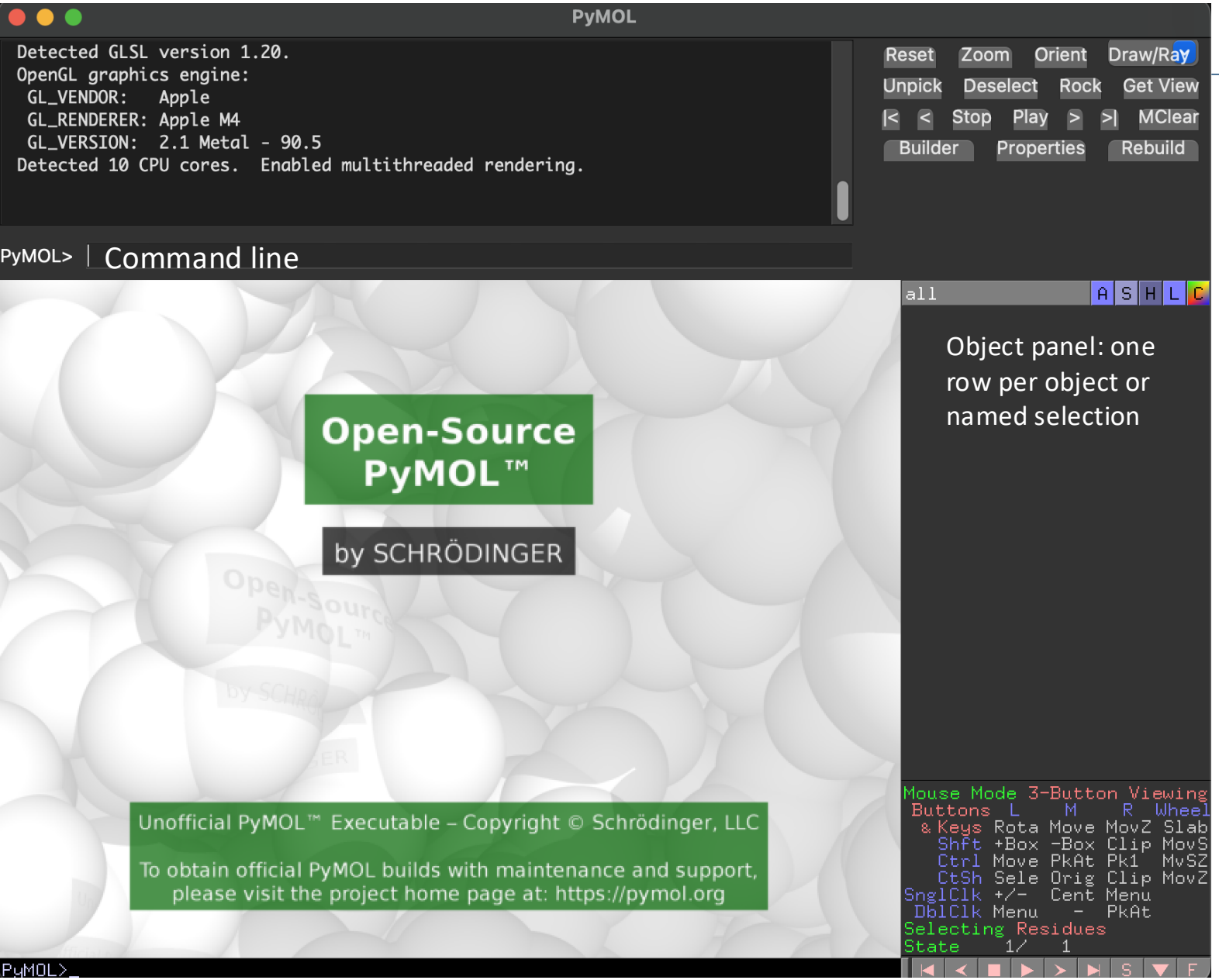
WHY A SEPARATE ENVIRONMENT

Cleaner to have separate tools in separate environments

IF THE SOLVER HANGS

- Use mamba, or conda install --solver=libmamba.

The window



Menus — everything here has a command equivalent

Object panel toggles:
Action, **S**how, **H**ide, **L**abel, **C**olor

Mouse Control Guide

Selection tools

`Mouse > Selection Mode` switches clicking between Atoms / Residues / Chains / Molecules.

Anatomy of a command

```
color   red,   resi 44 and chain A
#  ^       ^     ^
#  cmd     arg1  arg2
```

- Arguments are separated by commas, not spaces.
- Most commands take an optional selection as the last argument.
  If not present the command applies to everything.
- Keyword arguments come last: png out.png, width=2000, ray=1

The wiki helps: pymolwiki.org

Selections

Half of PyMOL is knowing how to say “these atoms and no others.”

PROPERTIES

`resi 114`	residue number
`resn MET`	residue name
`name CA`	atom name
`chain A`	chain
`elem S`	element
`ss H`	secondary structure
`b > 60`	B-factor

CLASSES

`polymer`	protein + nucleic acid
`solvent`	water
`organic`	small-molecule ligands
`inorganic`	ions, metals
`backbone`	and sidechain — within polymer
`hydro`	hydrogens

OPERATORS

`and or not`	Logic. and narrows, or widens.
`byres`	Grow to whole residues. Use it or you get half a sidechain.
`s1 within 5 of s2`	Atoms of s1 that are near s2
`s1 expand 5`	s1 plus its neighbours
`s1 around 5`	The neighbours only — s1 itself excluded

1YCR

```
fetch 1YCR, async=0

hide everything
show cartoon, polymer
color grey70

# colour N-to-C so you can read directionality
spectrum count, blue_white_red, polymer and name CA

# Select residues, name the selected residues patch
select patch, resi 8+44+68+70
show sticks, patch and sidechain
color orange, patch

orient
```

Representations and colour

SHOW / HIDE

`show`, `hide`, and `as`.
`as` replaces everything else

```
as cartoon
show surface, polymer

# surfaces only:
set transparency, 0.4
set surface_color, grey70
```

Two structures: adenylate kinase

`4AKE` E. coli adenylate kinase, no ligand, open.
`1AKE` The same enzyme clamped shut around AP5A, a two-substrate mimic.

```
fetch 4ake, opened, async=0
fetch 1ake, closed, async=0
```

`4AKE` has two copies in the asymmetric unit. `1AKE` has one. Split first:

```
# Extract chain A from opened
# Extract chain B from closed
# Delete initial structures

as cartoon
color grey70, chA_opened
color skyblue, chB_closed

align chA_opened, chB_closed
orient
```

`align`	Sequence alignment, then fit, then outlier rejection. Default for near-identical sequences.
`super`	Structure-driven. Use when sequence identity is low.

Ray tracing and saving


```
bg_color white
set ray_opaque_background, 0
set antialias, 2
set ambient_occlusion_mode, 1
set light_count, 8
set ray_trace_mode, 0

png figure1.png, width=2000, height=1500, dpi=150, ray=1
```

`width, height`	Pixels. These are what determine resolution.
`dpi=300`	Metadata, so layout software scales it right.
`ray=1`	Ray-traces first
`bg_color`	The viewport you work in.
`ray_opaque_background`	The file you export. 0 gives a transparent PNG.
`ambient_occlusion_mode`	Darkens crevices. Big readability win on surfaces.
`ray_trace_mode`	0 photoreal, 1 adds black outlines, 2 line art, 3 cel-shaded.

Reference

Every wiki page has worked examples. Read them instead of guessing.

Main Page	Start here	**Align**	Sequence-based fit
Fetch	Pull from the PDB	**Super**	Structure-based fit
Load	Local files and maps	**Distance**	Measure, find H-bonds
Show	Representations	**Ray**	Rendering
Color	Named colours, spectrum	**Simple Scripting**	.pml and Python

Cheat sheet

LOAD

```
fetch 1ubq, async=0          from the PDB
load file.pdb, name          from disk
load map.map, edmap          density
delete name                  remove
```

LOOK

```
hide everything              reset
as cartoon, polymer          replace reps
show sticks, sel             add rep
color grey70, sel

orient sel                   rotate + zoom
zoom sel, 5                  zoom only
```

COMPARE

```
align a, b                                  by sequence
super a, b                                  by structure
align a, b, transform=0                     measure only
distance d, s1, s2, 3.5, mode=2             H-bonds
```

RENDER

```
bg_color white
png f.png, width=2000, ray=1                always ray=1
```

DEBUG

```
help <cmd>
print(cmd.count_atoms("sel"))
iterate sel, print(resi,
resn)
get_view                                    camera
```

BASIC ✓

Profilin 1: Wild Type vs. M114T

`4X1L`	Wild-type profilin 1
`4X25`	M114T profilin 1 — an ALS-linked variant

Make a **ray-traced** figure showing any differences between the two proteins. Write a caption. Put your name on it.

SUBMIT

Upload your figure(s) with a caption and your name to GradeScope.

EXTRA ✓+

A cryo-EM map, and a missing ion

1. Visualise the density map for 7M6Q.
   Coordinates from PDB; Map from EMDB.
2. Find evidence of a chloride ion.
3. Comment on anything else you notice.

KNOW WHAT YOU ARE LOOKING AT

7M6Q is a full-length α1 **glycine receptor**, pentameric, in a lipid nanodisc, with glycine and THC bound. The map is **EMD-23704**.

The glycine receptor is an anion channel. Look into the channel.