Tutorial for the PyMOL Basics

Speaker: S. C. Yen

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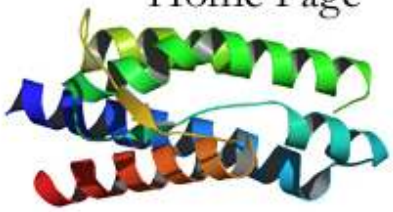
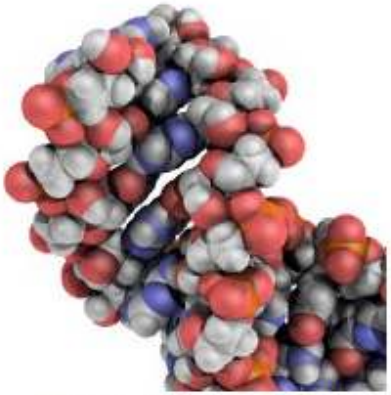
PyMOL Home Page





PyMOL v1.1 Released!

PyMOL Runs On:

Linux (or any Unix)

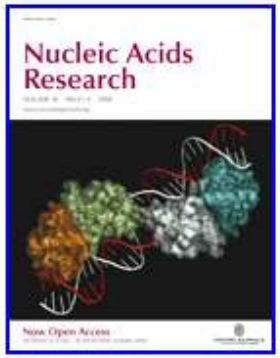
MacOS and Windows

Click to Sponsor

PyMOL is a USER-SPONSORED molecular visualization system on an OPEN-SOURCE foundation. *Please support our mission to create open, effective, and affordable tools for research by purchasing a subscription to maintenance and/or support. Thanks!*

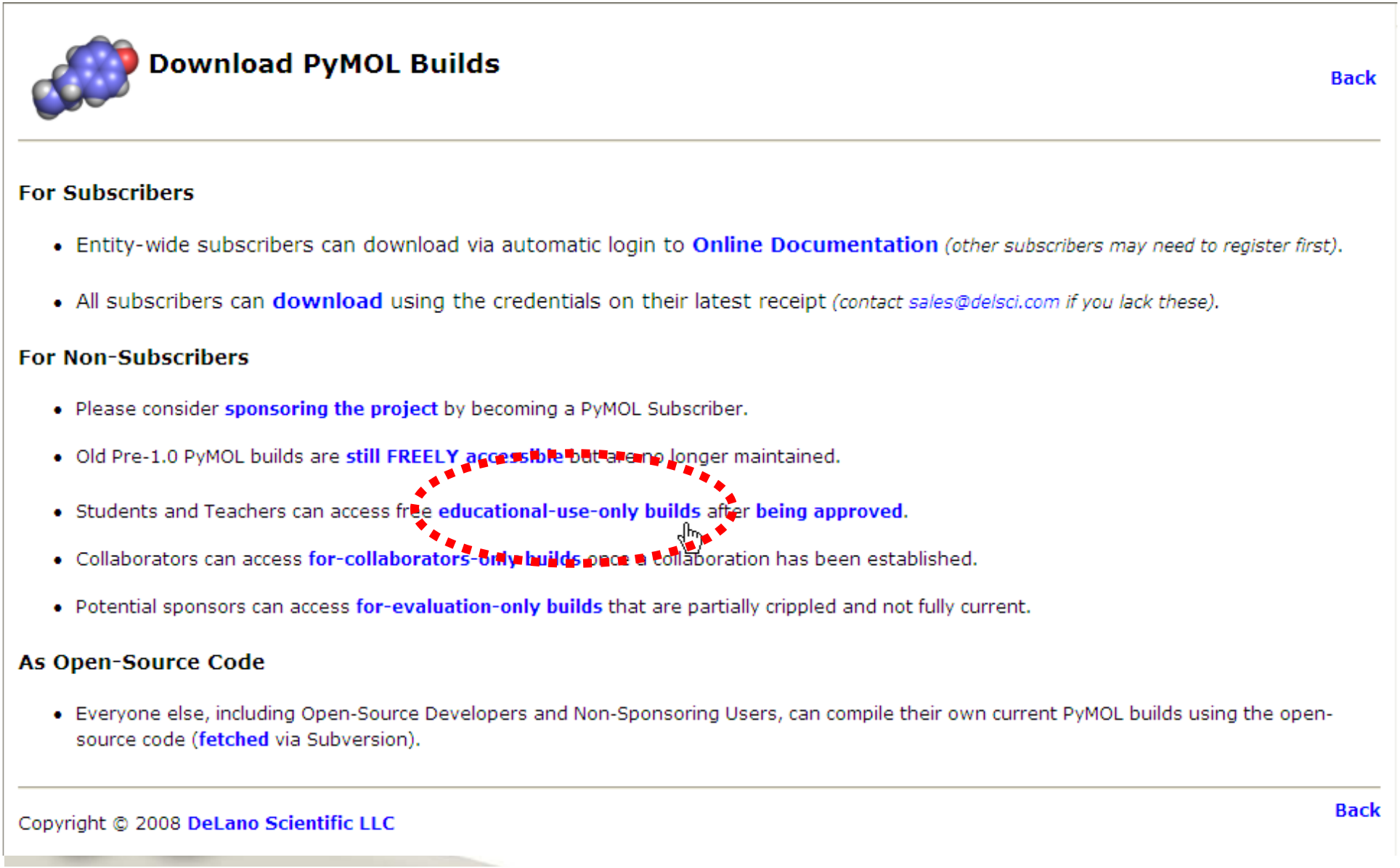
Latest News

- **August 21, 2008: Another PyMOL-based Cover:** McGeehan et al. *Structural analysis of the genetic switch that regulates the expression of restriction-modification genes.* **Nucleic Acids Research, 2008, Vol. 36, No. 14 4778-4787.**



Download PyMOL:
http://pymol.sourceforge.net/

Students and Teachers can access free educational-use-only builds after being approved.



Download PyMOL Builds

Back

For Subscribers

- Entity-wide subscribers can download via automatic login to **Online Documentation** *(other subscribers may need to register first)*.
- All subscribers can **download** using the credentials on their latest receipt *(contact sales@delsci.com if you lack these)*.

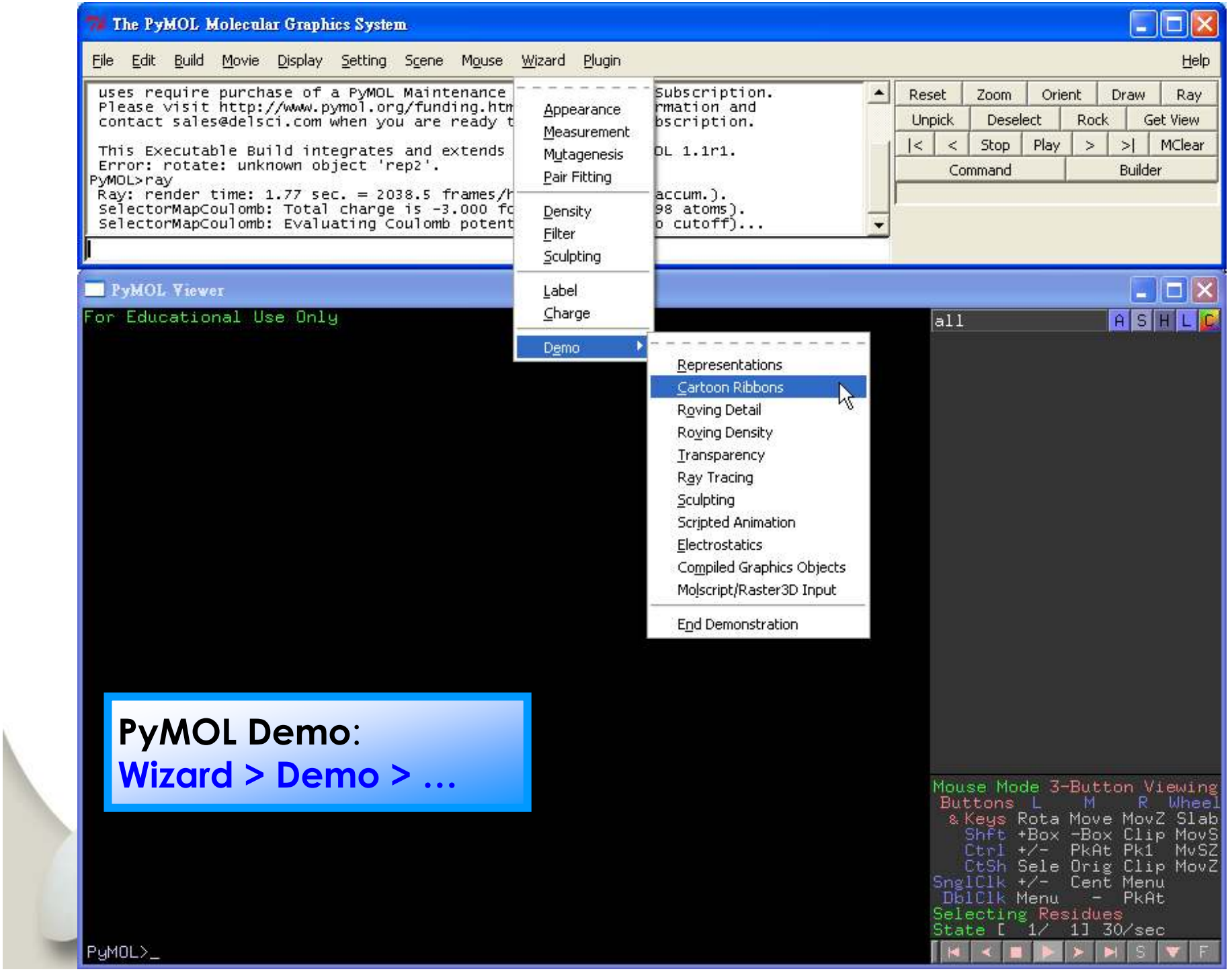
For Non-Subscribers

- Please consider **sponsoring the project** by becoming a PyMOL Subscriber.
- Old Pre-1.0 PyMOL builds are **still FREELY accessible** but are no longer maintained.
- Students and Teachers can access free **educational-use-only builds** after **being approved**.
- Collaborators can access **for-collaborators-only builds** once a collaboration has been established.
- Potential sponsors can access **for-evaluation-only builds** that are partially crippled and not fully current.

As Open-Source Code

- Everyone else, including Open-Source Developers and Non-Sponsoring Users, can compile their own current PyMOL builds using the open-source code (**fetched** via Subversion).

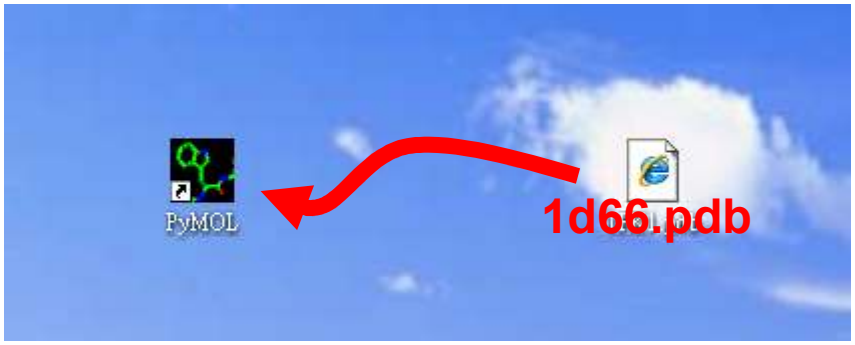
Back


The PyMOL Molecular Graphics System
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help
uses require purchase of a PyMOL Maintenance
Please visit http://www.pymol.org/funding.htm
contact sales@delsci.com when you are ready t
This Executable Build integrates and extends
Error: rotate: unknown object 'rep2'.
PyMOL>ray
Ray: render time: 1.77 sec. = 2038.5 frames/h
SelectorMapCoulomb: Total charge is -3.000 fo
SelectorMapCoulomb: Evaluating Coulomb potent
Subscription.
rmation and
bscription.
OL 1.1r1.
accum.).
98 atoms).
o cutoff)...
Reset Zoom Orient Draw Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear
Command Builder
Appearance
Measurement
Mutagenesis
Pair Fitting
Density
Filter
Sculpting
Label
Charge
Demo
Representations
Cartoon Ribbons
Roving Detail
Roving Density
Transparency
Ray Tracing
Sculpting
Scripted Animation
Electrostatics
Compiled Graphics Objects
Molscript/Raster3D Input
End Demonstration
PyMOL Viewer
For Educational Use Only
all
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
DblClk Menu - PkAt
Selecting Residues
State [1/ 1] 30/sec
S F
PyMOL>_
PyMOL Demo:
Wizard > Demo > ...

1. 開啓檔案

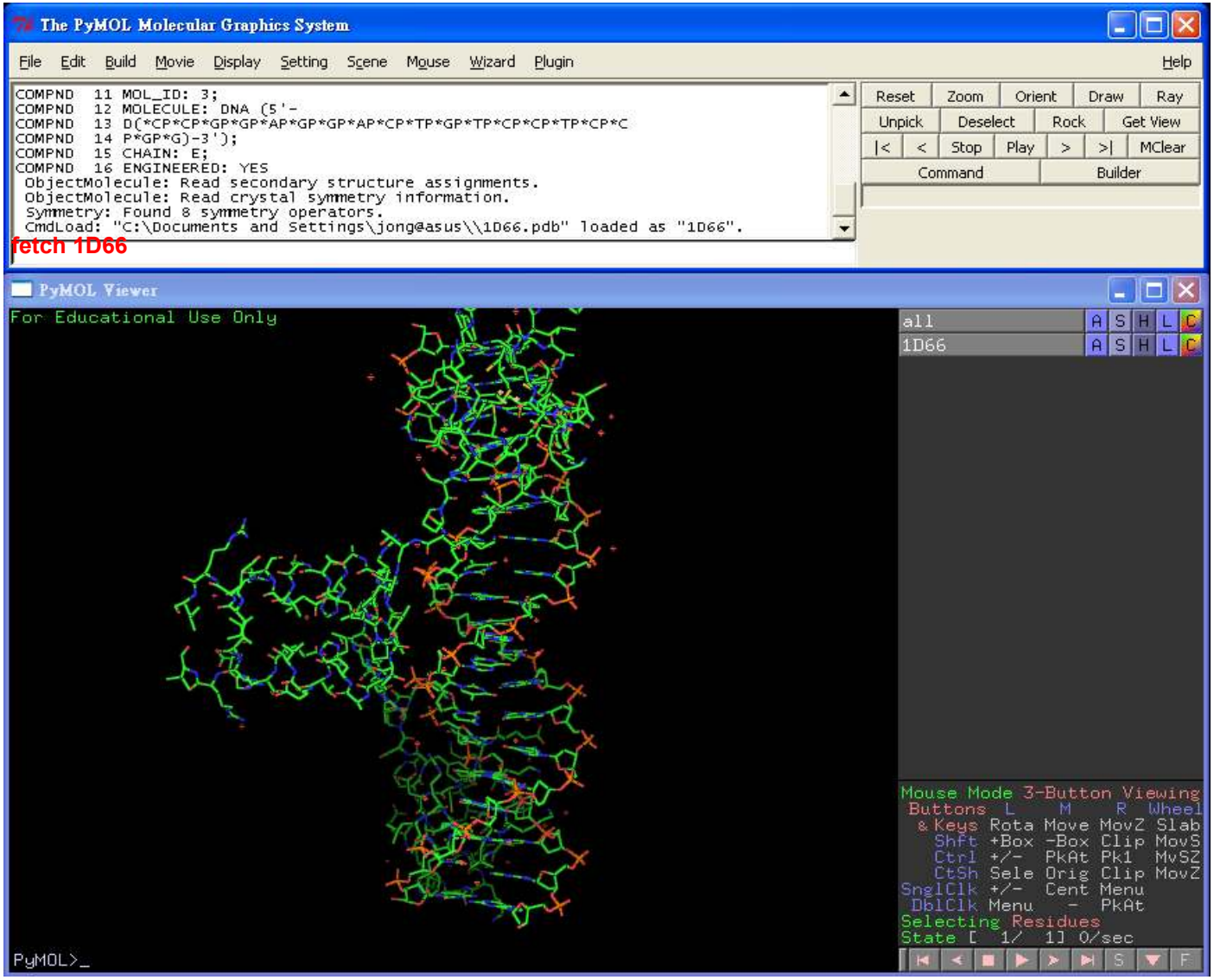
1. Download a PDB file: 1D66

2. Open PyMOL and load 1d66.pdb

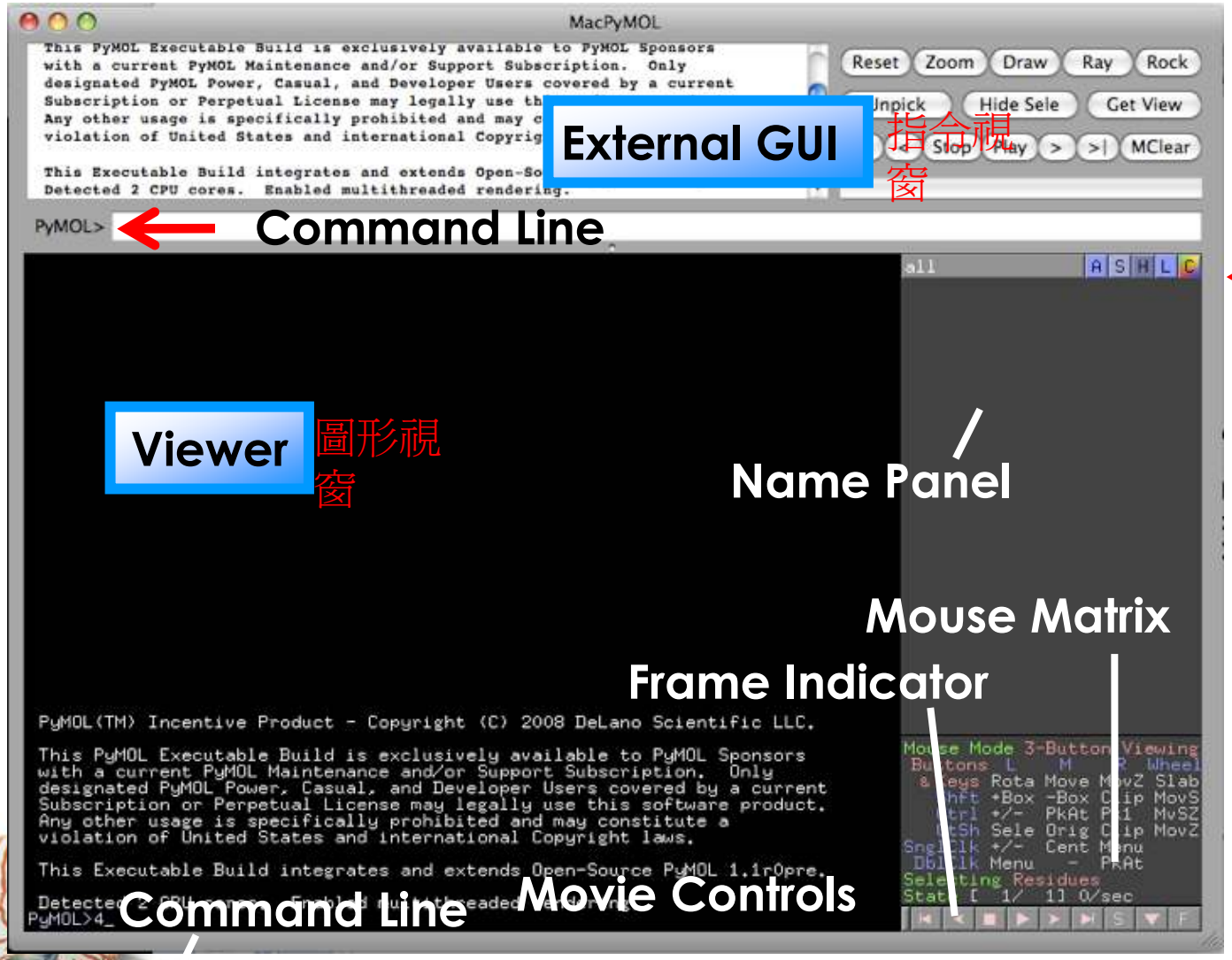


1. 開啓檔案-指令輸入

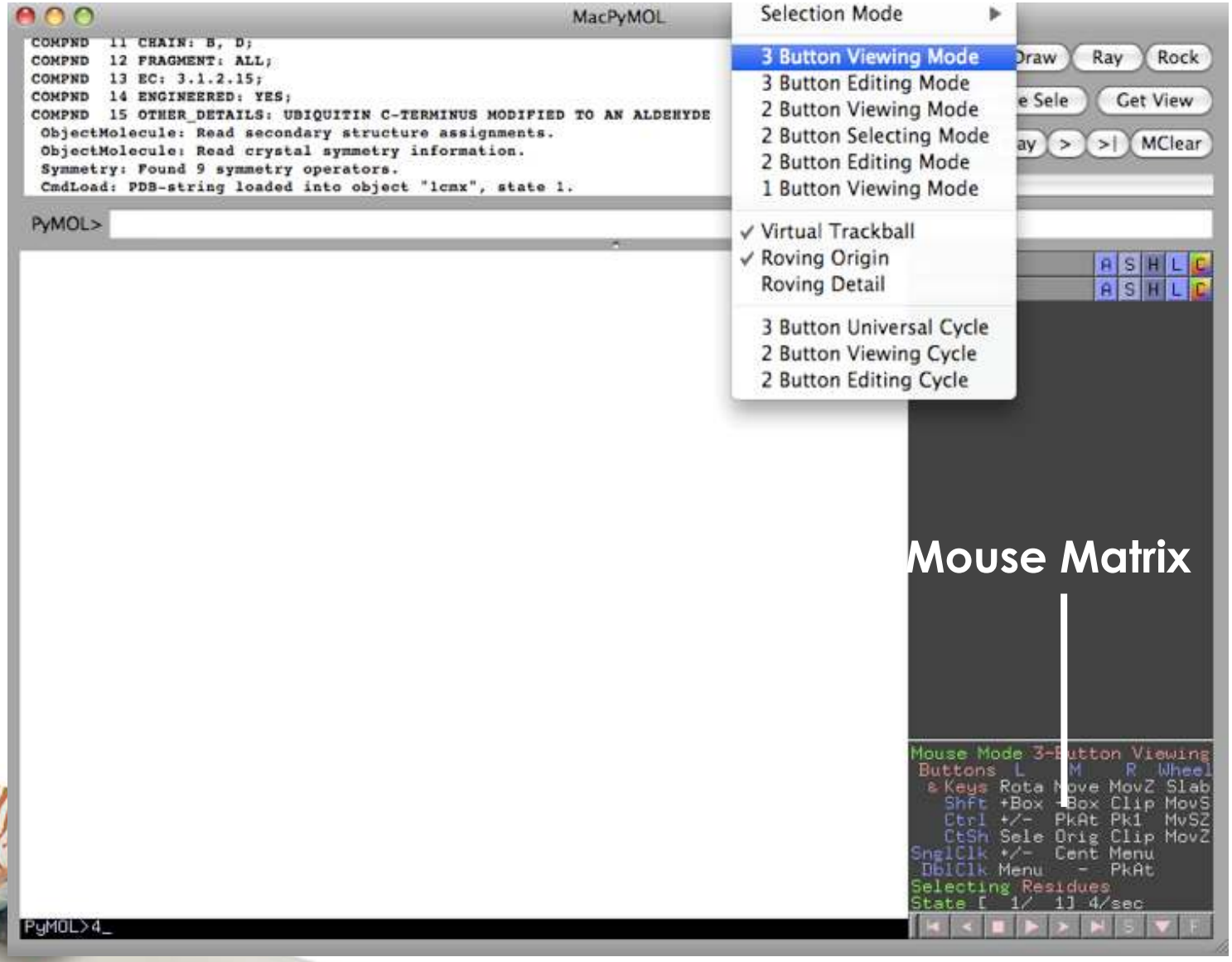
fetch - 下載PDB並顯示



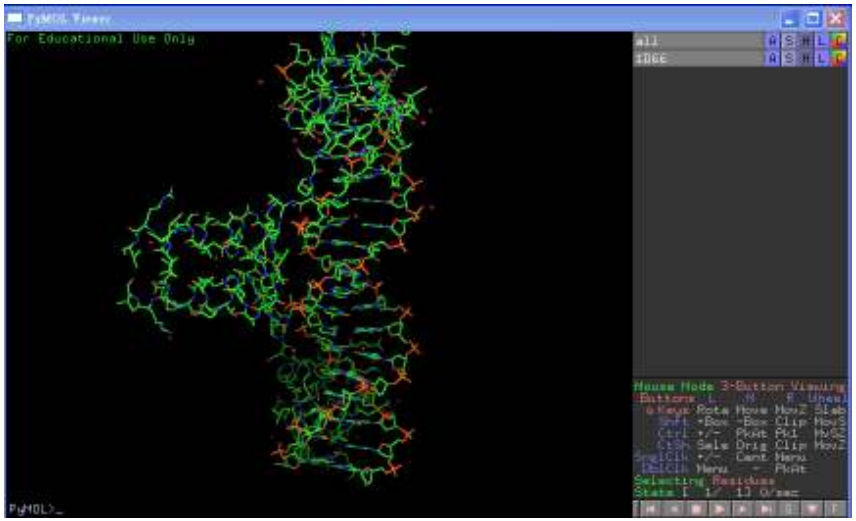
PyMOL Interface



Basic control skills

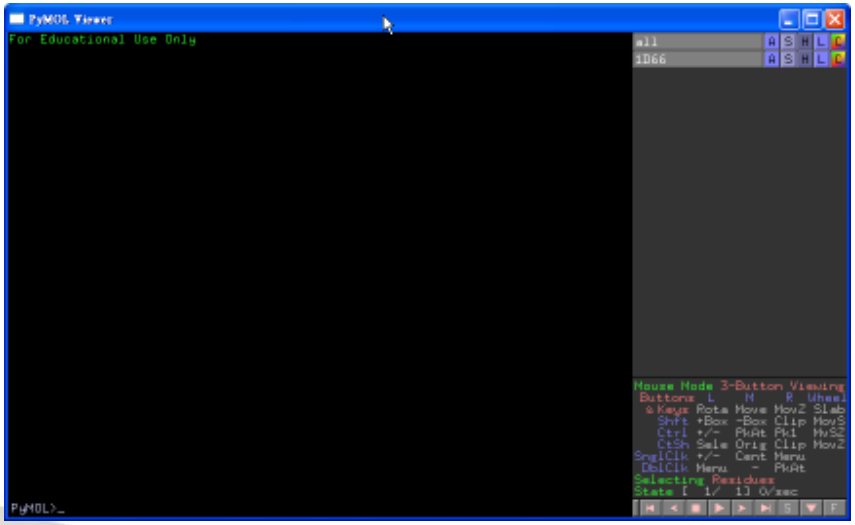


Show & Hide



A S H L C

Hide:
everything
lines
nonbonded
sticks
ribbon
cartoon
labels
cell
dots
spheres
nb_spheres
mesh
surface



Show:
as
lines
sticks
ribbon
cartoon
label
cell
nonbonded
dots
spheres
nb_spheres
mesh
surface

不同的表示法

- Using 

  H > hide everything

  S > show line

  C > by ss > Helix Sheet Loop (can change color)

  S > show sticks

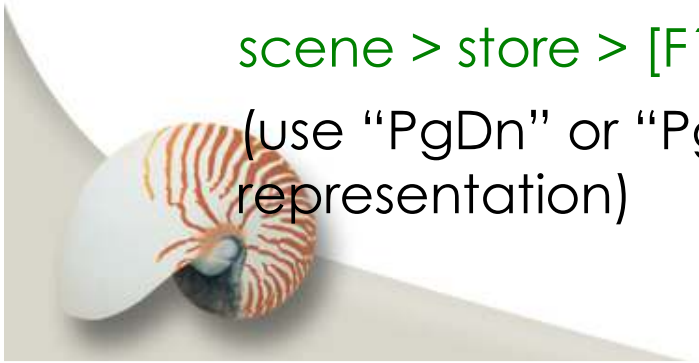
  S > show ribbon

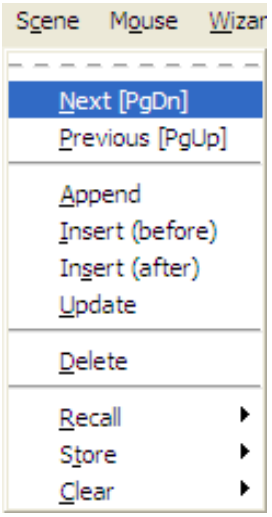
  S > show cartoon

- Save each representation in different channels, to do this go to….

  scene > store > [F1-F12]

  (use “PgDn” or “PgUp” to view each representation)





Exercise 1.

- Download 1cmx
- Hide 1cmx atoms
- Show 1cmx in cartoon
- Show 1cmx color from N-terminal to C-terminal

Action preset menus

From default to more complex

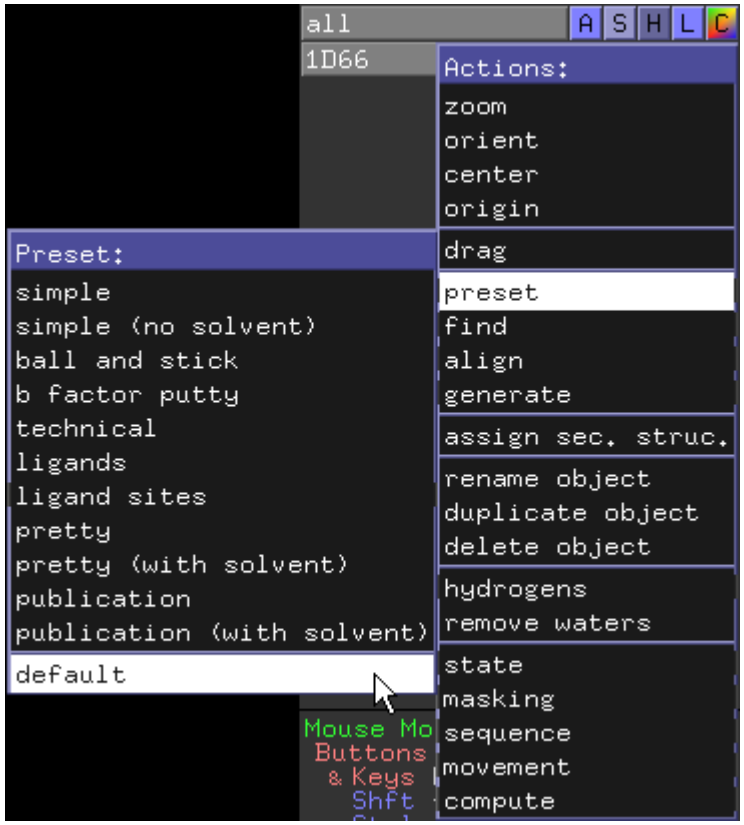
1D66 > A > preset > default

This command has a similar effect but is not the same as the following cascade: hide everything and show lines:

1D66 > H > everything

and

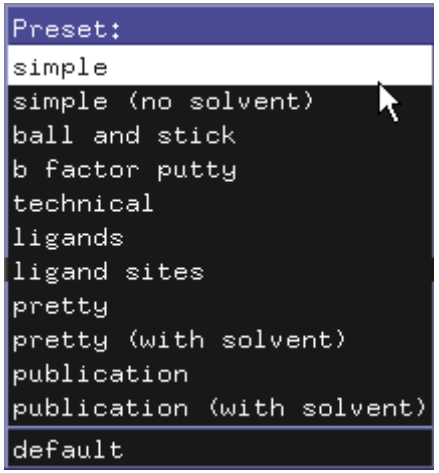
1D66 > S > lines

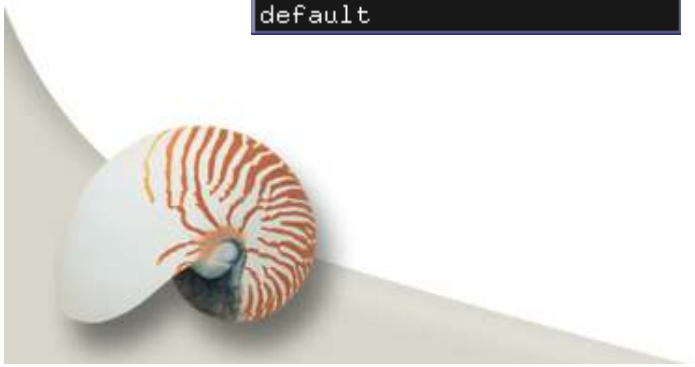


Action preset menus

Explore the other menus of this series.

1D66 > A > preset > simple





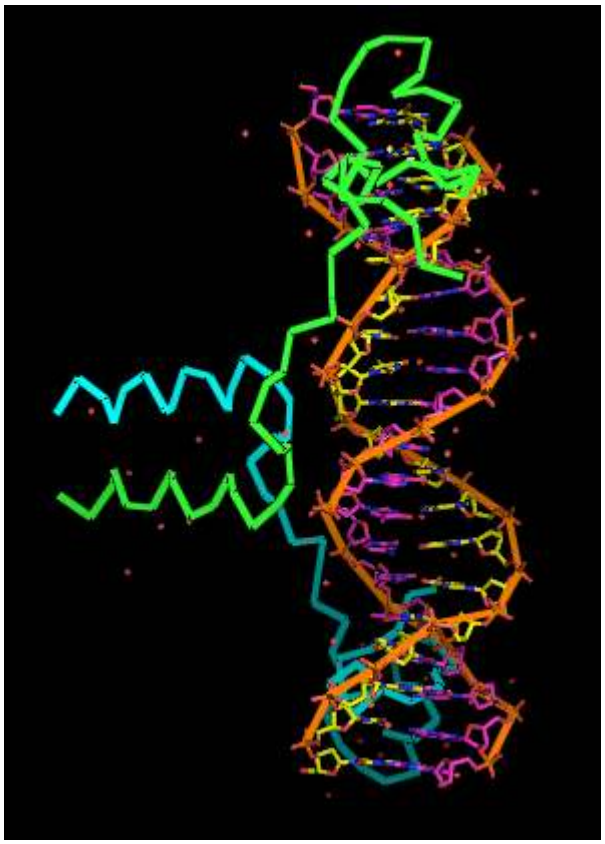
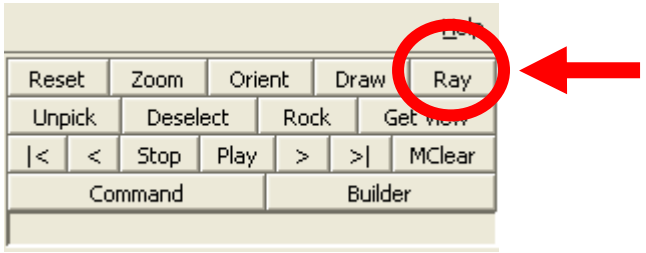
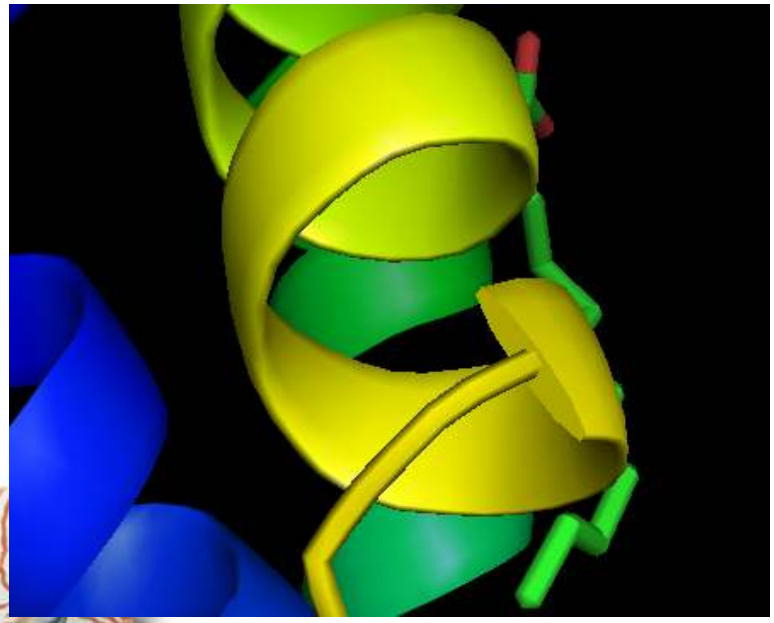


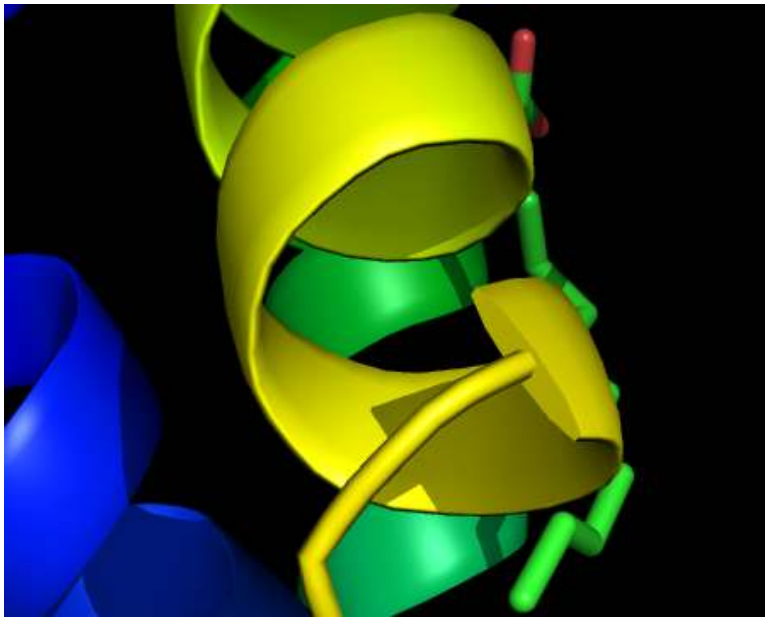
Image Resolution

Use Ray

PyMol offers an internal "**ray tracer**" to create stunning rendered images with a high visual quality much more pleasant to the eye and ideal for publication.





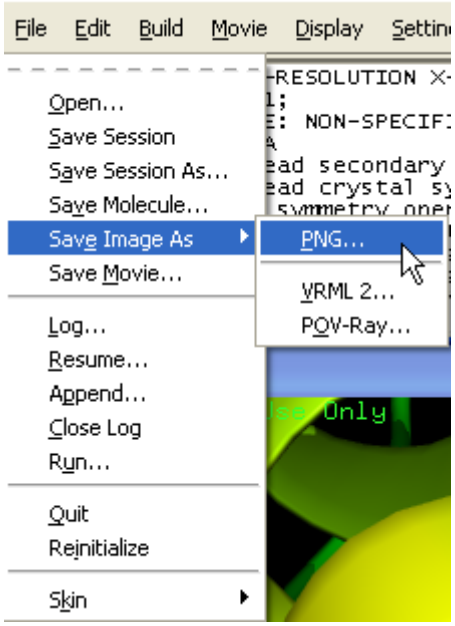


***Default size is 640 x 480 pixels when PyMol is first opened.**

Save Image

- **File > Save Image…**

→ The image will be saved as a PNG image on the desktop



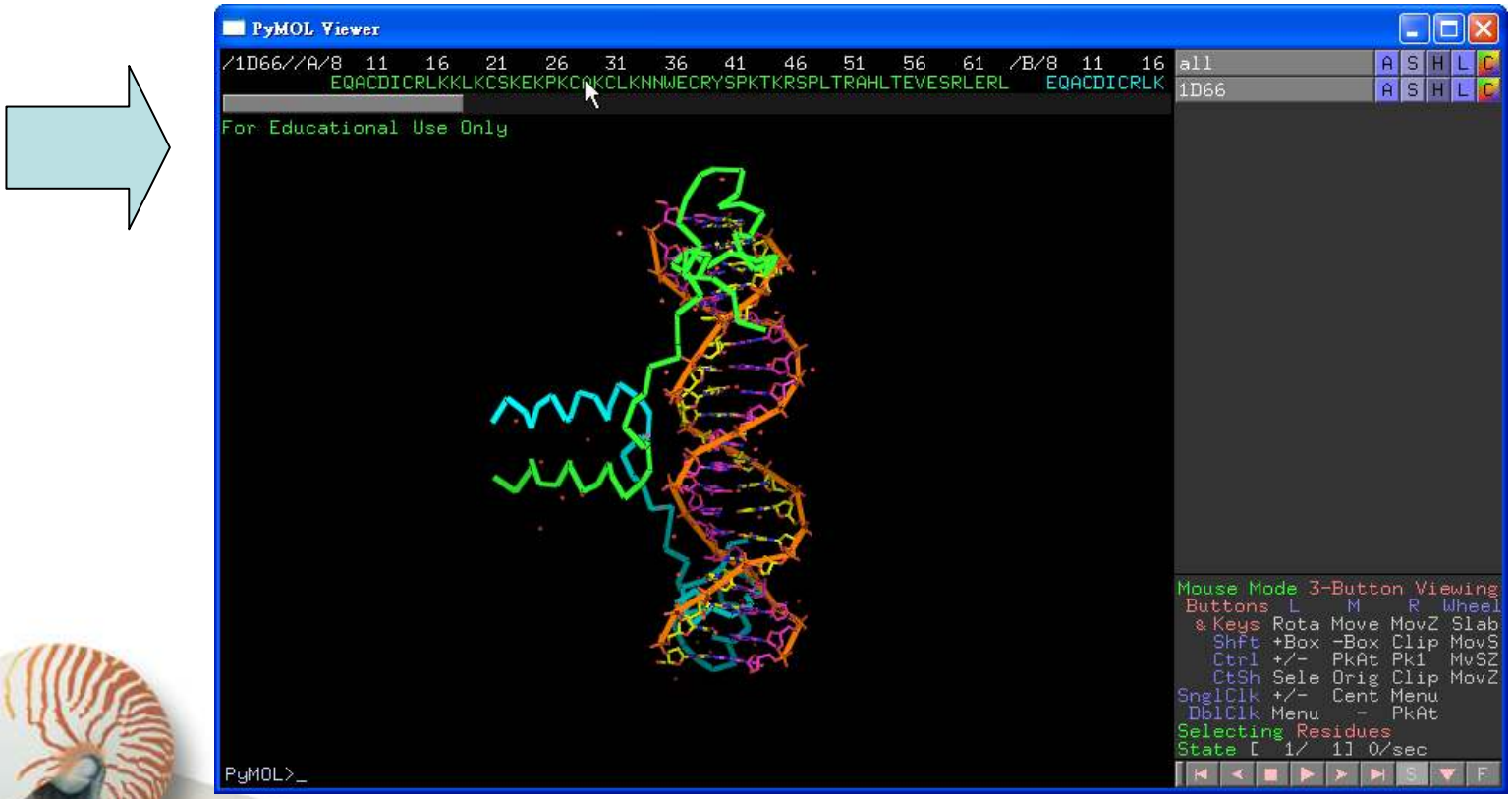
- Within the top PyMOL> command line, **type the following commands**:

> png filename.png

4. Show Sequence

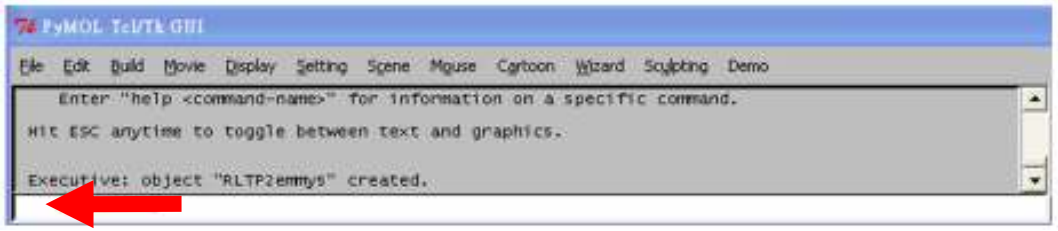
- **Display > Sequence**

→ will display residue codes, residues, chains, atoms and states



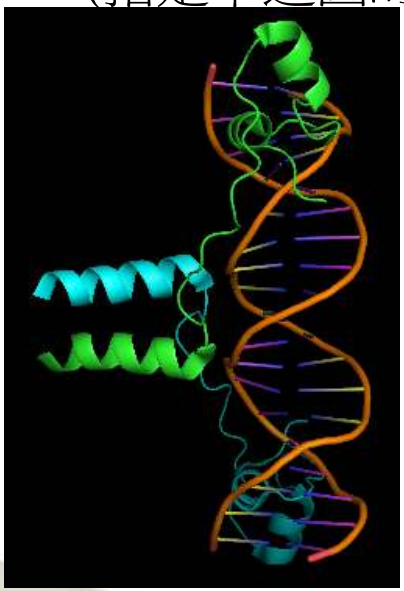
5. 鍵入指令

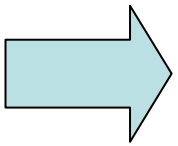
在下面箭頭的地方鍵入下列的所有指令。



show cartoon, all　　(將所有的東西以卡通圖的方式呈現)

color orange　　(指定卡通圖的顏色是橘色；也可以“color orange, all”來表示)





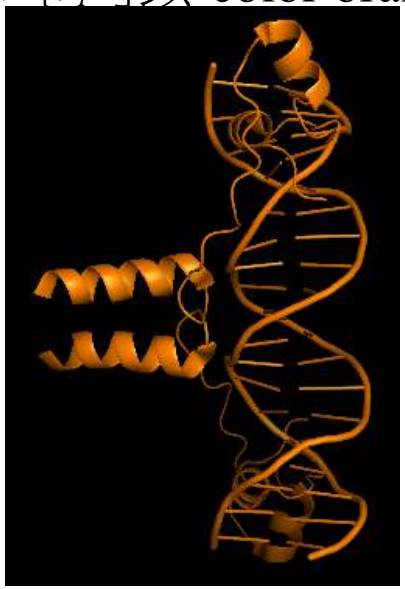


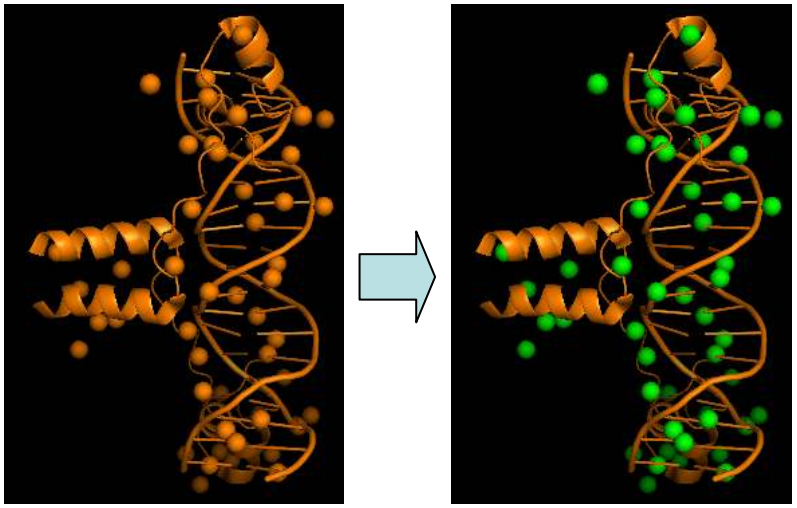
Table with pre-defined colours

white		black		blue		green		red	
cyan		yellow		magenta		salmon		lime	
slate		hotpink		orange		yellowgreen		bluegreen	
blueviolet		marine		olive		purple		teal	
ruby		forest		deep		grey		carbon	
nitrogen		oxygen		hydrogen		brightorange		pink	
firebrick		chocolate		wheat		violet		density	

6. 顯示水或非protein和DNA物質

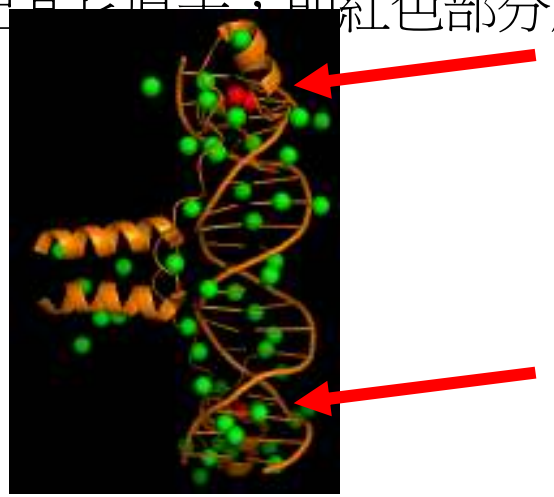
- 可以用下列方式顯示所有水分子。

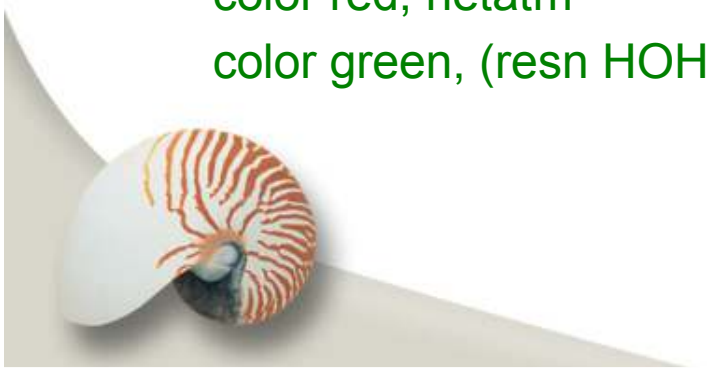
```
show spheres, (resn HOH)
color green, (resn HOH)
```



- 若是直接選hetro-atom，可能會選出其它原子，即紅色部分所示。

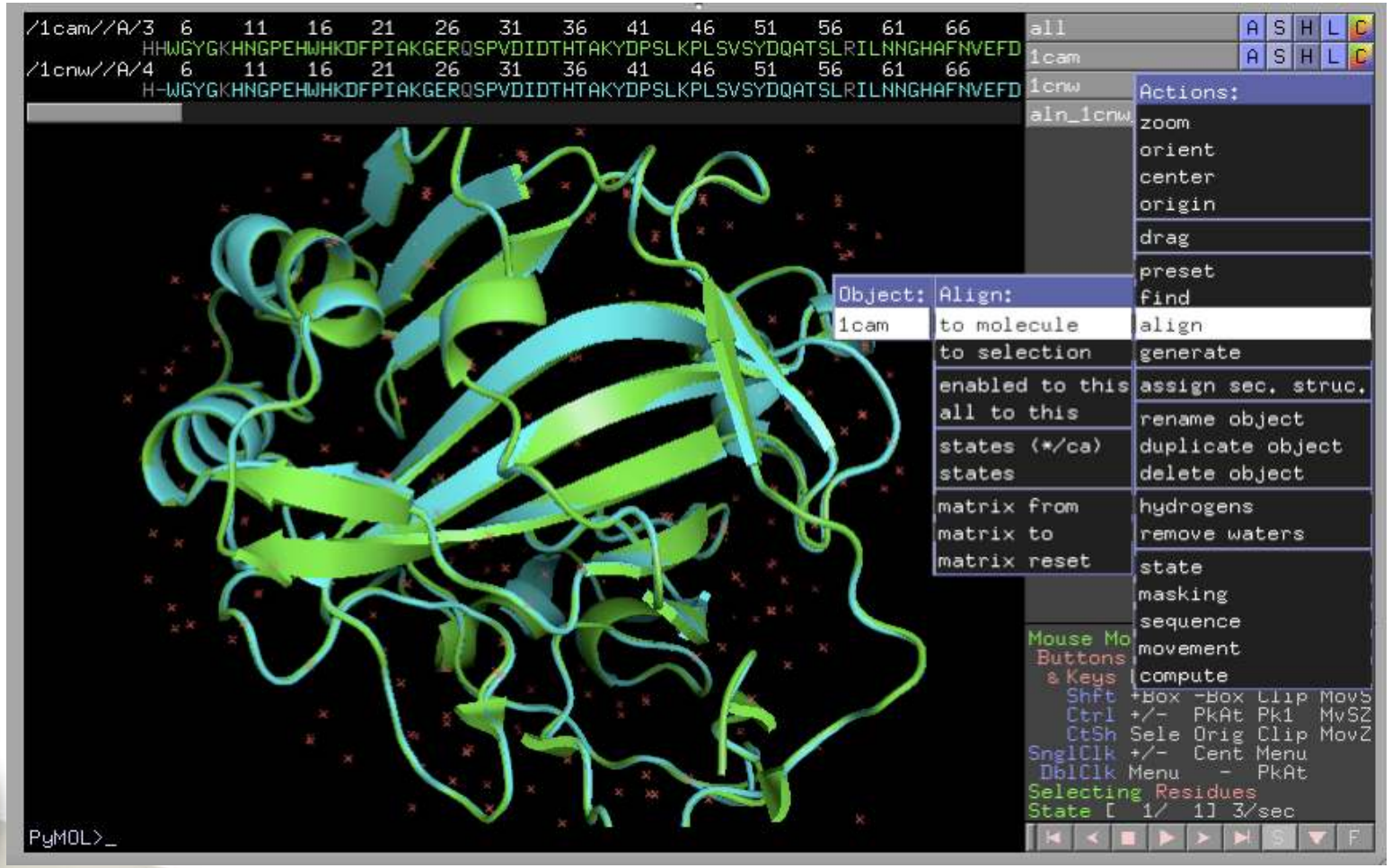
```
show spheres, hetatm
color red, hetatm
color green, (resn HOH)
```



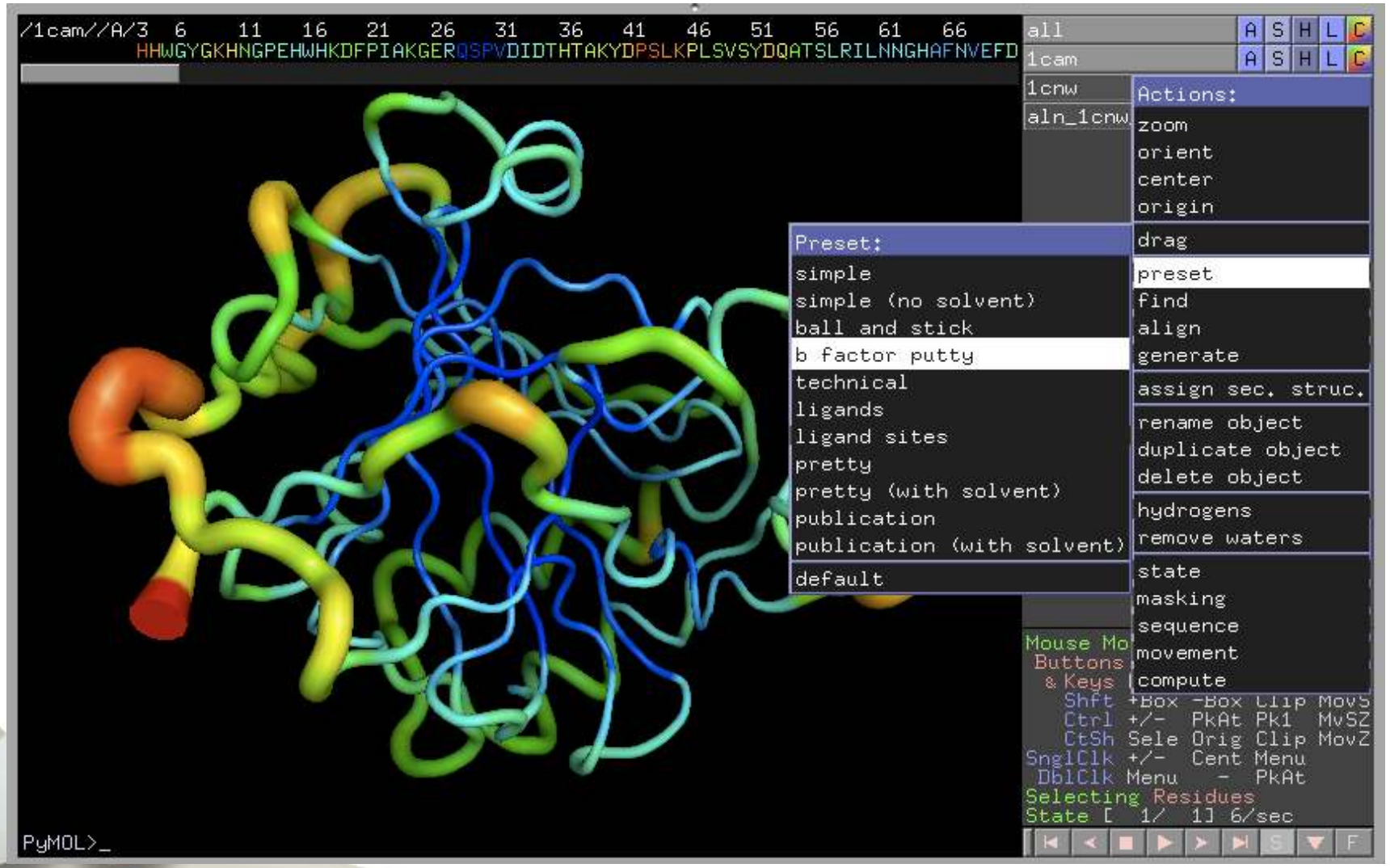


7.Pymol align is sequence alignment

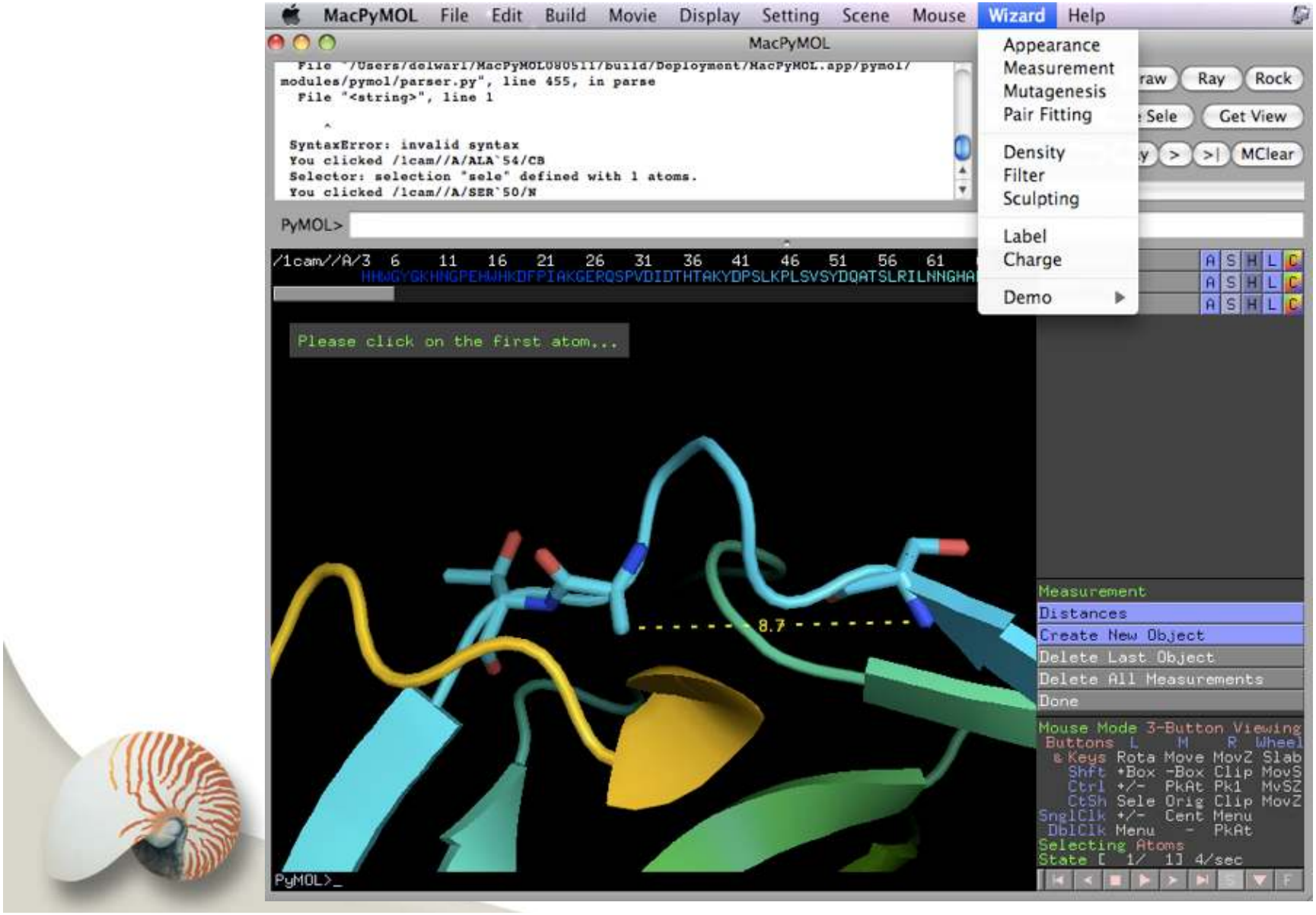
- Download 1cam & 1cnw



8. B-factor


/1cam//A/3 6 11 16 21 26 31 36 41 46 51 56 61 66
HHWGYGKHNGPEHWHKDFPIAKGERQSPVDIDTHTAKYDPSLKPLSVSYDQATSLRILNNGHAFNVEFD
all
1cam
1cnw
aln_1cnw
Actions:
zoom
orient
center
origin
drag
preset
find
align
generate
assign sec. struc.
rename object
duplicate object
delete object
hydrogens
remove waters
state
masking
sequence
movement
compute
Preset:
simple
simple (no solvent)
ball and stick
b factor putty
technical
ligands
ligand sites
pretty
pretty (with solvent)
publication
publication (with solvent)
default
Selecting Residues
State [1/ 1] 6/sec
PyMOL>_

9. 算距離


MacPyMOL File Edit Build Movie Display Setting Scene Mouse Wizard Help
MacPyMOL
File "/Users/delwar1/MacPyMOL080511/build/Deployment/MacPyMOL.app/pymol/modules/pymol/parser.py", line 455, in parse
File "<string>", line 1
SyntaxError: invalid syntax
You clicked /1cam//A/ALA`54/CB
Selector: selection "sele" defined with 1 atoms.
You clicked /1cam//A/SER`50/N
PyMOL>
Appearance
Measurement
Mutagenesis
Pair Fitting
Density
Filter
Sculpting
Label
Charge
Demo
Ray
Rock
Get View
MClear
Please click on the first atom...
8.7
Measurement
Distances
Create New Object
Delete Last Object
Delete All Measurements
Done
Mouse Mode 3-Button Viewing
Selecting Atoms
PyMOL>_

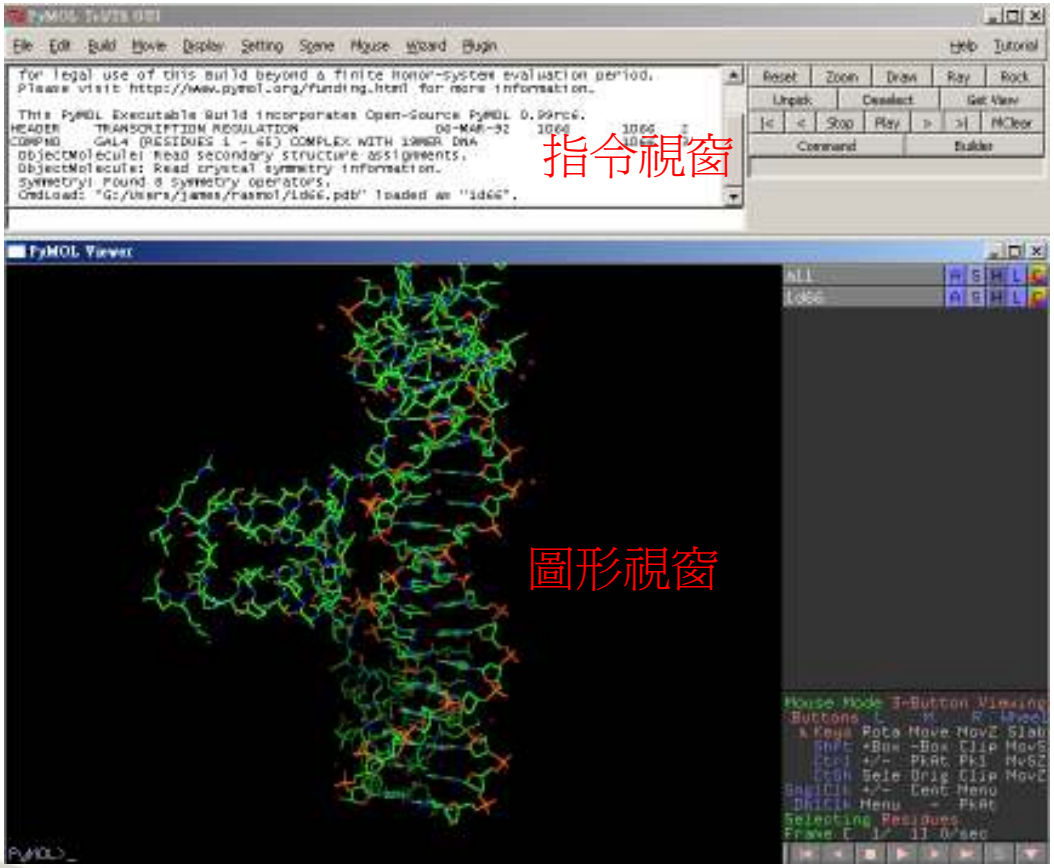
指令縮寫參考:

name <atom names>	n; <atom names>
resn <residue names>	r; <residue names>
resi <residue identifiers>	i; <residue identifiers>
chain <chain ID>	c; <chain ID>
segi <segment identifier>	s; <segment identifier>
elem <element symbol>	e; <element symbol>
flag <number>	f; <number>
alt <code>	
numeric_type <numeric type>	nt; <numeric type>
text_type <text type>	tt; <text type>
hydrogen	h;
all	*
visible	v;
id <original-index>	
hetatm	
ss <secondary structure>	
around <distance>	a; <distance>
expand <distance>	e; <distance>
gap <distance>	
in <selection>	
like <selection>	l; <selection>
<selection> and <selection>	<selection> & <selection>
<selection> or <selection>	<selection> | <selection>
<selection> not <selection>	<selection> ! <selection>
<selection> and not <selection>	<selection> & ! <selection>
byres <selection>	br; <selection>
byobject <selection>	bo; <selection>

Surface

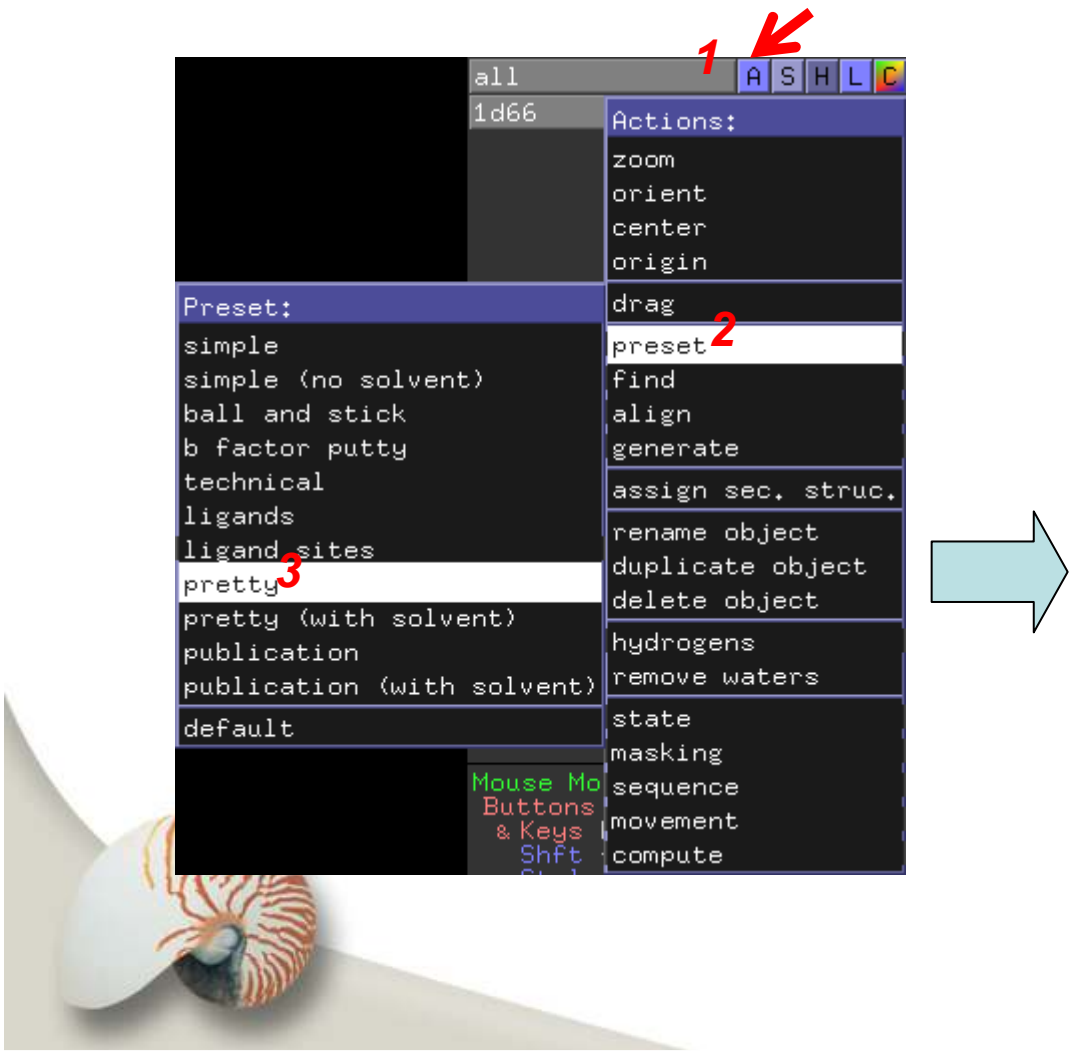
開啓檔案

- PDB: 1D66。
- 開啓PyMOL軟體，並讀入1D66檔案。

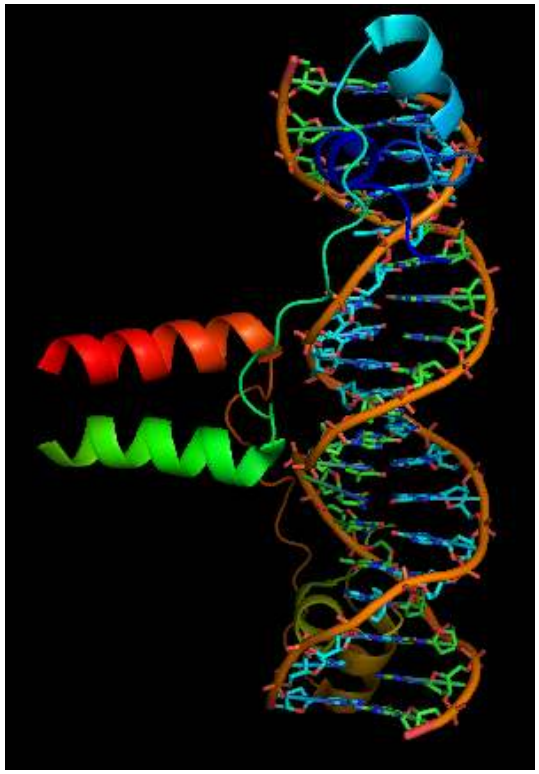


Surface

Action > Preset > Pretty (調整至適當方向)

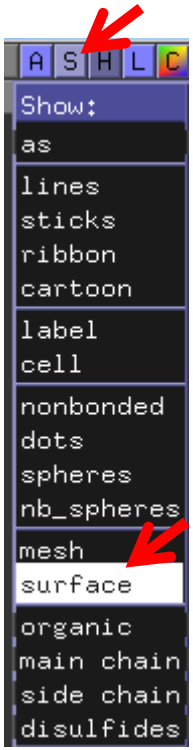


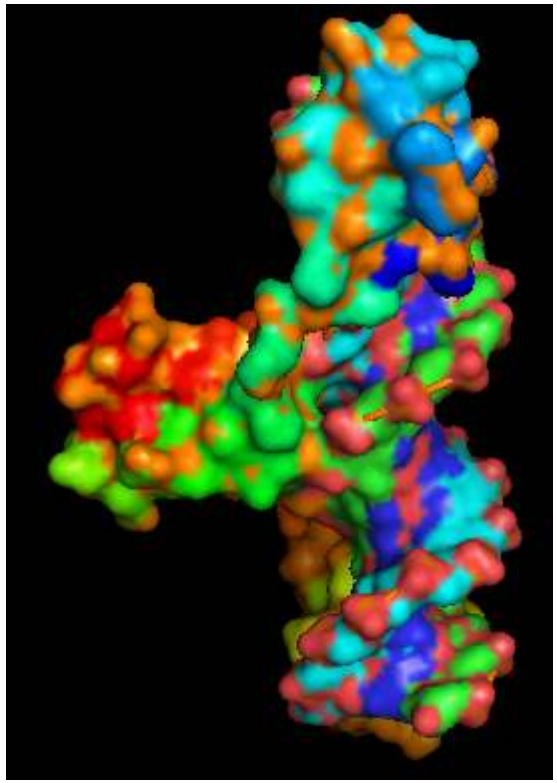
PDB: 1D66



Surface

Show > surface

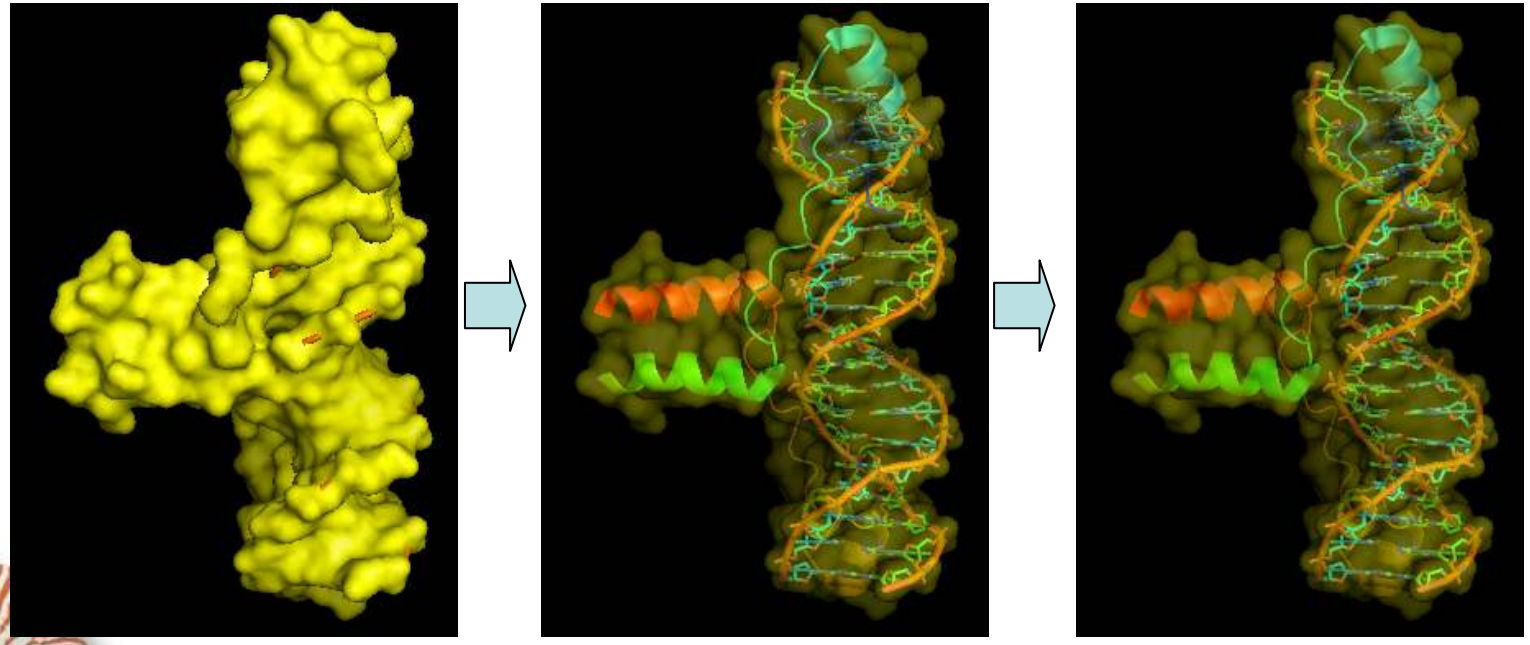




透明的surface

- 利用透明外觀形式來呈現蛋白質的結構。

```
set surface_color,yellow
set transparency, 0.6
set cartoon_transparency, 0.2
```

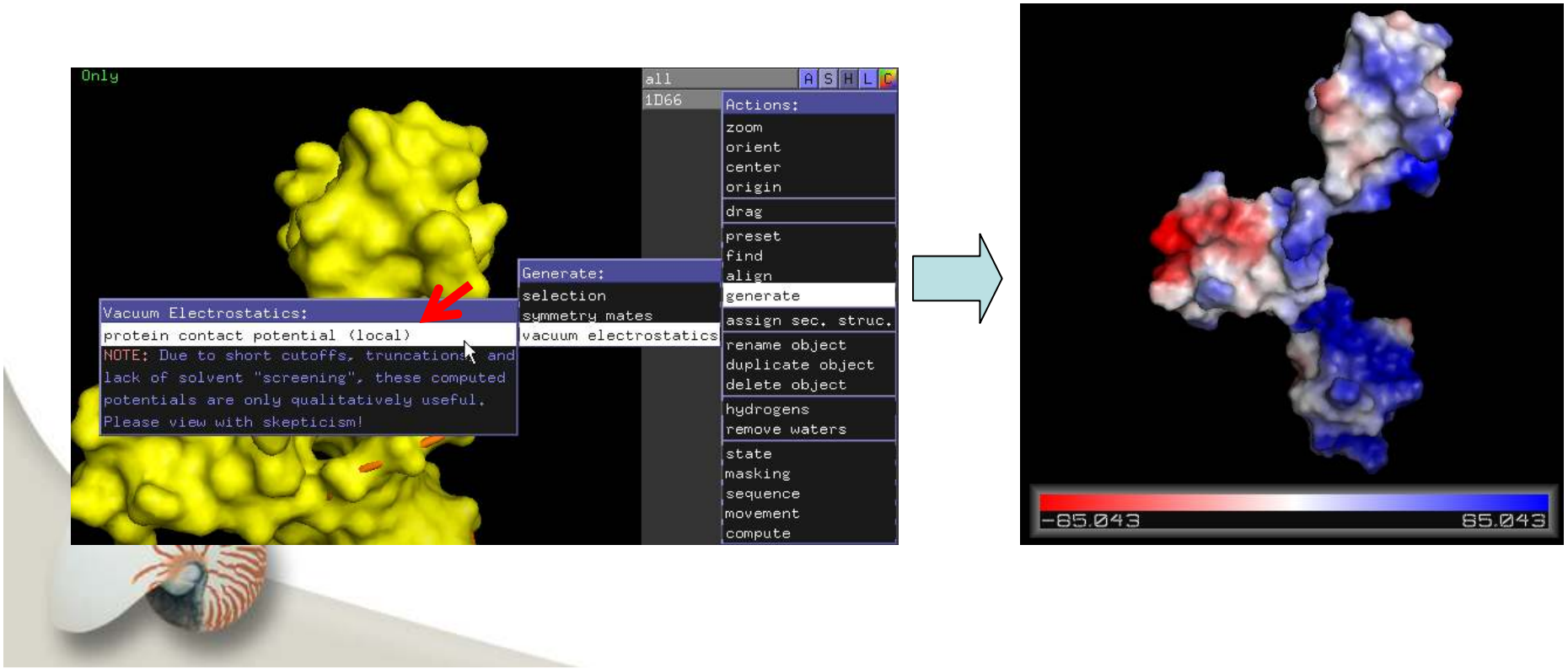


Surface

- 顯示蛋白質表面的電荷:

set transparency, 0 先取消透明度

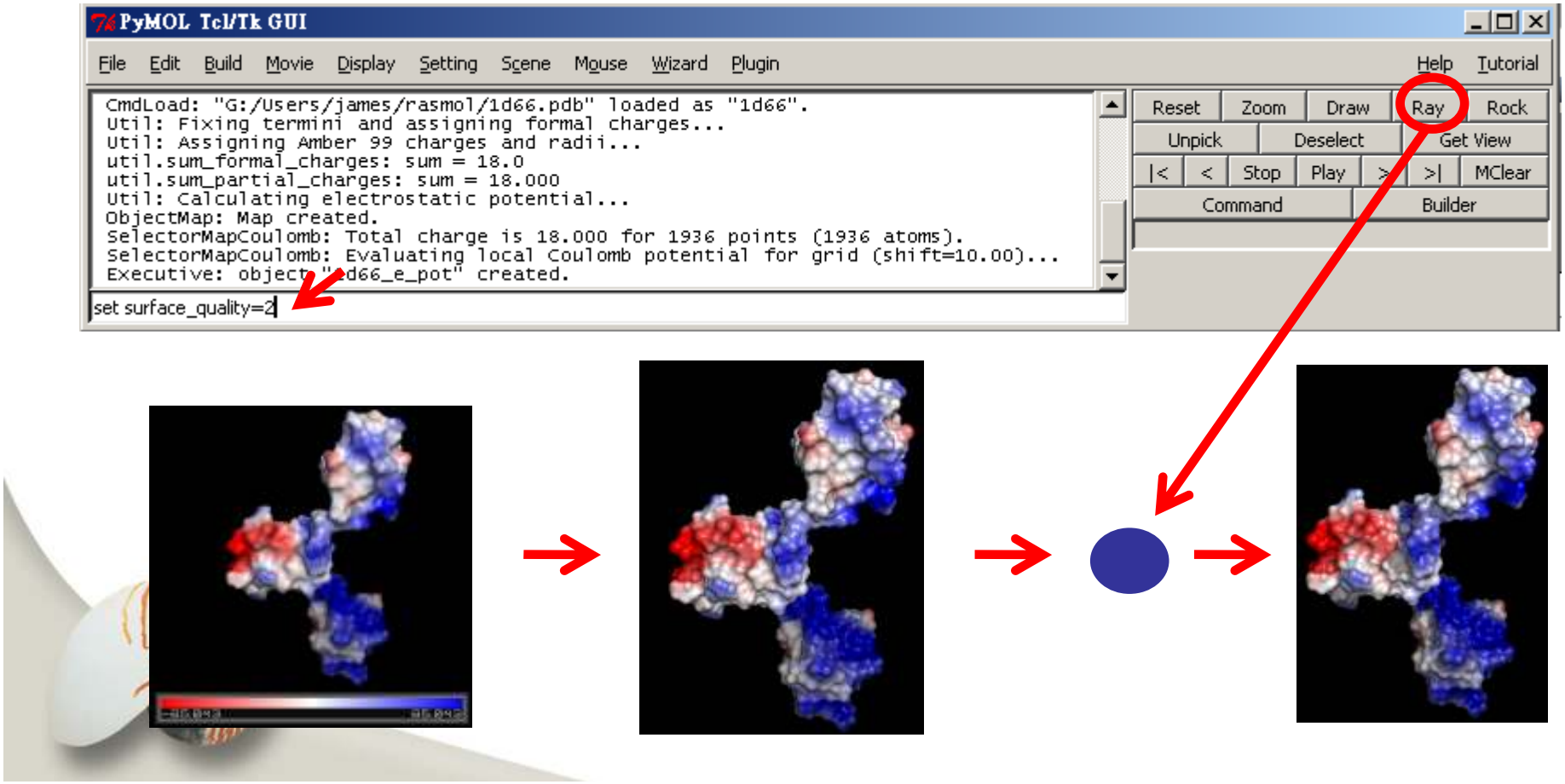
Action > generate > vacuum electrostatics > protein contact potential (local)



Surface

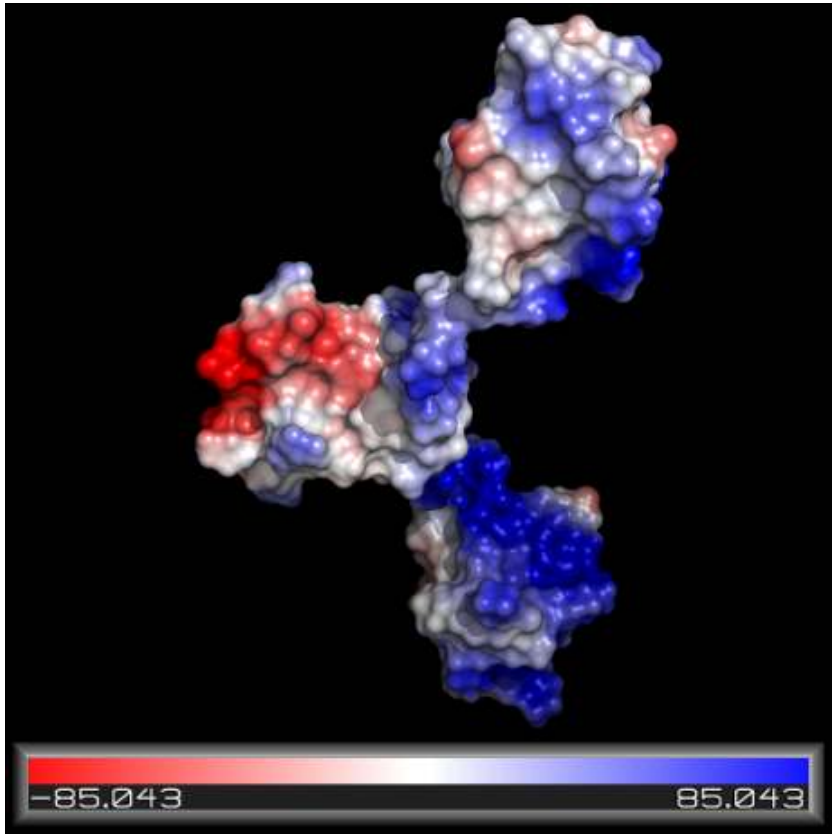
- 以較高的品質顯示蛋白質surface:

  type “set surface_quality=2” in command line



Surface

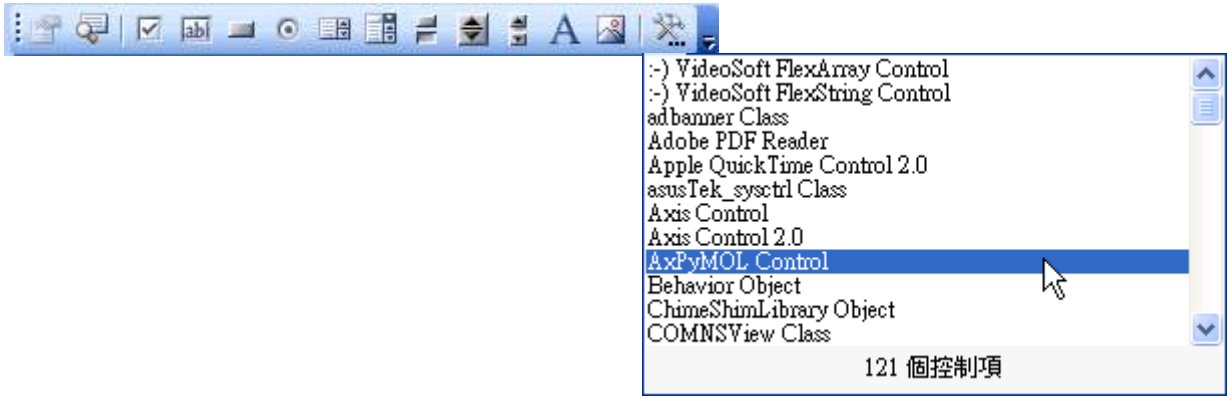
- 旋轉以檢視不同角度:
- 按著”Ctrl”+滑鼠中鍵，就可以在藍白紅的bar上調整正負電的scale

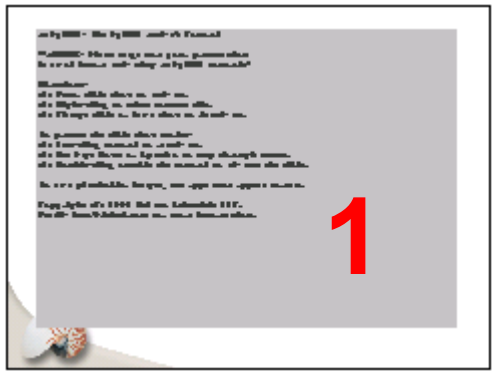


AxPyMOL

- The **PyMOL ActiveX control** which can be used in **Powerpoint**
- Installing AxPyMOL: **http://delsci.com/axpymol/**
- Usage:

Click here !!





2

3

Key in the pathway of structure

4

Play the slide