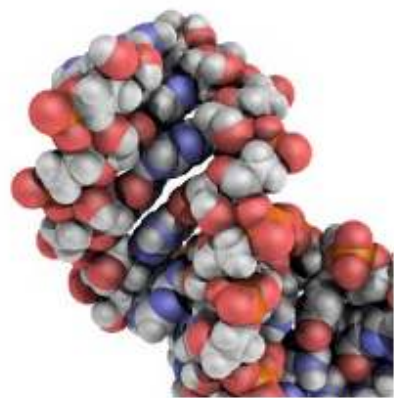
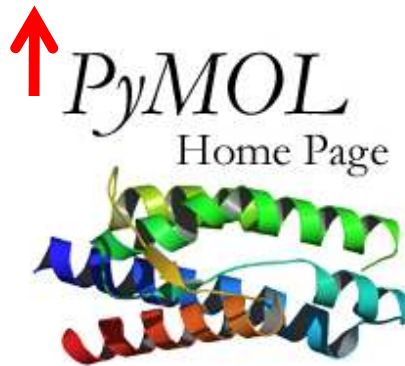


# Tutorial for the PyMOL Basics

Speaker: S. C. Yen





PyMOL v1.1 Released!

PyMOL Runs On:



Linux (or any Unix)



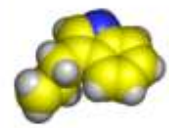
MacOS  
and



Windows



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!



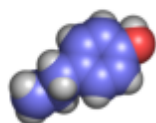
### Latest News

- **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](mailto: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- Old Pre-1.0 PyMOL builds are [still FREELY accessible](#) but are no longer maintained.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).

The PyMOL Molecular Graphics System

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

uses require purchase of a PyMOL Maintenance Subscription. Please visit <http://www.pymol.org/funding.htm> or contact [sales@delsci.com](mailto:sales@delsci.com) when you are ready to purchase.

This Executable Build integrates and extends the PyMOL core. Error: rotate: unknown object 'rep2'.

PyMOL>ray  
Ray: render time: 1.77 sec. = 2038.5 frames/second  
SelectorMapCoulomb: Total charge is -3.000 for 98 atoms.  
SelectorMapCoulomb: Evaluating Coulomb potential (0 cutoff)...

Appearance  
Measurement  
Mutagenesis  
Pair Fitting  
Density  
Filter  
Sculpting  
Label  
Charge  
Demo

Reset Zoom Orient Draw Ray  
Unpick Deselect Rock Get View  
< < Stop Play > >| MClear  
Command Builder

DL 1.1r1.  
accum.).  
98 atoms).  
0 cutoff)...

PyMOL Viewer  
For Educational Use Only

all A S H L

Representations  
Cartoon Ribbons  
Roving Detail  
Roving Density  
Transparency  
Ray Tracing  
Sculpting  
Scripted Animation  
Electrostatics  
Compiled Graphics Objects  
Molscript/Raster3D Input  
End Demonstration

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

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

The screenshot displays the PyMOL Molecular Graphics System interface. The main window shows the command prompt with the following text:

```
COMPND 11 MOL_ID: 3;  
COMPND 12 MOLECULE: DNA (5'-  
COMPND 13 D(*CP*CP*GP*GP*AP*GP*GP*AP*CP*TP*GP*TP*CP*CP*TP*CP*C  
COMPND 14 P*GP*G)-3');  
COMPND 15 CHAIN: E;  
COMPND 16 ENGINEERED: YES  
ObjectMolecule: Read secondary structure assignments.  
ObjectMolecule: Read crystal symmetry information.  
Symmetry: Found 8 symmetry operators.  
CmdLoad: "C:\Documents and Settings\jong@asus\1D66.pdb" loaded as "1D66".  
fetch 1D66
```

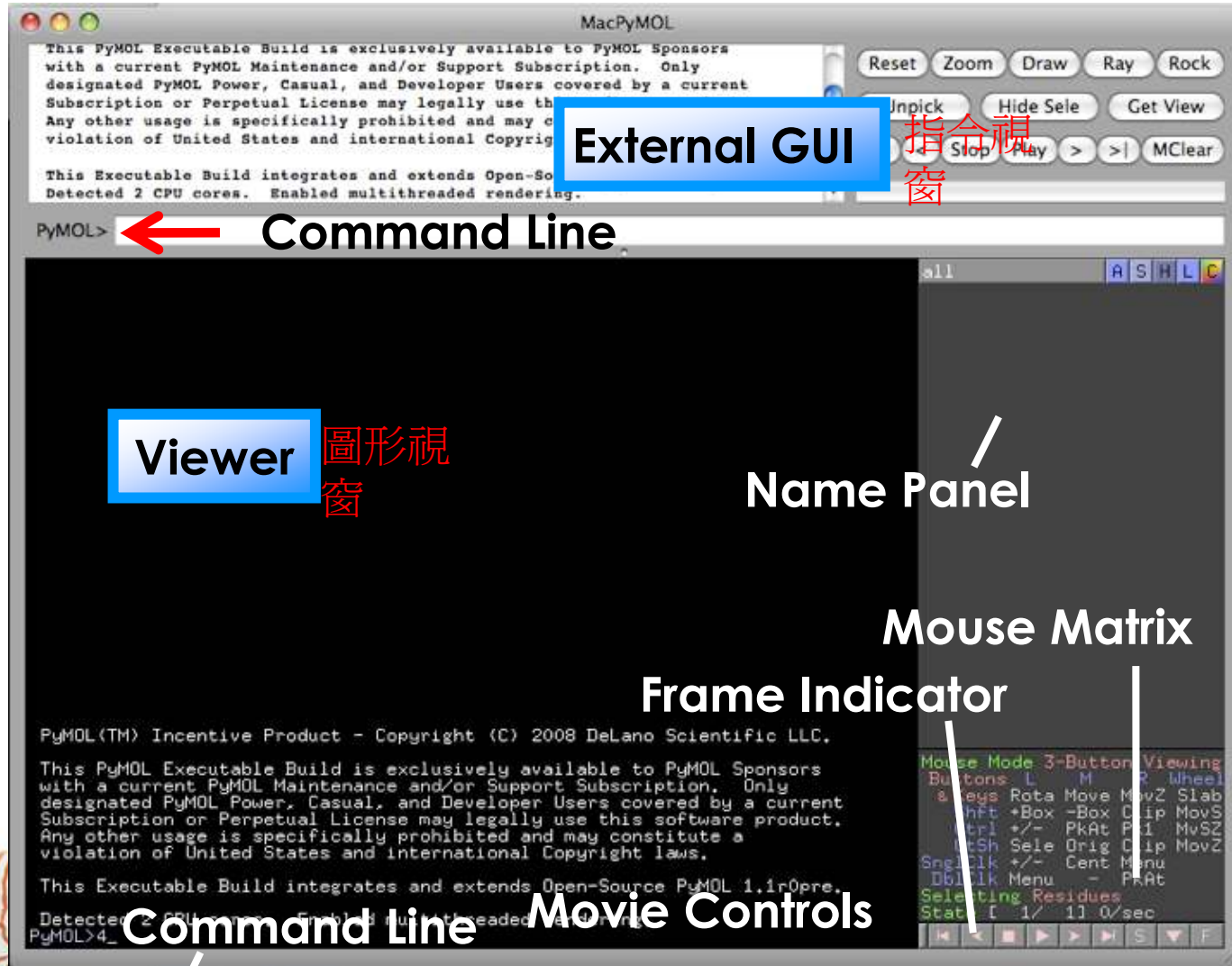
The interface also shows a 3D molecular model of a protein structure, rendered in green and orange, with a blue ribbon representation. The PyMOL Viewer window displays the command prompt with the text "For Educational Use Only" and "PyMOL>". The right-hand side of the interface shows a list of objects and a mouse control panel.

Object	A	S	H	L
all				
1D66				

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 Drig Clip MovZ  
SnglClk +/- Cent Menu  
DblClk Menu - PkAt  
Selecting Residues  
State [ 1/ 1] 0/sec



# PyMOL Interface



External GUI

指令視窗

Command Line

Viewer

圖形視窗

Name Panel

Mouse Matrix

Frame Indicator

Movie Controls

Command Line

A: action  
S: show  
H: hide  
L: label  
C: color

# Basic control skills

The screenshot displays the MacPyMOL application window. The top-left pane shows a list of compounds and their details:

```
COMPND 11 CHAIN: B, D;  
COMPND 12 FRAGMENT: ALL;  
COMPND 13 EC: 3.1.2.15;  
COMPND 14 ENGINEERED: YES;  
COMPND 15 OTHER_DETAILS: UBIQUITIN C-TERMINUS MODIFIED TO AN ALDEHYDE  
ObjectMolecule: Read secondary structure assignments.  
ObjectMolecule: Read crystal symmetry information.  
Symmetry: Found 9 symmetry operators.  
CmdLoad: PDB-string loaded into object "1cmx", state 1.
```

The main PyMOL window is currently empty. A 'Selection Mode' menu is open, listing various modes:

- 3 Button Viewing Mode (highlighted)
- 3 Button Editing Mode
- 2 Button Viewing Mode
- 2 Button Selecting Mode
- 2 Button Editing Mode
- 1 Button Viewing Mode

Below the menu, there are checked options: Virtual Trackball, Roving Origin, and Roving Detail. Further down, there are cycle options: 3 Button Universal Cycle, 2 Button Viewing Cycle, and 2 Button Editing Cycle.

On the right side of the interface, there are buttons for 'Draw', 'Ray', 'Rock', 'e Sele', 'Get View', 'ay >', '>|', and 'MClear'. Below these are two rows of colored buttons labeled 'A S H L E'.

A 'Mouse Matrix' window is open in the bottom-right corner, displaying the following information:

```
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] 4/sec
```

At the bottom of the Mouse Matrix window, there are navigation buttons: left arrow, right arrow, double left arrow, double right arrow, 'S', and 'F'.

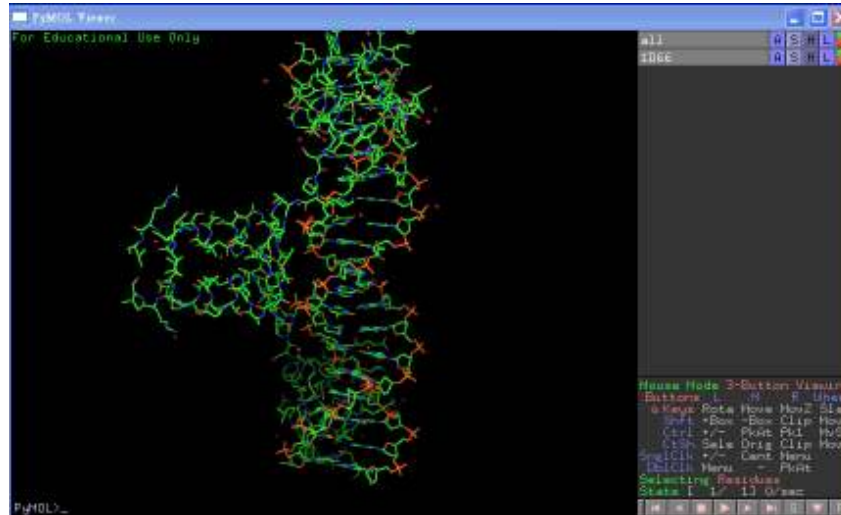


# Show & Hide

A S H L C

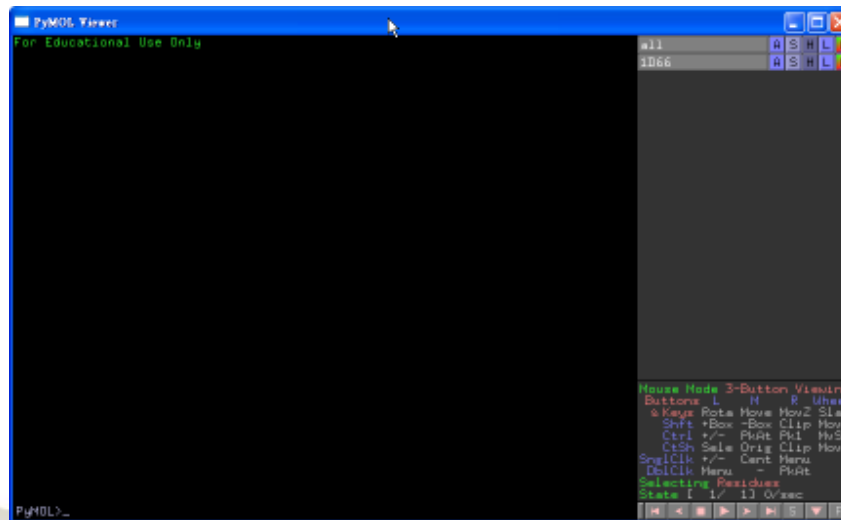
Hide:

- 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



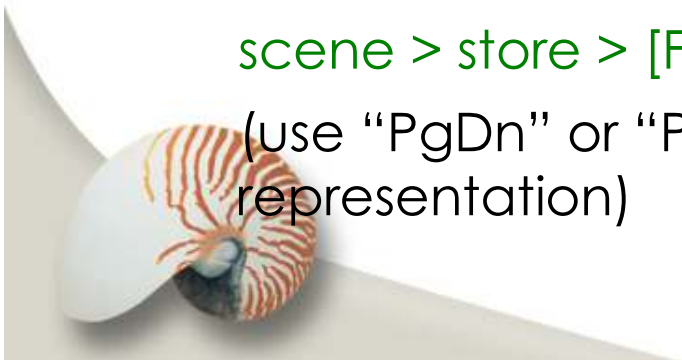
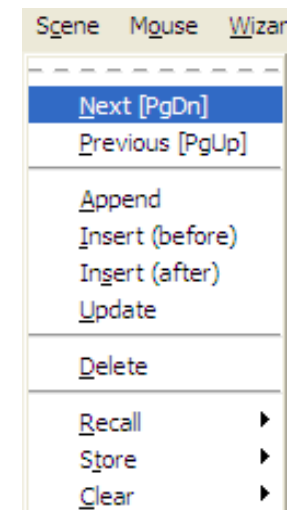
# 不同的表示法

- Using A S H L C
  - 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

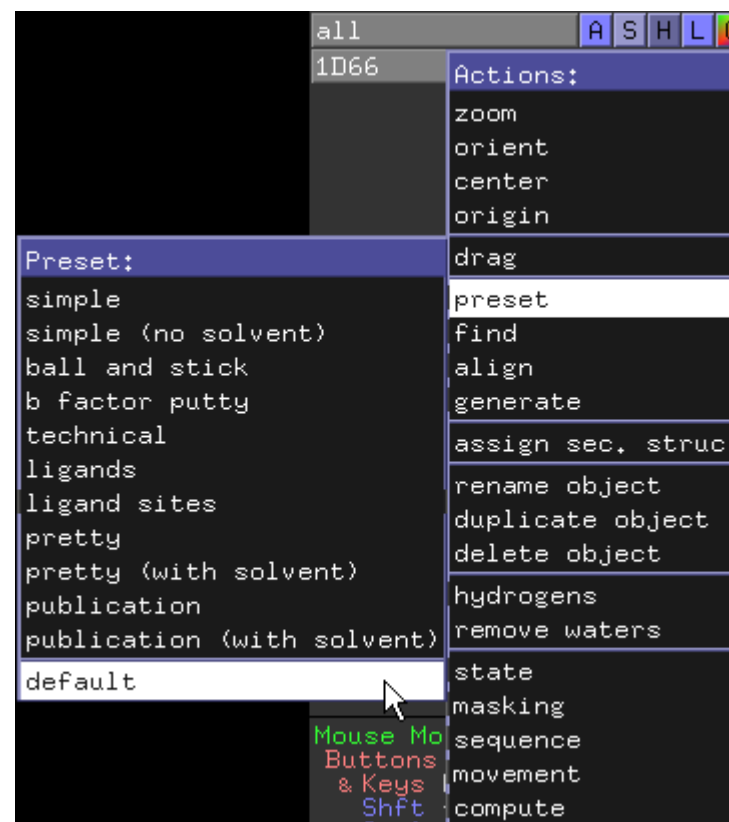
**1D66 > A > preset > default**

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**

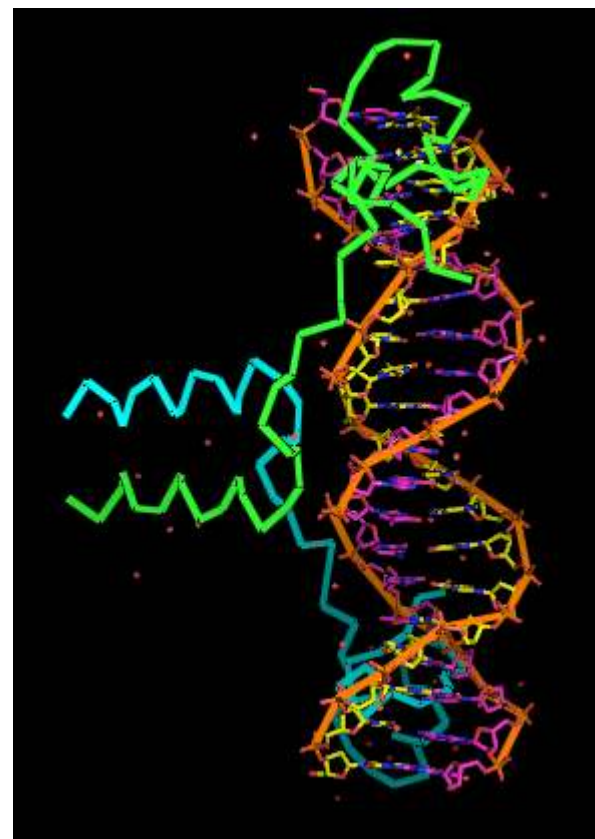
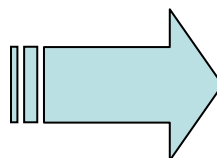
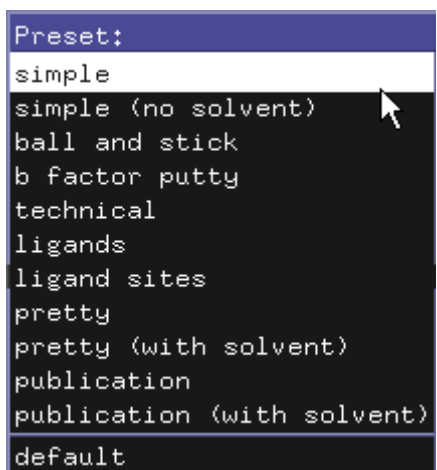




# Action preset menus

Explore the other menus of this series.

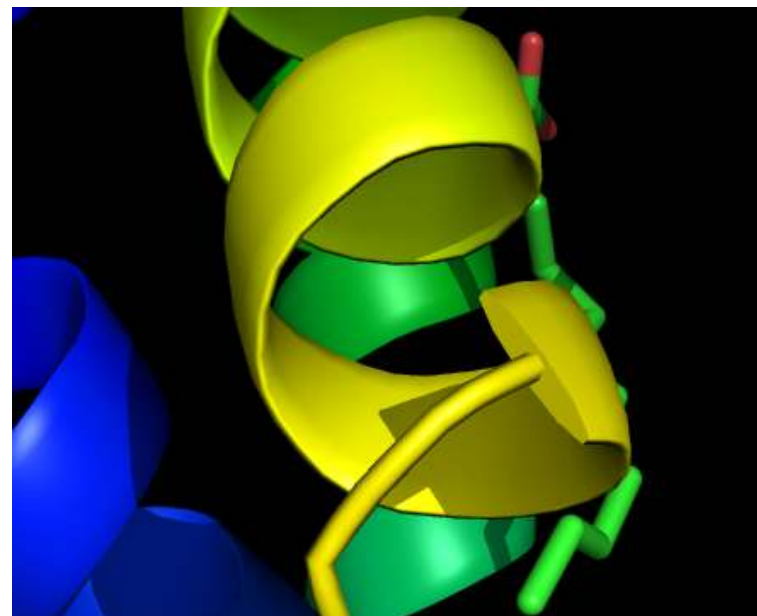
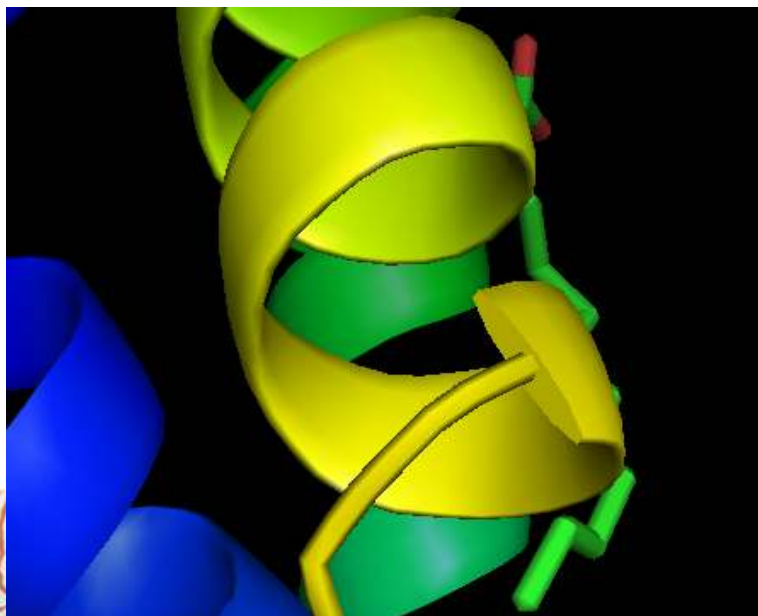
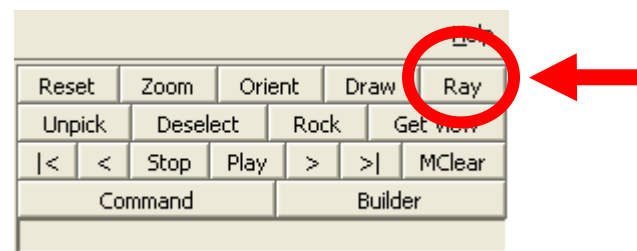
1D66 > A > preset > simple



# 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.

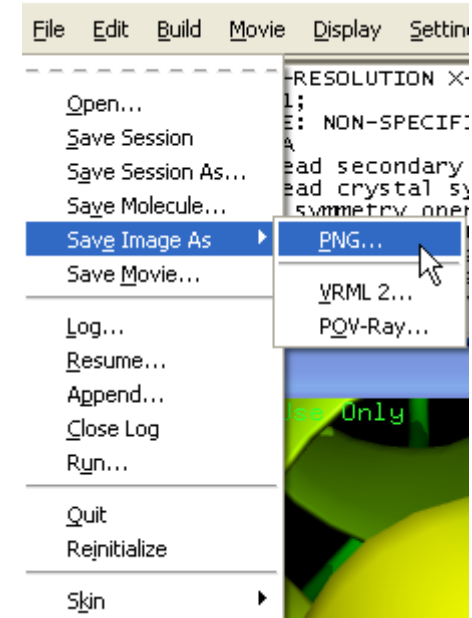
# Save Image

- **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:**

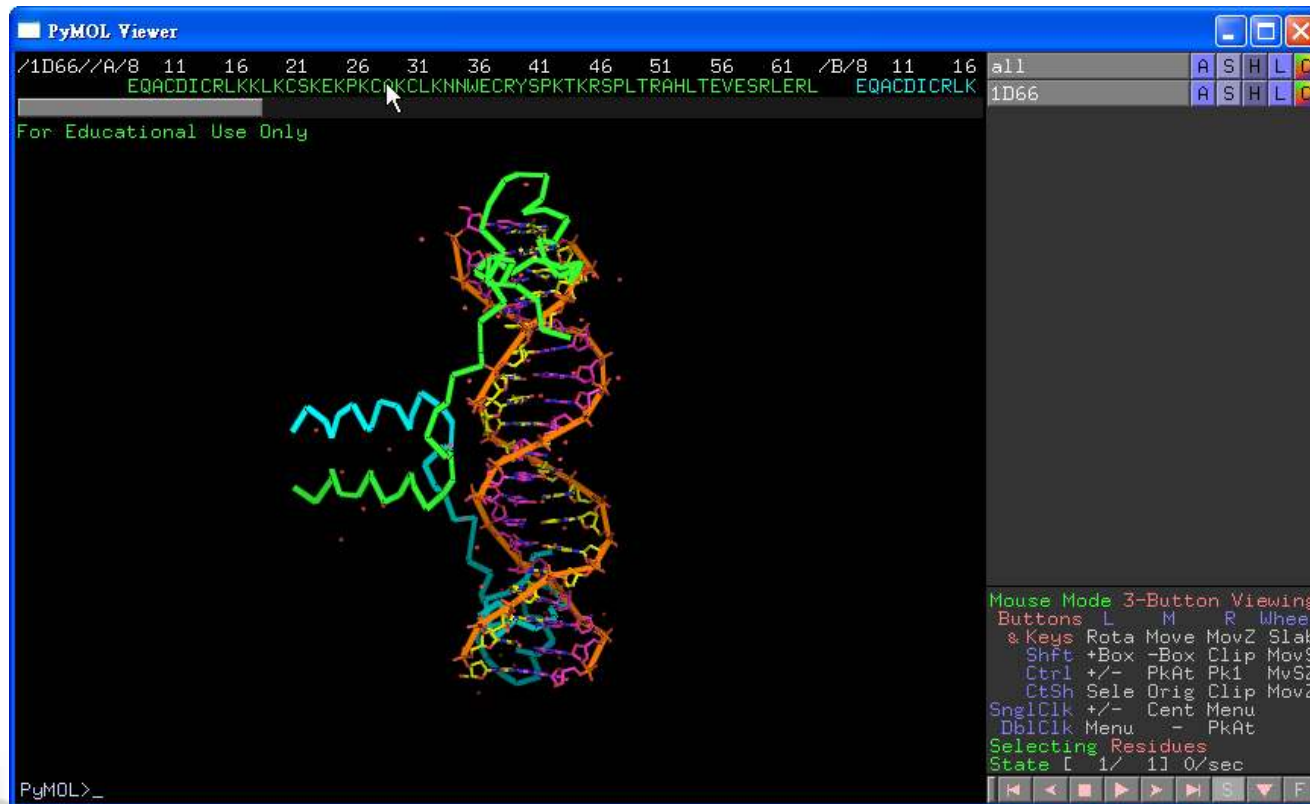
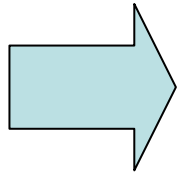
> png filename.png



# 4. Show Sequence

## ■ Display > Sequence

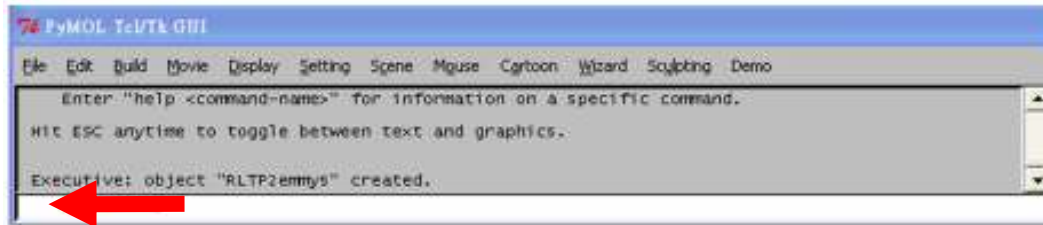
→ will display residue codes, residues, chains, atoms and states





# 5. 鍵入指令

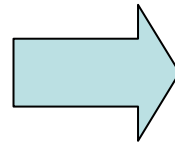
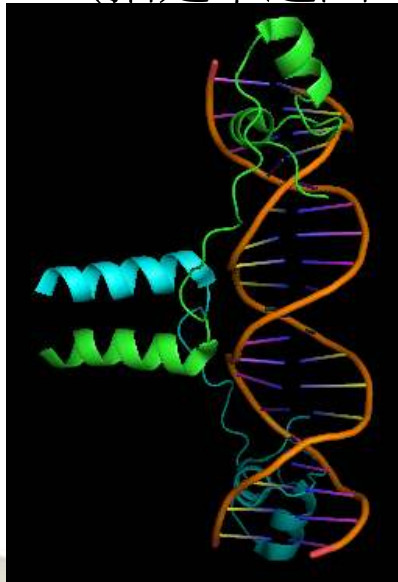
在下面**箭頭**的地方鍵入下列的所有指令。



**show cartoon, all**  
**color orange**

(將所有的東西以卡通圖的方式呈現)

(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	

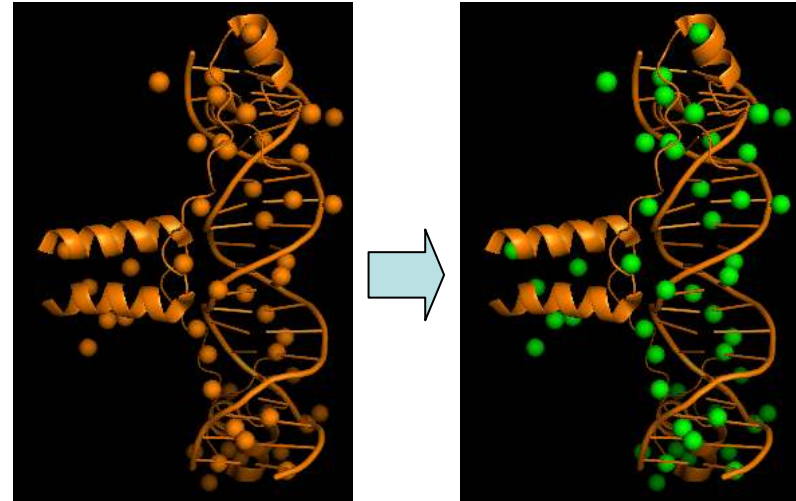


## 6. 顯示水或非protein和DNA物質

- 可以用下列方式顯示所有水分子。

show spheres, (resn HOH)

color green, (resn HOH)

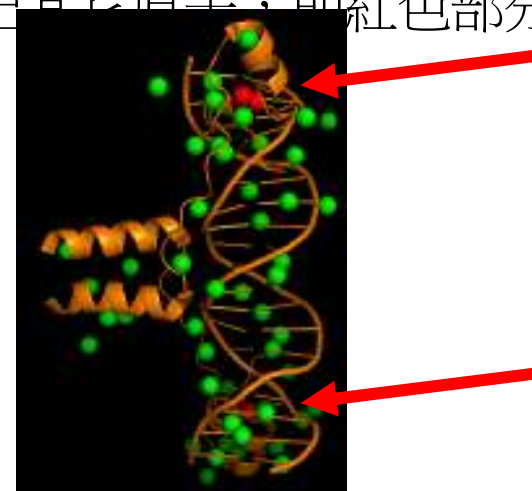


- 若是直接選heto-atom，可能會選出其它原子，即紅色部分所示。

show spheres, hetatm

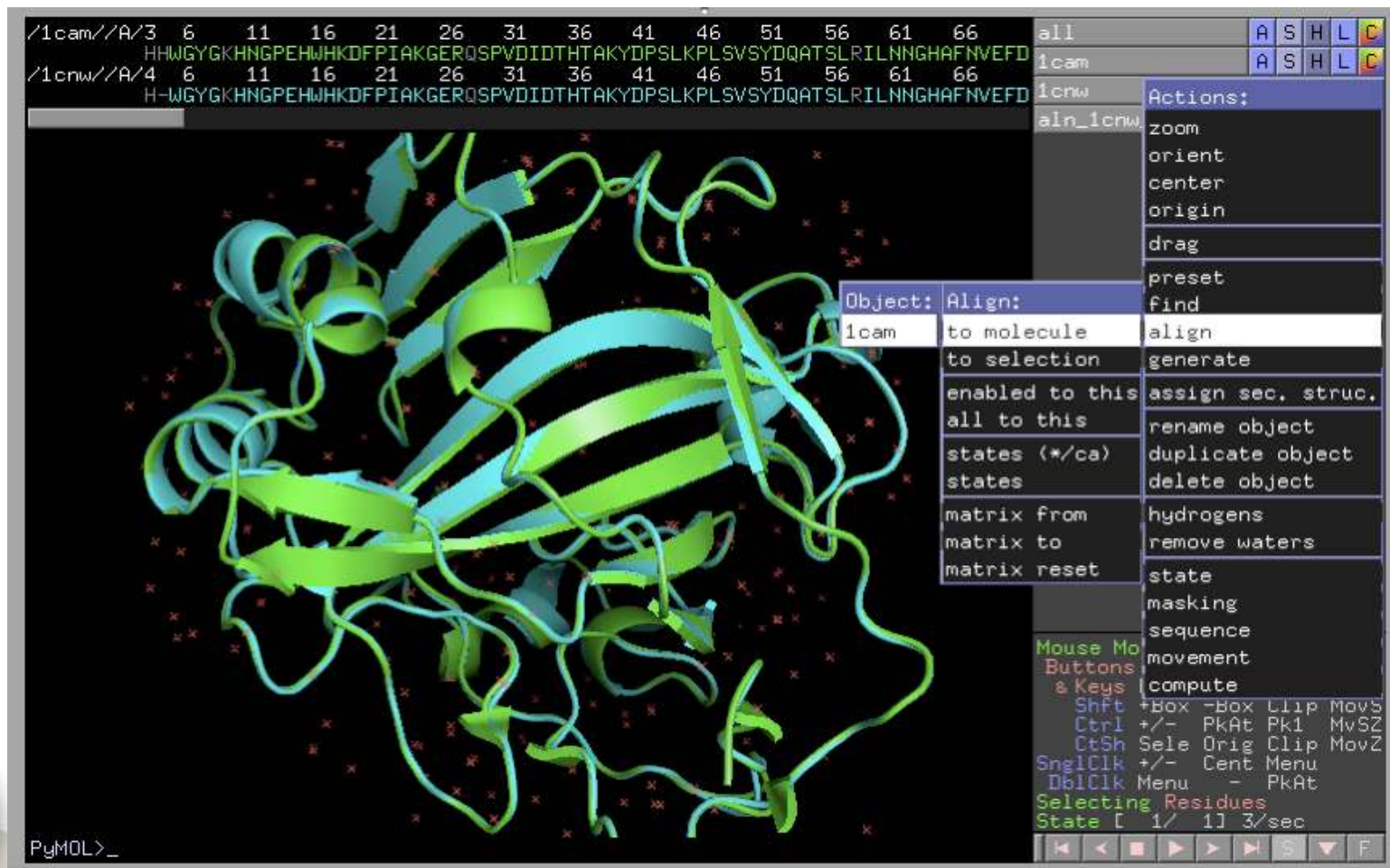
color red, hetatm

color green, (resn HOH)



# 7.Pymol align is sequence alignment

- Download 1cam & 1cnw



The screenshot displays the PyMOL interface. At the top, a sequence alignment is shown between two protein structures, 1cam and 1cnw. The sequences are identical: HHWGYGKHNNGPEHWHKDFPIAKGERQSPVDIDTHTAKYDPSLKPLSVSYDQATSLRILNNGHAFNVEFD. The alignment is visualized in a 3D ribbon representation, with the 1cam structure in cyan and the 1cnw structure in green. The background is black with red asterisks indicating alignment points. On the right side, a context menu is open for the '1cam' object, showing various actions such as 'align', 'generate', 'assign sec. struc.', 'duplicate object', 'delete object', 'hydrogens', 'remove waters', 'state', 'masking', 'sequence', 'movement', and 'compute'. The bottom of the interface shows the PyMOL command line and a keyboard shortcuts table.

```
/1cam//A/3 6 11 16 21 26 31 36 41 46 51 56 61 66  
HHWGYGKHNNGPEHWHKDFPIAKGERQSPVDIDTHTAKYDPSLKPLSVSYDQATSLRILNNGHAFNVEFD  
/1cnw//A/4 6 11 16 21 26 31 36 41 46 51 56 61 66  
H-WGYGKHNNGPEHWHKDFPIAKGERQSPVDIDTHTAKYDPSLKPLSVSYDQATSLRILNNGHAFNVEFD
```

Object:	Align:
1cam	to molecule
	to selection
enabled to this	assign sec. struc.
all to this	rename object
states (* /ca)	duplicate object
states	delete object
matrix from	hydrogens
matrix to	remove waters
matrix reset	state
	masking
	sequence
	movement
	compute

Mouse Mo  
Buttons  
& Keys

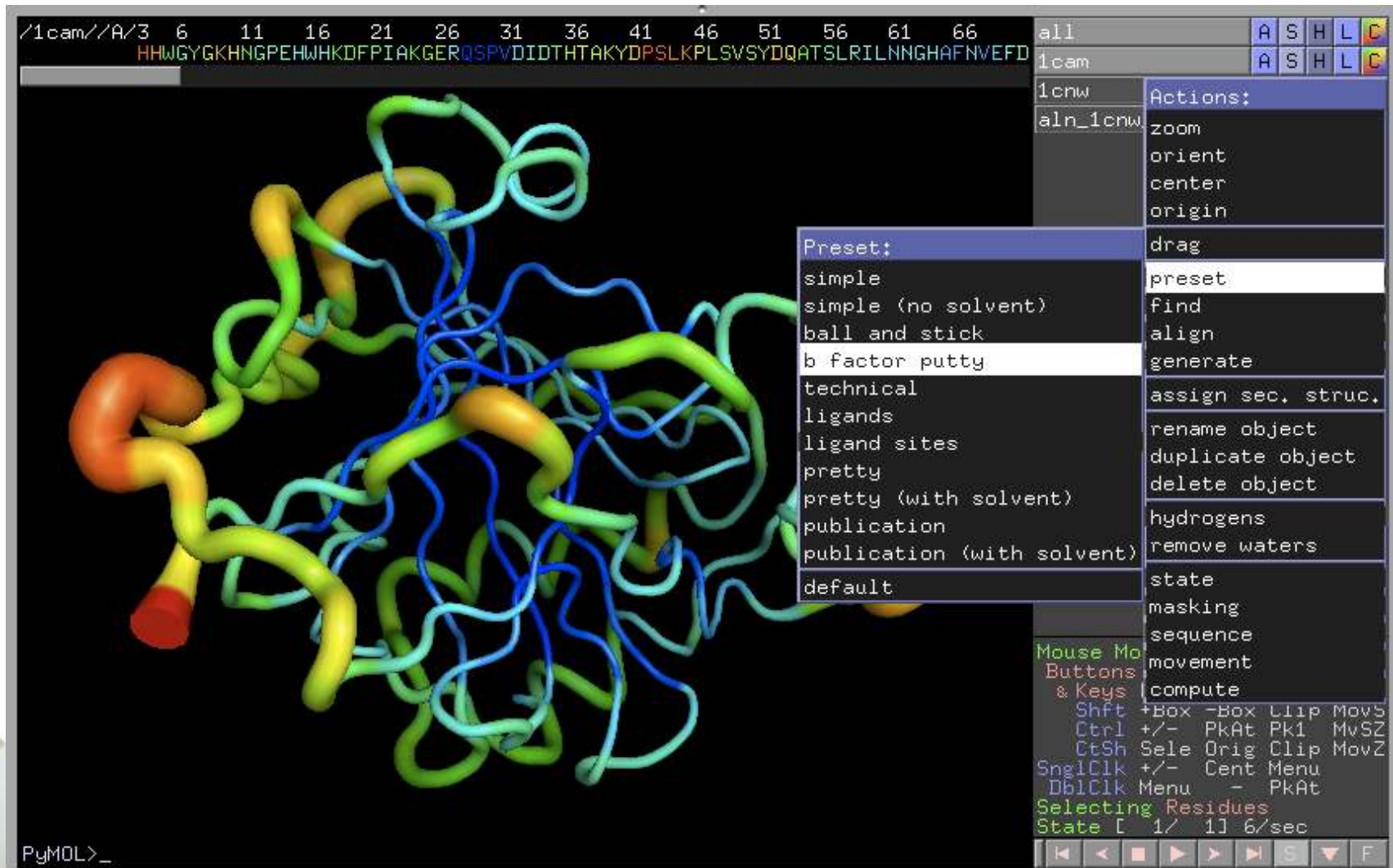
Shft	+Box	-Box	Clip	MovS
Ctrl	+/-	PkAt	Pk1	MvSZ
CtSh	Sele	Orig	Clip	MovZ
SnglClk	+/-	Cent	Menu	
Db1Clk	Menu	-	PkAt	

Selecting Residues  
State [ 1/ 11 3/sec





# 8. B-factor



The image shows a PyMOL interface with a protein structure rendered in a ribbon format. The structure is colored by B-factor, with a gradient from red (high B-factor) to blue (low B-factor). A context menu is open over the structure, showing the 'Preset:' list with 'b factor putty' selected. The interface includes a command line at the top with the protein sequence: `/1cam//A/3 6 11 16 21 26 31 36 41 46 51 56 61 66 HHWGYGKHNGPEHWKDFPIAKGERQSPV D I D T H T A K Y D P S L K P L S V S Y D Q A T S L R I L N N G H A F N V E F D`. The right sidebar shows a list of actions for the selected object, including 'zoom', 'orient', 'center', 'origin', 'drag', 'preset', 'find', 'align', 'generate', 'assign sec. struc.', 'rename object', 'duplicate object', 'delete object', 'hydrogens', 'remove waters', 'state', 'masking', 'sequence', and 'movement'. The bottom status bar shows 'PyMOL>\_' and 'State [ 1 / 1 ] 6/sec'.

```
all A S H L C
1cam A S H L C
1cnw Actions:
aln_1cnw zoom
orient
center
origin
drag
Preset:
simple
simple (no solvent)
ball and stick
b factor putty
technical
ligands
ligand sites
pretty
pretty (with solvent)
publication
publication (with solvent)
default
preset
find
align
generate
assign sec. struc.
rename object
duplicate object
delete object
hydrogens
remove waters
state
masking
sequence
movement
compute
Mouse Mo
Buttons
& Keys
Shift +Box -Box Liip Mov5
Ctrl +/- PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State [ 1 / 1 ] 6/sec
```

# 9. 算距離

The screenshot displays the MacPyMOL software interface. At the top, the menu bar includes 'MacPyMOL', 'File', 'Edit', 'Build', 'Movie', 'Display', 'Setting', 'Scene', 'Mouse', 'Wizard', and 'Help'. The 'Wizard' menu is open, showing options: Appearance, Measurement, Mutagenesis, Pair Fitting, Density, Filter, Sculpting, Label, Charge, and Demo. The main window shows a protein structure with a yellow dashed line indicating a distance of 8.7 Å between two atoms. The command window at the top left shows a syntax error: 'SyntaxError: invalid syntax' and 'You clicked /lcam//A/ALA 54/CB'. The sequence viewer below the command window shows the protein sequence: /lcam//A/3 6 11 16 21 26 31 36 41 46 51 56 61. The measurement panel at the bottom right shows 'Measurement' and 'Distances' options. The mouse mode is set to '3-Button Viewing'.

```
File ~/Users/delwari/MacPyMOL080511/build/Deployment/MacPyMOL.app/pymol/modules/pymol/parser.py", line 455, in parse
File "<string>", line 1

^
SyntaxError: invalid syntax
You clicked /lcam//A/ALA 54/CB
Selector: selection "sele" defined with 1 atoms.
You clicked /lcam//A/SER 50/N

PyMOL>

/lcam//A/3 6 11 16 21 26 31 36 41 46 51 56 61
HHWGYGKINGPEHWJKDFPIAKGERQSPVDIDHTAKYDPSLKP LSVSYDQATSLRILNNGHA

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
Buttons L M R Wheel
s Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl +/- PkAt Pk1 MovSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DbIClk Menu - PkAt

Selecting Atoms
State [ 1/ 1] 4/sec
```



## 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>



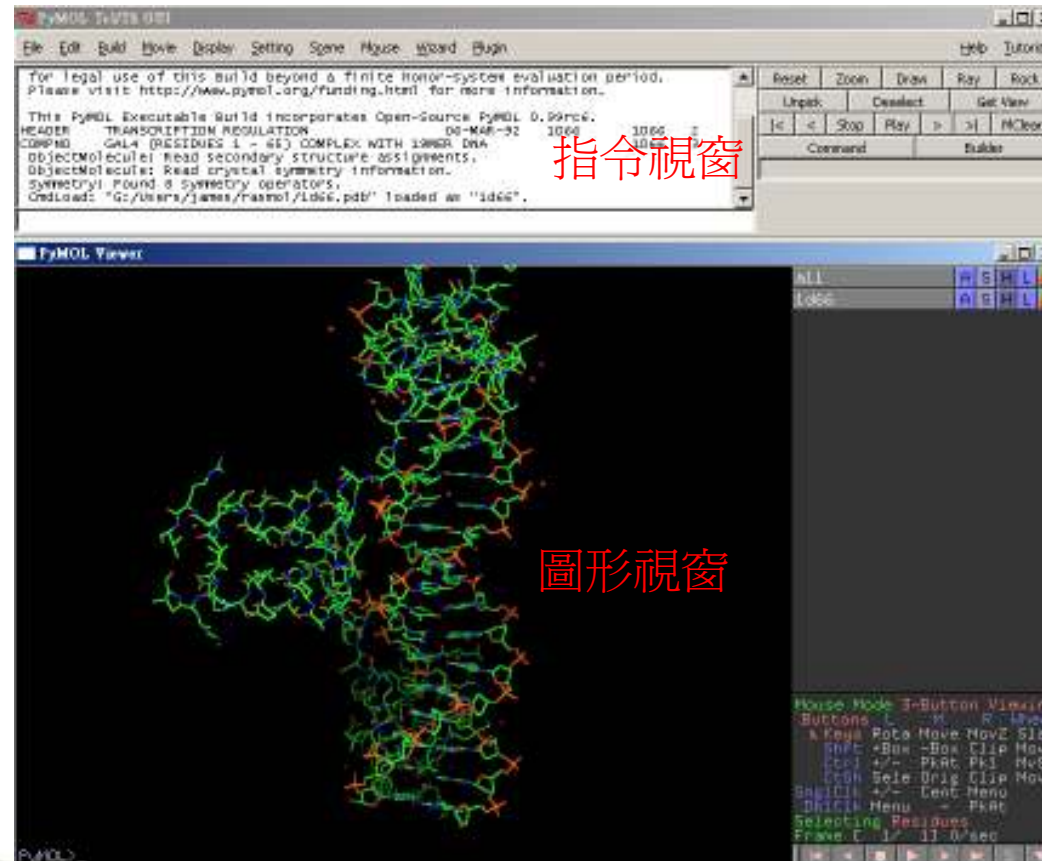
# Surface





# 開啓檔案

- PDB: 1D66。
- 開啓PyMOL軟體，並讀入1D66檔案。



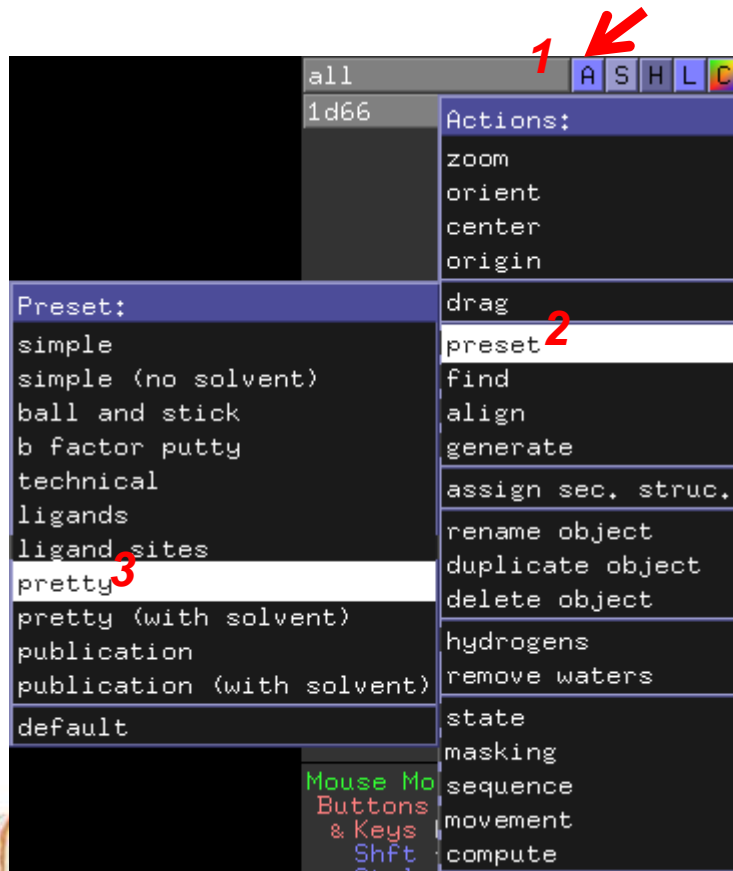
指令視窗

圖形視窗



# Surface

Action > Preset > Pretty (調整至適當方向)

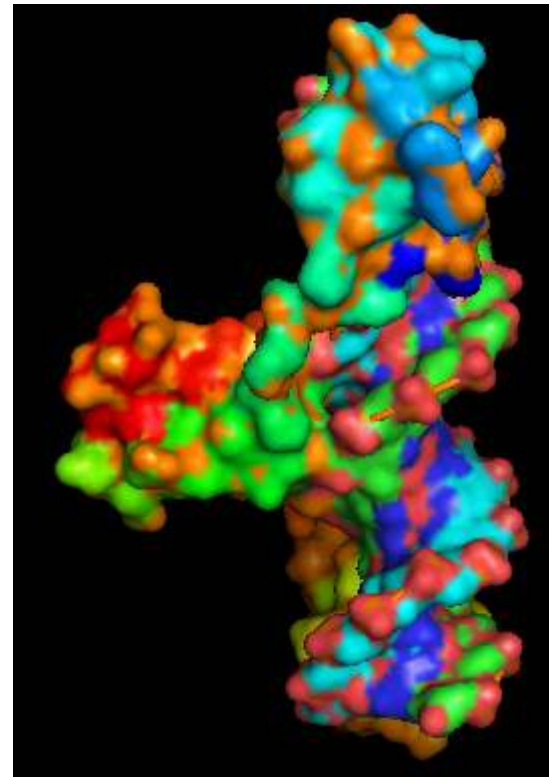
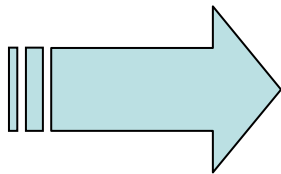
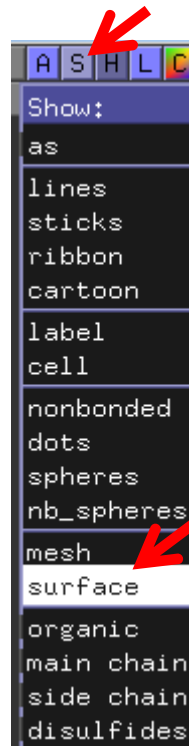


PDB: 1D66



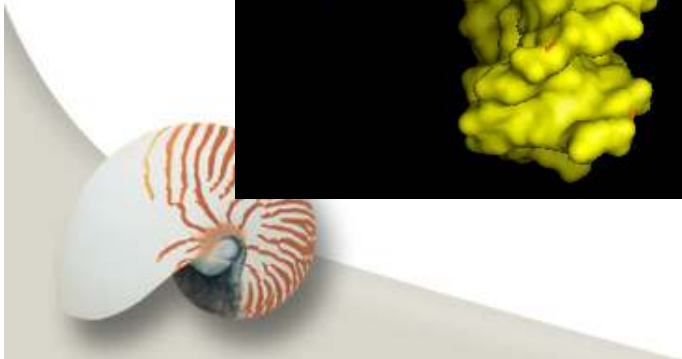
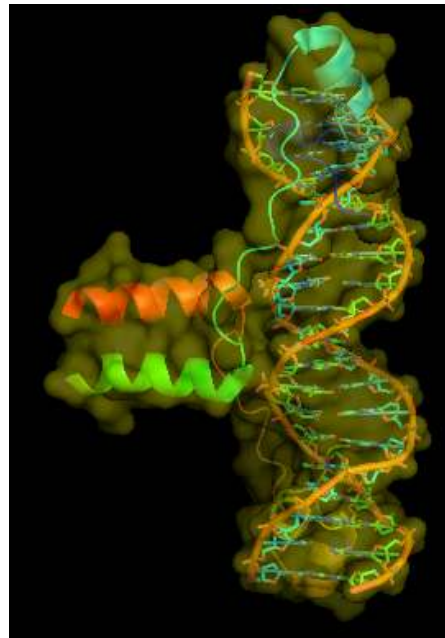
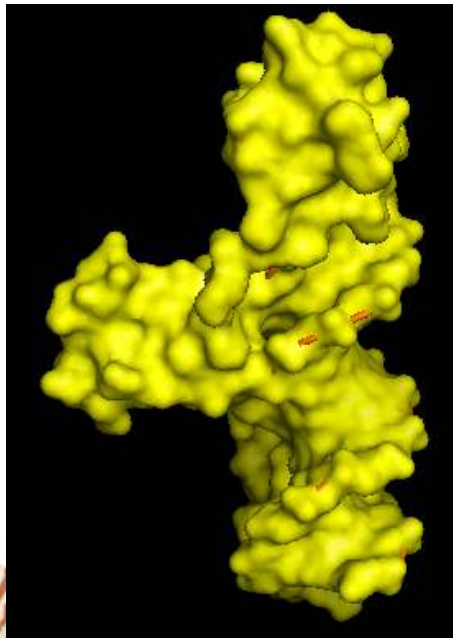
# Surface

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

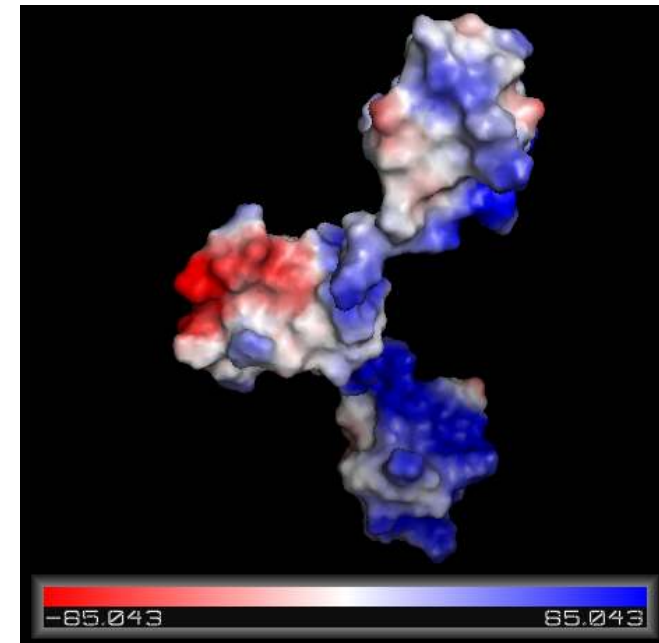
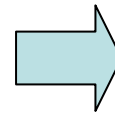
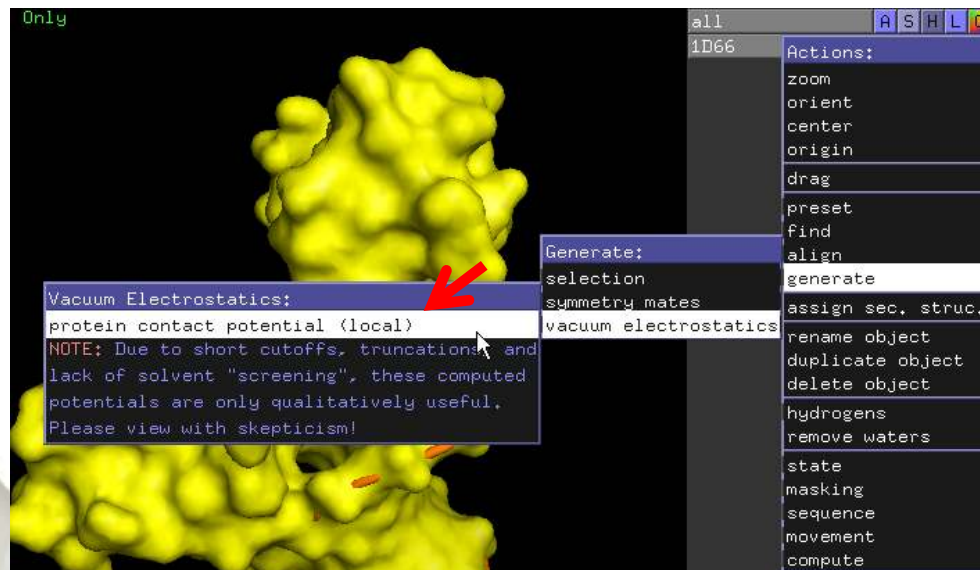


# Surface

- 顯示蛋白質表面的電荷:

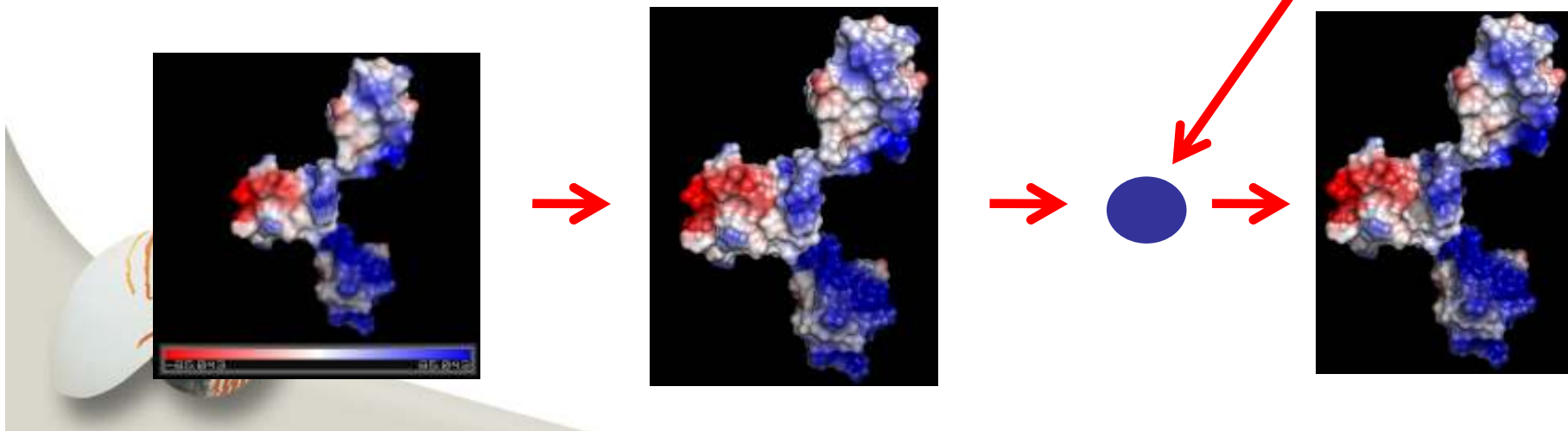
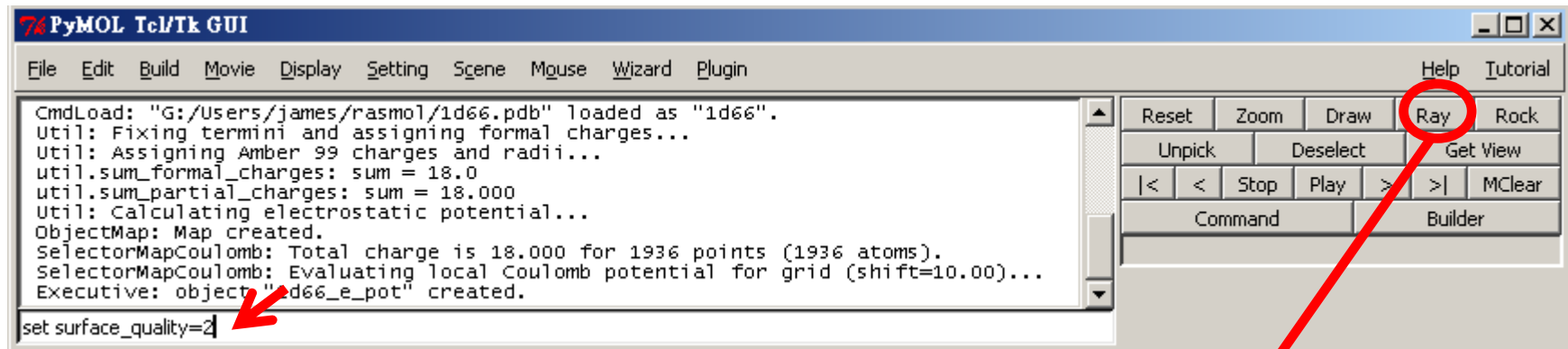
set transparency, 0 先取消透明度

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



# Surface

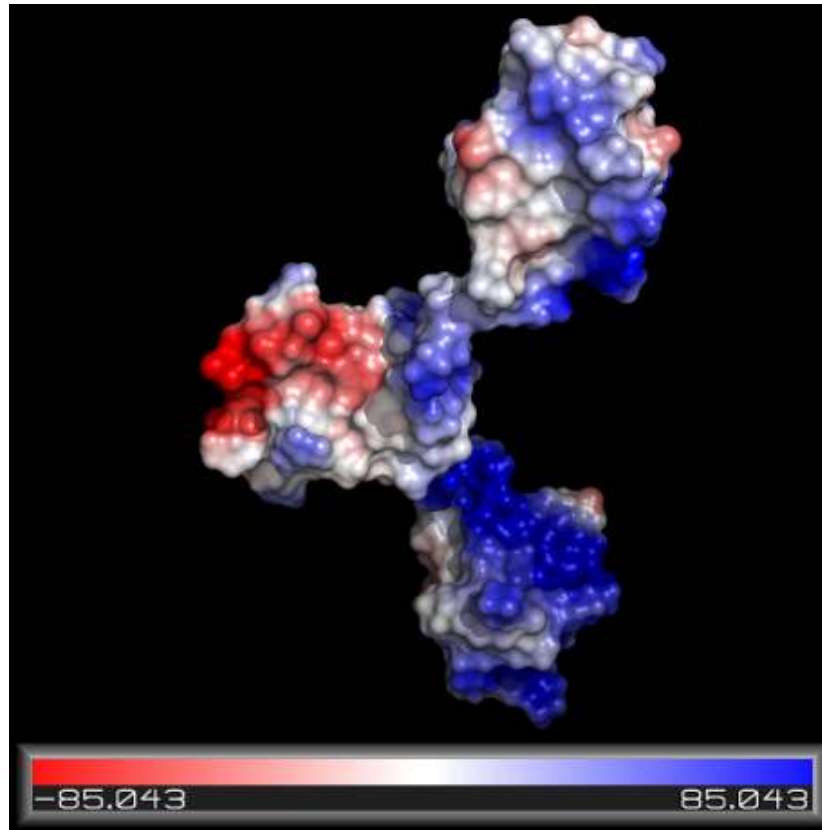
- 以較高的品質顯示蛋白質surface:  
type “set surface\_quality=2” in command line





# Surface

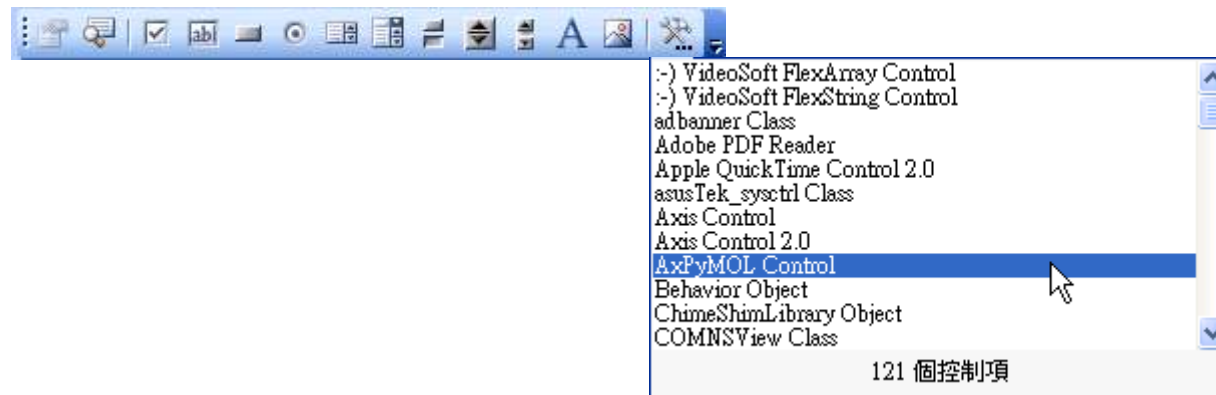
- 旋轉以檢視不同角度:
- 按著”Ctrl”+滑鼠中鍵，就可以在藍白紅的bar上調整正負電的scale

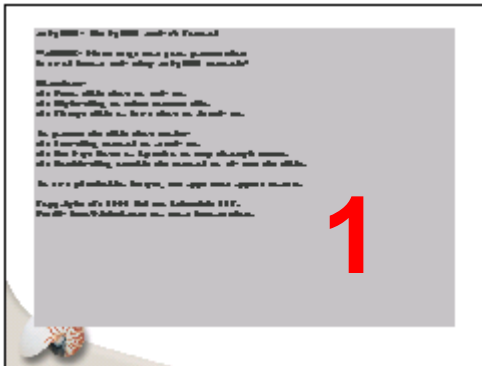


# AxPyMOL

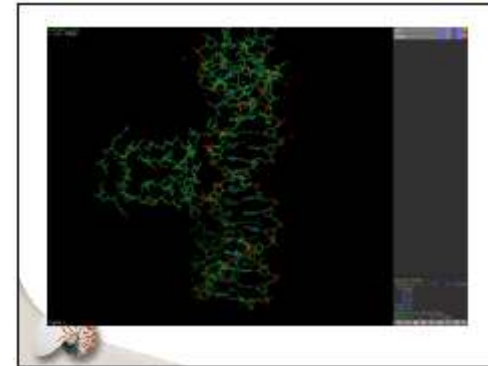
- The **PyMOL ActiveX control** which can be used in **Powerpoint**
- Installing AxPyMOL: <http://delsci.com/axpymol/>
- Usage:

**Click here !!**





4   
Play the slide



2



3

Key in the pathway of structure



