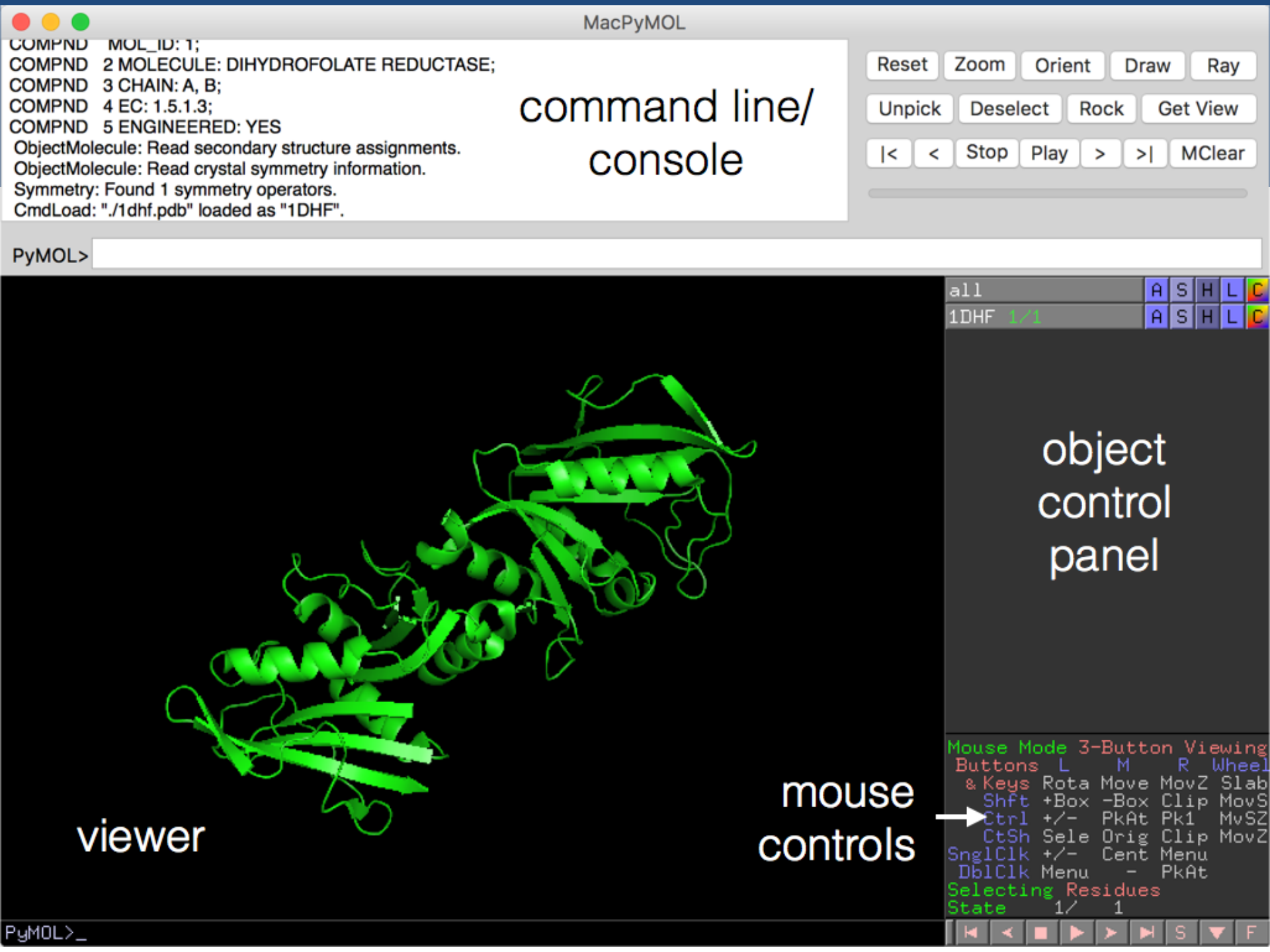
Protein structure and PyMOL scripting


MacPyMOL
COMPND MOL_ID: 1;
COMPND 2 MOLECULE: DIHYDROFOLATE REDUCTASE;
COMPND 3 CHAIN: A, B;
COMPND 4 EC: 1.5.1.3;
COMPND 5 ENGINEERED: YES
ObjectMolecule: Read secondary structure assignments.
ObjectMolecule: Read crystal symmetry information.
Symmetry: Found 1 symmetry operators.
CmdLoad: "./1dhf.pdb" loaded as "1DHF".
command line/ console
Reset
Zoom
Orient
Draw
Ray
Unpick
Deselect
Rock
Get View
|<
<
Stop
Play
>
>|
MClear
PyMOL>
all
1DHF 1/1
object control panel
viewer
mouse controls
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl +/- PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1
PyMOL>_

Object control panel

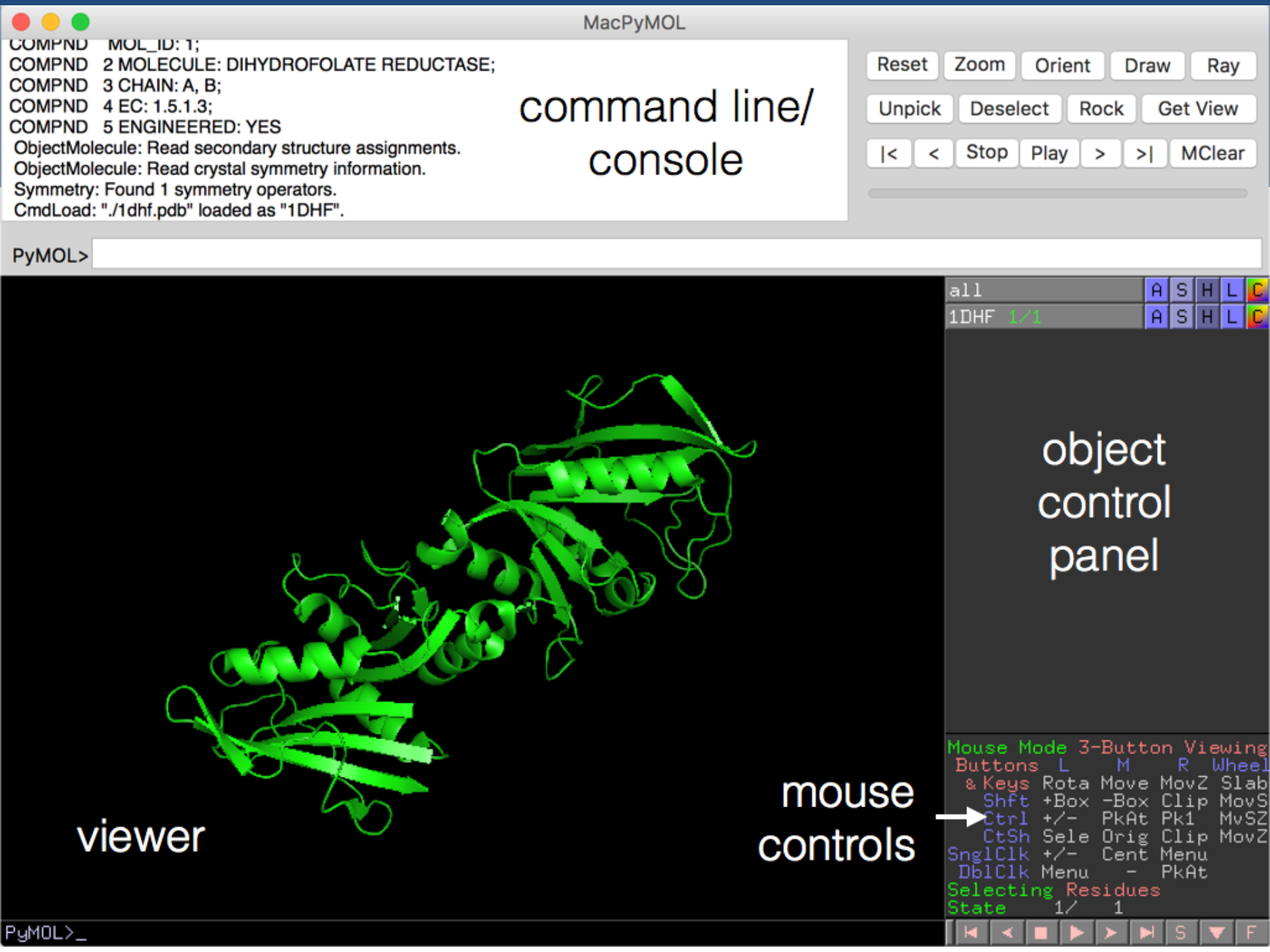
A (Actions): Rename, duplicate, remove

S (Show): Change the way things appear, e.g. change to stick or cartoon view.

H (Hide): Things that are shown using **S** accumulate, and don't automatically replace the last view. **H** is the opposite of **S** and hides unwanted representations.

L (Label): Label atoms, residues, etc.

C (Color): Change the color of atoms and groups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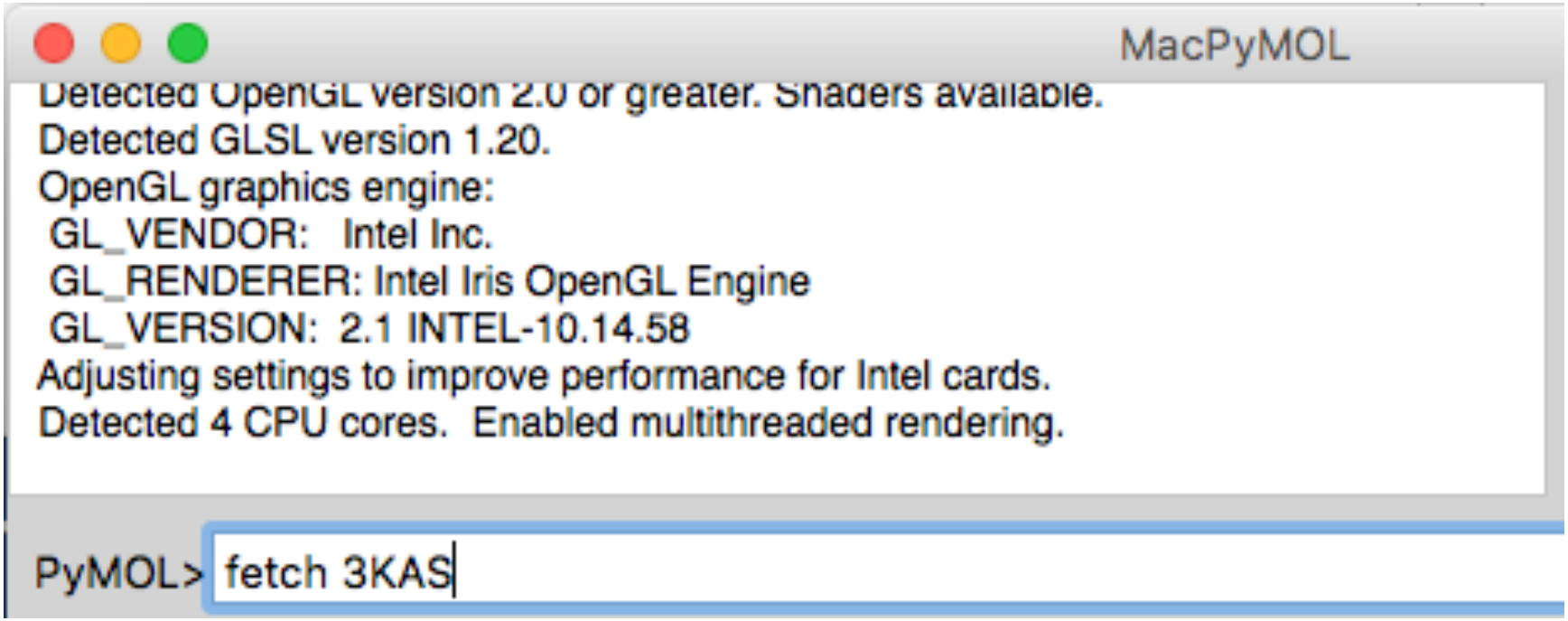
Selecting Residues
State 1/ 1
PyMOL>_

Anything you can do with a menu, you can do with a command

```
command arg1, arg2, arg3
```

```
>fetch 3KAS
```



Anything you can do with a menu, you can do with a command

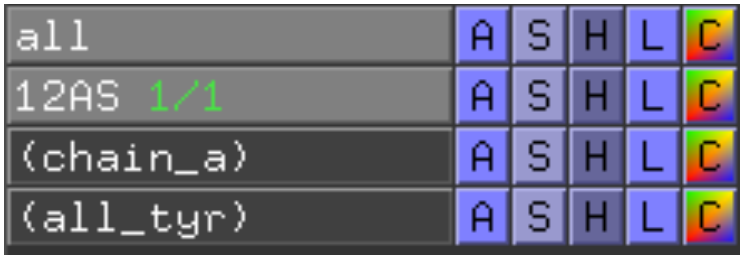
`select` *`name`*`,` *`selector`*

select chain A

```
>select chain_a, chain A
```

select all tyrosines

```
>select all_tyr, resn TYR
```



More on selector syntax

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

Anything you can do with a menu, you can do with a command

hide everything

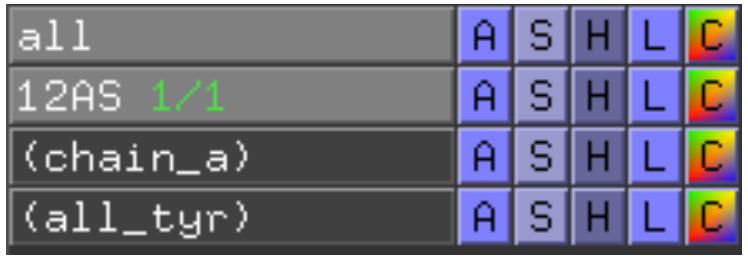
```
>hide all
```

show selection as ribbon

```
>show ribbon, (chain_a)
```

color selection blue

```
>color blue, (all_tyr)
```



PyMOL exercises

1. Download & open structure 3KAS:
   `fetch 3KAS`
   - Display in various forms (cartoon, stick, spheres, …)
   - Color different chains

2. Download & open structure 1DLW
   - Display as cartoon
   - Show heme as sticks

Every PyMOL command has a python counterpart

PyMOL:`>select chain_a, chain A`

Python: `cmd.select("chain_a","chain A")`

Need help? (PyMOL command line)

`>help select`

PYMOL API

cmd.select(string name, string selection)

You can navigate through your file system with the PyMOL console

Show the current working directory:

```
>pwd
```

(print working directory)

List all files and directories in the current working directory:

```
>ls
```

You can navigate through your file system with the PyMOL console

Change directories

```
>cd directory_name
```

Navigate to a directory called downloads

```
>cd Downloads
```

Navigate to a parent directory

```
>cd ..
```

PyMOL Excercises

- Use the PyMOL console to navigate to your Downloads folder
- Use the PyMOL console to navigate to your Desktop

An aside about text editors

- Text editors edit plain or raw text (no bold, italic, underline, etc.)
- Microsoft Word is **not** a text editor

- Windows: Notepad
- Mac OSX: TextEdit (Format > Make plain text)

- Cross-platform: Atom
  - www.atom.io

A simple python script to view a protein structure

- Open a new text file
- Add the contents:

```
cmd.fetch("3KAS")
```

- Save as "myscript.py" (or any name you want)
  - Text files can have any extension, but for python scripts we use ".py" by convention
- Using the PyMOL console, navigate to the directory where you saved your script
- In the PyMOL console:

```
>run myscript.py
```

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PyMOL exercises

Write a python script to do the following:

1. Download & open structure 3KAS:
   `fetch 3KAS`
   - Display in various forms (cartoon, stick, spheres, …)
   - Color different chains

2. Download & open structure 1DLW
   - Display as cartoon
   - Show heme as sticks