

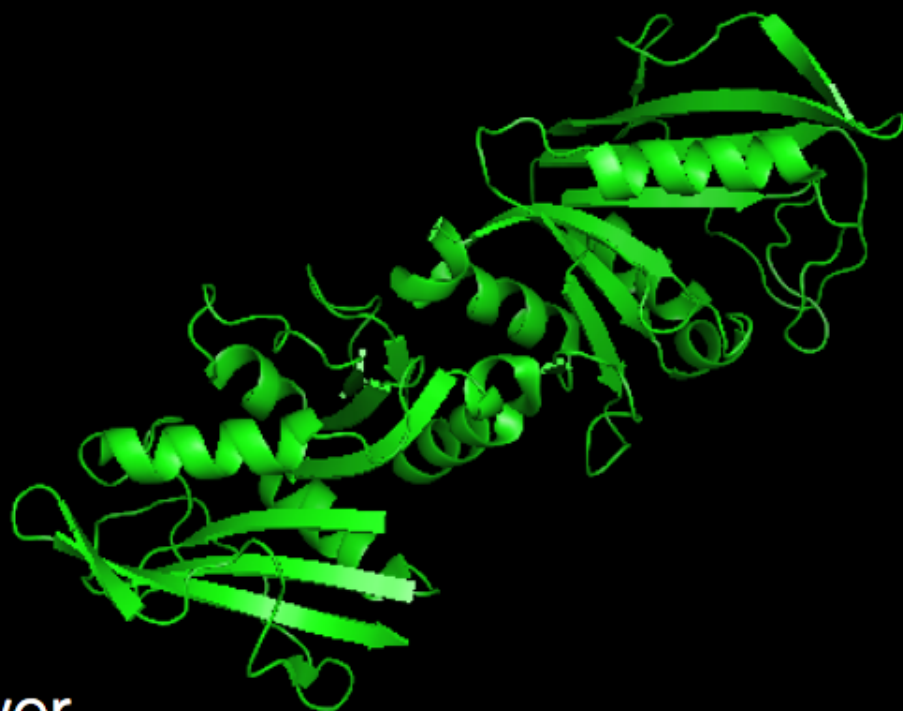
Protein structure and PyMOL scripting

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>



viewer

object
 control
 panel

mouse
 controls

all	A	S	H	L	C
1DHF 1/1	A	S	H	L	C

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
 Db1Clk 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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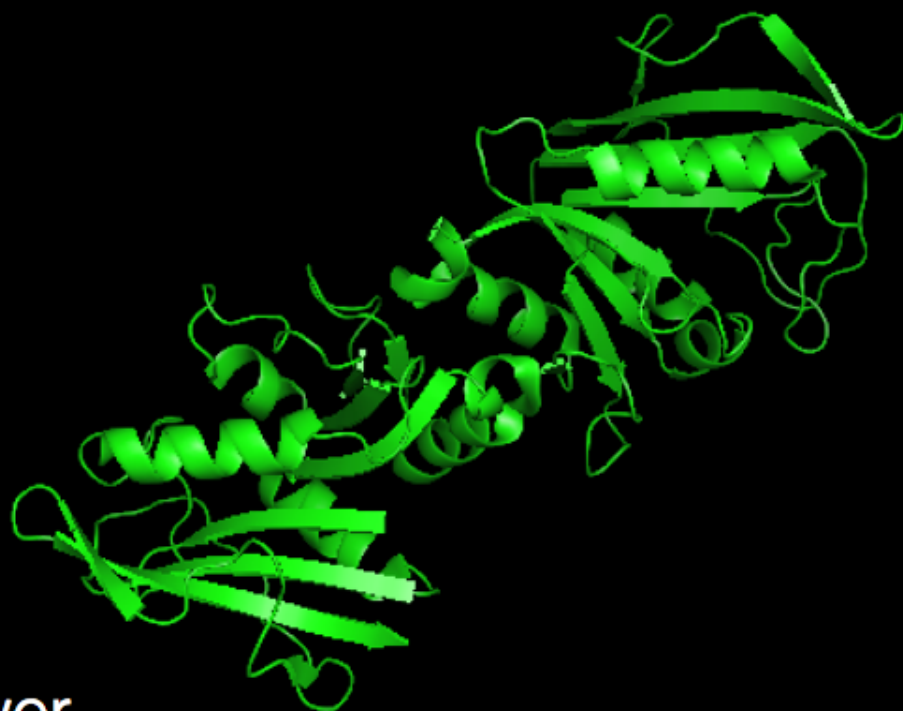
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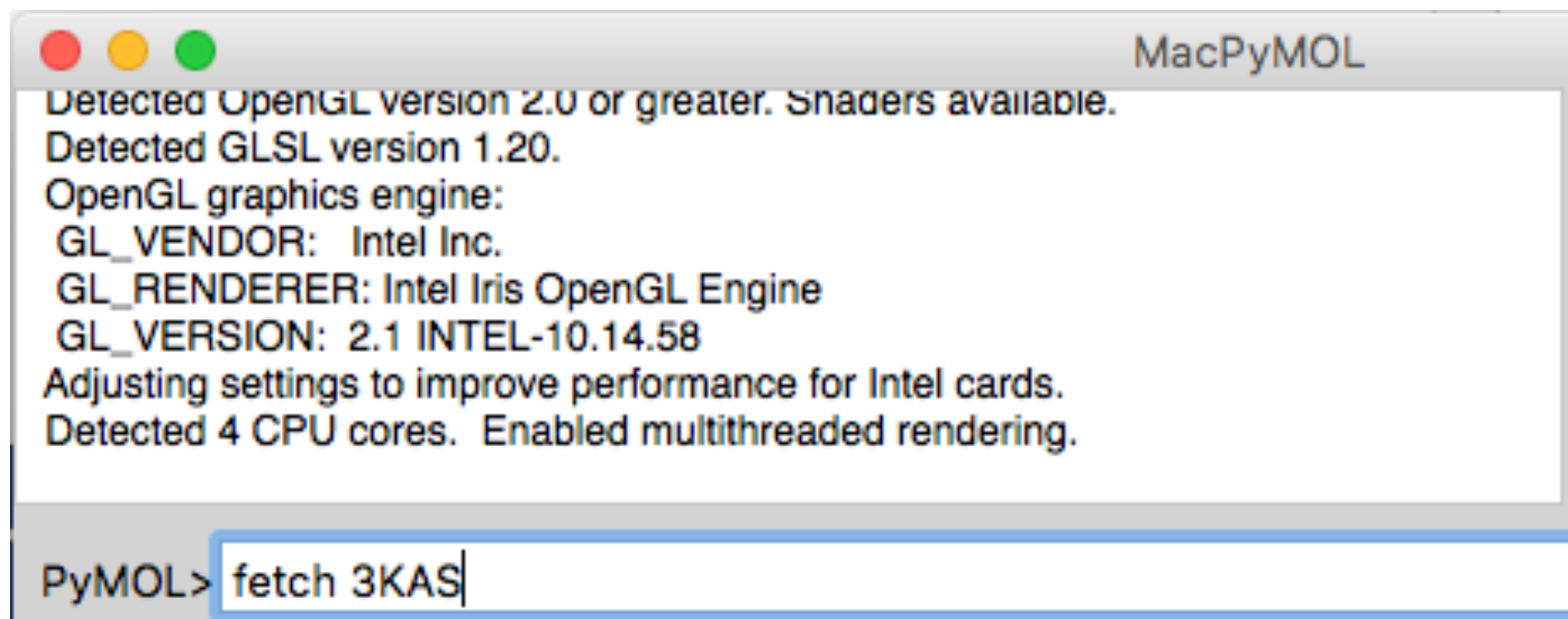
Navigation icons: Home, Left, Stop, Right, End, S, Down, F

PyMOL>_

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

`command arg1, arg2, arg3`

`>fetch 3KAS`



The image shows a screenshot of a MacPyMOL terminal window. The window title is "MacPyMOL". The terminal output displays the following text:

```
Detected OpenGL version 2.0 or greater. Shaders available.  
Detected GLSL version 1.20.  
OpenGL graphics engine:  
GL_VENDOR: Intel Inc.  
GL_RENDERER: Intel Iris OpenGL Engine  
GL_VERSION: 2.1 INTEL-10.14.58  
Adjusting settings to improve performance for Intel cards.  
Detected 4 CPU cores. Enabled multithreaded rendering.
```

At the bottom of the terminal, the prompt "PyMOL>" is followed by the command "fetch 3KAS" which is currently being entered, indicated by a blue cursor.

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

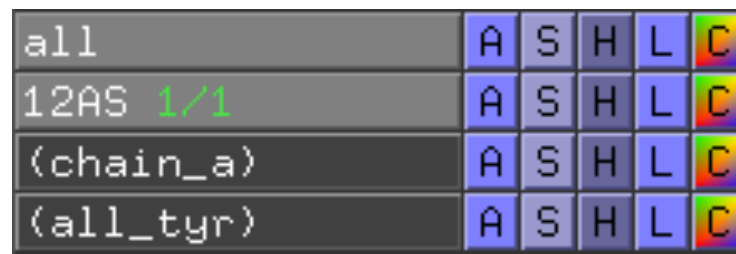
`select name, selector`

select chain A

`>select chain_a, chain A`

select all tyrosines

`>select all_tyr, resn TYR`



all	A	S	H	L	C
12AS 1/1	A	S	H	L	C
(chain_a)	A	S	H	L	C
(all_tyr)	A	S	H	L	C

More on selector syntax

http://pymolwiki.org/index.php/Property_Selectors

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)

all	A	S	H	L	C
12AS 1/1	A	S	H	L	C
(chain_a)	A	S	H	L	C
(all_tyr)	A	S	H	L	C

PyMOL exercises

1. Download & open structure 3KAS:
`fetch 3KAS`
 - Display as cartoon
 - Color chain A in blue and chain B in green
2. Download & open structure 1DLW
 - Display chain A as cartoon, colored in brown
 - Show heme as sticks, colored in standard atom colors

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 Exercises

- 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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