

Visualizing Protein Structures — A Practical Introduction to PyMOL

MOL305 - Proteins: structure and function

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1 Introduction

This introduction to PyMOL uses the porin proteins OmpF and OmpK36, from *Escherichia coli* and *Klebsiella pneumoniae* respectively, as examples. Porin proteins make water-filled channels in the outer membrane of Gram-negative bacteria.

Descriptions of how PyMOL works is written in normal text.

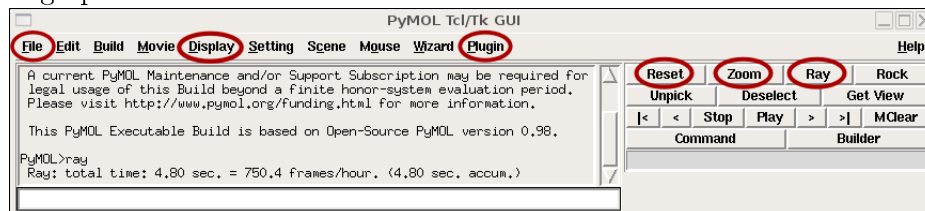
Direct instructions for interactions with PyMOL are written in sans serif font.

Commands are written in typewriter font.

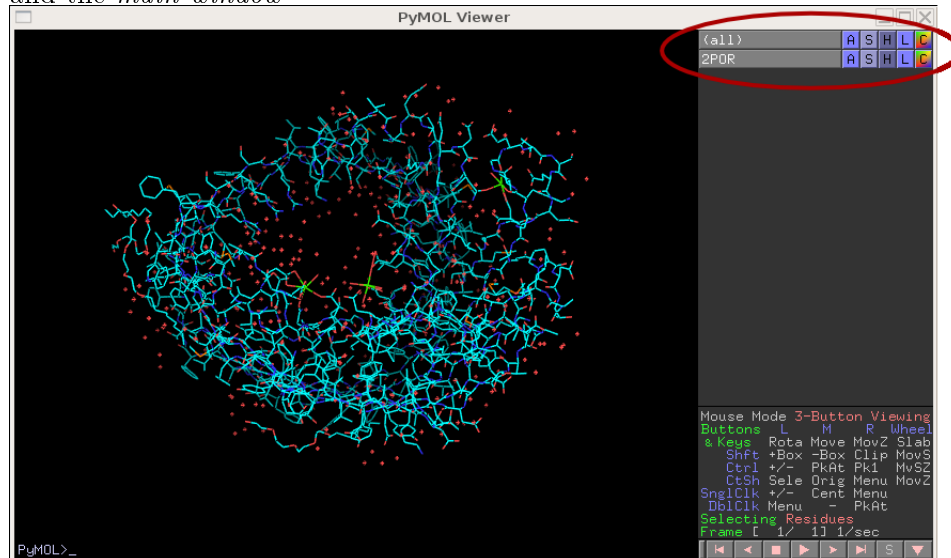
Menu selections are referred to like this: FILE>OPEN.

2 The PyMOL graphical user interface

The graphical user interface is divided in two – the *menu window*



and the *main window*



For the purpose of this introduction we will only focus on the parts of the user interface encircled in red.

2.1 Load the structure coordinates

Protein structure coordinates can be read in either from file or directly from the PDB database through the internet. To read from file – simply use the File menu: FILE>OPEN.

To read directly from the PDB database – use the PDB Loader Service plugin: `PLUGIN>PDB LOADER SERVICE` – and enter the the PDB identifier code.

Open the coordinates for the *Escherichia coli* porin protein OmpF – **2OMF**.

Use both methods to load the OmpF structure coordinates. (The first requires you to download the PDB file from the PDB database.)

2.2 Use the mouse to rotate, zoom and move the structure

The mouse can be used to perform different manipulations of the view of the structure.

Rotate

Click with the left mouse button and move the mouse.

Zoom

Click with the right mouse button and move the mouse.

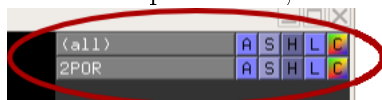
Move

Click the middle mouse button and move the mouse.

Tip To get back the initial view, click on the RESET button (menu window).

2.3 Objects and selections

The PDB identifier of the OmpF structure that was loaded is listed at the upper right of the main window. More than one structure can be loaded at the same time, and each will have a separate line, and are considered by PyMOL to be separate *objects*.



When selections of parts of the structures are made these will be listed as new lines. To separate selections from objects, the selection names are always surrounded by parenthesis. One special selection is always present, namely the first line marked **(all)**. It always represents all objects.

Click on one of the amino acid residues in the structure. (You may need to also press the CTRL key here.)

Note two things:

1. A new line named **(sel01)** appears – the amino acid is selected.
2. The identity of the residue is listed in the *menu window*.

Objects and selections can be made active or inactive by clicking on the grey bar containing the name.

Click on the 2OMF line.

Note that the the structure disappears. Clicking one more time brings the structure back in view.

2.4 The main window menus

Each object or selection has a separate set of menus attached that are accessible by clicking on the letters to the right of the name:



A Action

S Show

H Hide

L Label

C Colour

By using the appropriate menu, different manipulations of the structures (objects) or parts of the structures (selections) can be made.

Only selected functions from the menus will be demonstrated here, but feel free to explore!

2.4.1 The action menu

One nice feature that can be found in the action menu is the PRESET functionality.

Select **A>PRESET** to get the PRESET sub-menu. Choose different preset views and observe the effects.

Also, hydrogen bonds can be visualized:

Select **A>FIND>POLAR CONTACTS>WITHIN SELECTION**.

If you need to remove objects and selections, this can be done from the action menu.

2.4.2 The show and hide menus

The show and hide menus can be used to choose between the different representations of structures such as lines, sticks, ribbon, cartoon, spheres (CPK) and surface.

Explore different representations by selecting from the show menu. Also try different combinations of representations.

Note that if you get lost, the hide *everything* feature is handy (**H>EVERYTHING**).

2.4.3 The colour menu

Try out different ways of colouring the structure.

Note that some colouring schemes only make sense in combination with particular representations. E.g. COLOUR BY ELEMENT can be used with lines, sticks, spheres and surface.

2.5 Displaying the sequence and selecting residues

One useful feature of PyMOL is the ability to display the sequence, and use it to make selections of single and multiple amino acid residues.

Display the sequence: DISPLAY>SEQUENCE. Try to mark residues by clicking on them. Choose different representations and/or colours for the selected residues.

2.6 Saving a session

Sessions can be saved for later: FILE>SAVE SESSION. To open a saved session: FILE>OPEN.

2.7 Making nice pictures with PyMOL

One of the nice features of PyMOL is the ability to make high (publication) quality images. The first step is to perform a so-called ray trace rendering of the structure.

Click on the RAY button in the menu window.

This may take a while, depending on the computer, structure and the chosen representation. Notice that the image becomes very nice and smooth. Next, you can save the image: FILE>SAVE IMAGE.

3 Manipulating the structures using PyMOL commands

Some things are difficult or impossible to do by mouse and menus only. Examples are selecting chains, secondary structure elements or amino acid residues by name or number. The way to do this is to issue commands. This can be done in several ways. Here we will mainly use the prompt at the bottom of the main window, and also demonstrate how commands can be collected into a script file.

To make things slightly more interesting we will now switch to the homologous OmpK36 from *Klebsiella pneumoniae* (PDB: 1OSM). The reason is that the coordinates for the native trimeric state is present for this structure.

3.1 Selecting chains

The OmpK36 structure has three (identical) chains. They are named A, B, and C. To select chain A:

```
select chain A
```

To name the selection:

```
select chain_A, chain A
```

Try to change representation and/or colour of chain A by using the chain_A menus. Issue the following command to bring chain A into focus:

```
zoom chain_A
```

Try to rotate the molecule. Bring back focus to the trimer (all chains):

```
zoom
```

3.2 Selecting secondary structure elements

Issue the following commands to make named selections of the secondary structure elements:

```
select helix, ss h
select sheet, ss s
select loops, ss l+'''
```

3.3 Selecting residues by name and number

Amino acid residues can be selected by their three letter code. To select all phenylalanines (PHE):

```
select resn PHE
```

To select a particular amino acid residue, you must refer to them by their numbers:

```
select resi 100
```

Note that this selection will select residue number 100 in all chains. To refer to a residue in a particular chain one can combine two statements in one select:

```
select chain A and resi 100
```

Named selections are useful to define groups of amino acids. For instance:

```
select aromatic, resn PHE+TYR+TRP
```

Note that you can combine the selection of multiple residues by separating them with +. In a similar manner ranges of amino acids can be selected using numbers:

```
select resi 1-100
```

3.4 Combine named selections

One powerful way of using named selections is to combine them by the boolean operators *and*, *or* and *not*. One example – make a selection of all aromatic residues located in the β -sheets (this requires that you already have made the above mentioned selections *sheet* and *aromatic*):

```
select sheet and aromatic
```

Try to use the other two boolean operators and observe the effects.

Note that to get e.g. sheets *and* helices, you need to use the *or* operator:

```
select sheet or helix
```

4 Visualization tasks

Based on what you have learned, try to make the visualizations suggested below. To save some work, a pre-made script can be loaded that will give you a set of named selections (<http://www.cbu.uib.no/~pal/1OSM.pml>). This script requires that the 1OSM.pdb file is located in the same directory as the script. The script can be invoked by FILE>RUN.

4.1 The constriction zone

The so-called constriction zone of the porins are important for screening which compounds are allowed to pass through the pore. The following illustration shows important residues involved in the constriction zone:

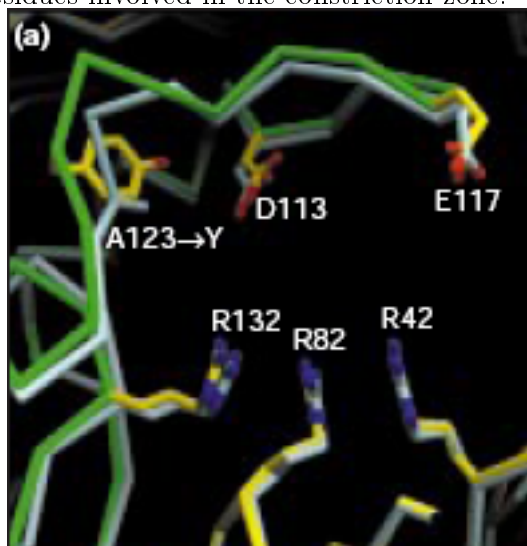


Figure from *Dutzler et al. Structure*, 1999, 7:425-434.

Visualize these residues in a similar manner and use PyMOL to get a better impression of where these amino acids are located.

4.2 The aromatic rings and the trimer interface

Aromatic residues play an important role in placing the protein correctly in the membrane. Select the aromatic residues in the β -sheets, and observe the pattern. Since these proteins are situated in membranes, what group of amino acids do you expect to find on the outside of the barrels (facing the membrane)? Try to visualize this group.

Is there a difference in the pattern of amino acids that face the membrane compared to the trimer interface?

4.3 Hydrogen bonding

Try to observe the hydrogen bonding pattern in the β -sheets and the α -helices.

5 I just can't get enough!

Compare the two structures we have been looking at by loading both structures. Then – make a structural alignment between the two:

```
align 10SM, 2OMF
```

6 Important links

PDB <http://www.rcsb.org/pdb/>

PyMOL <http://pymol.sourceforge.net/>