

# IBT 432 Aplikasi Bioinformatika

## Visualisasi protein modelling

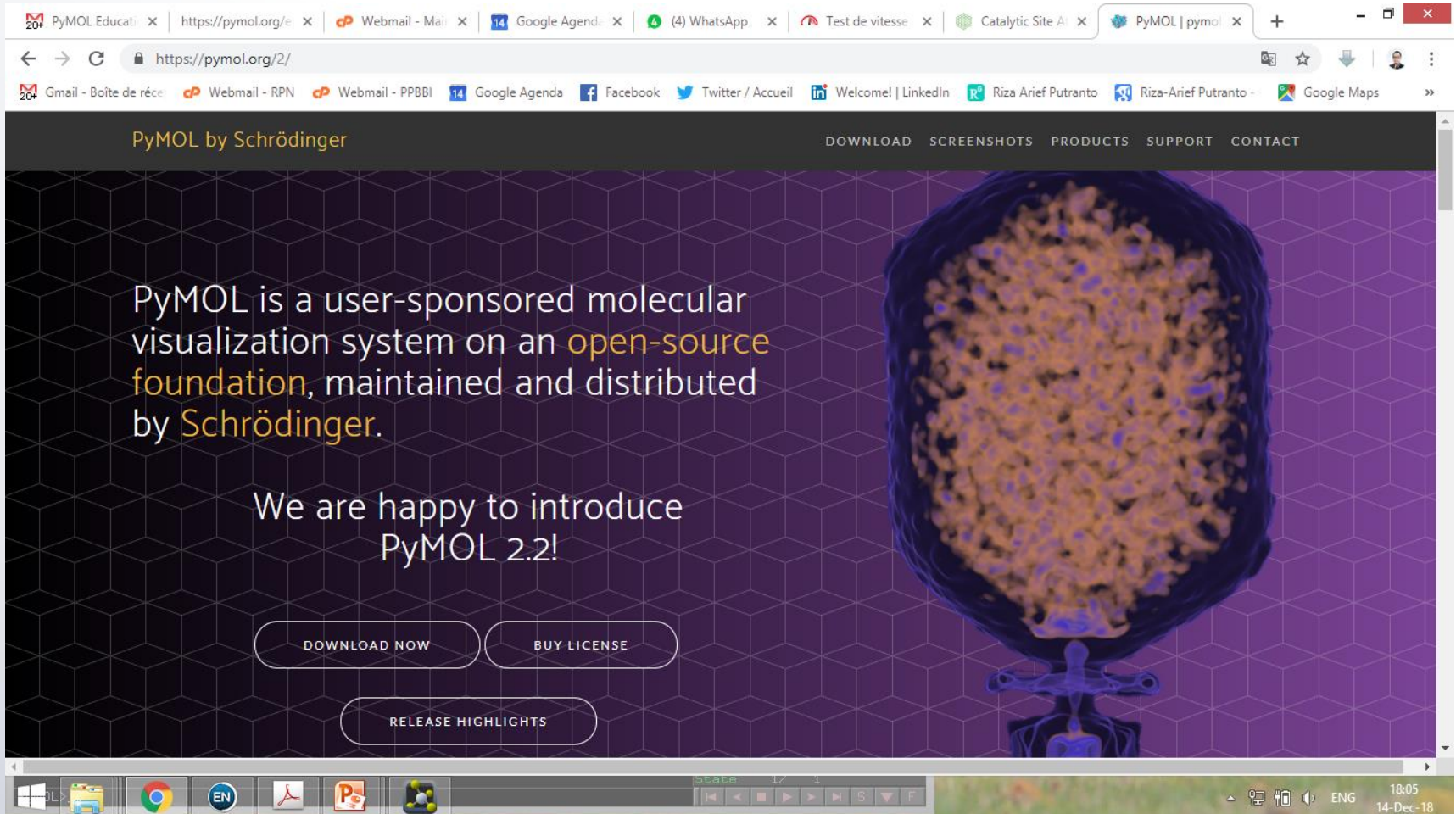
**Riza Arief Putranto**

# Rencana Perkuliahan

- ~~1. Kontrak belajar dan pengenalan bioinformatika aplikatif~~
- ~~2. Database sekuen dan analisis genomika~~
- ~~3. Anotasi sekuen ke genom - Praktik~~
- ~~4. Analisis komparasi genomika I~~
- ~~5. Analisis komparasi genomika II~~
- ~~6. Analisis komparasi genomika III~~
- ~~7. Analisis komparasi genomika - Praktik~~
- ~~8. Protein modelling I~~
- ~~9. Protein modelling II~~
- ~~10. Protein modelling III~~
- ~~11. Protein modelling - Praktik~~
12. Visualisasi protein modelling
13. Visualisasi protein modelling - Praktik
14. Presentasi mahasiswa

# Visualization of protein model: PyMOL

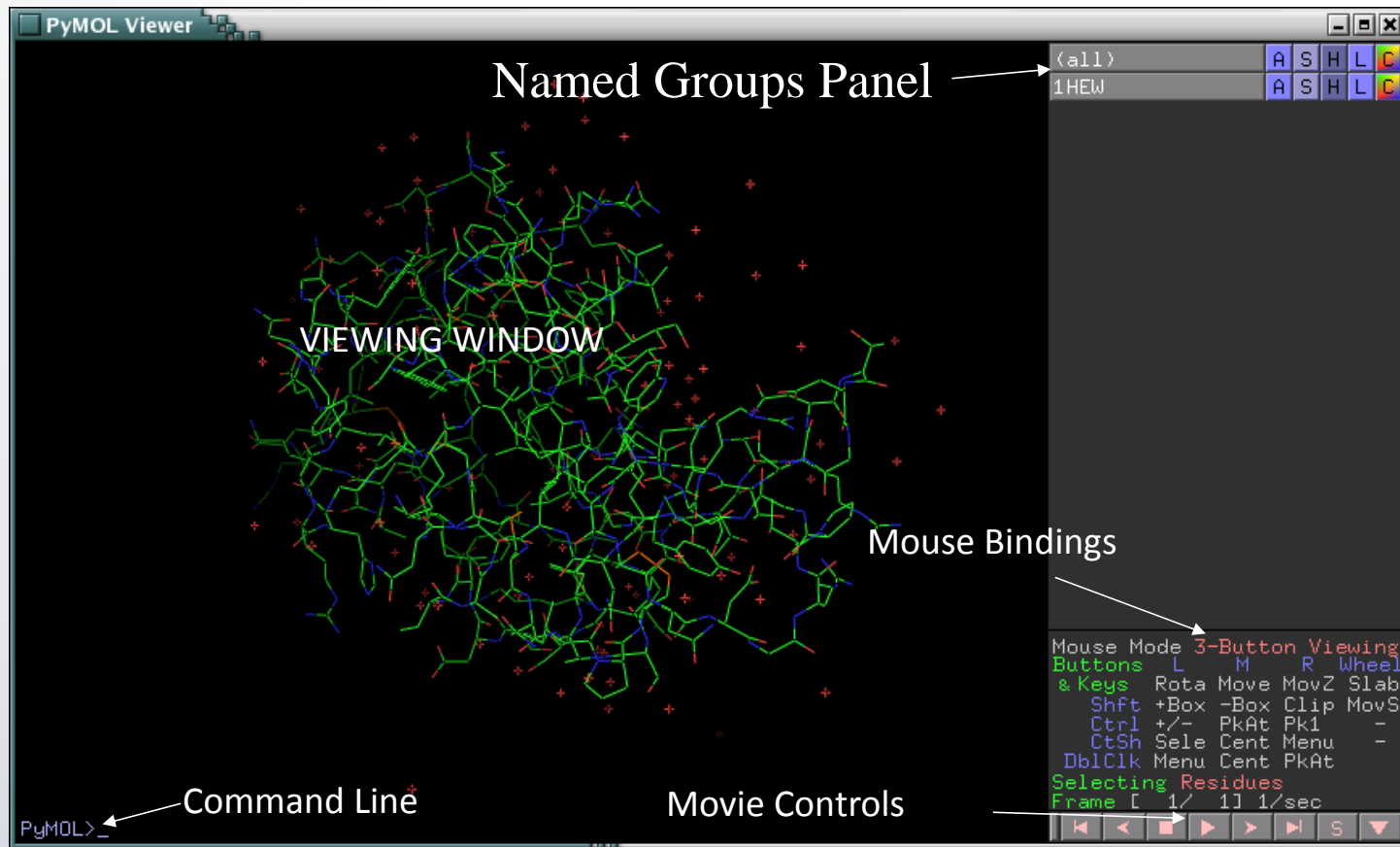
<http://www.pymol.org/>



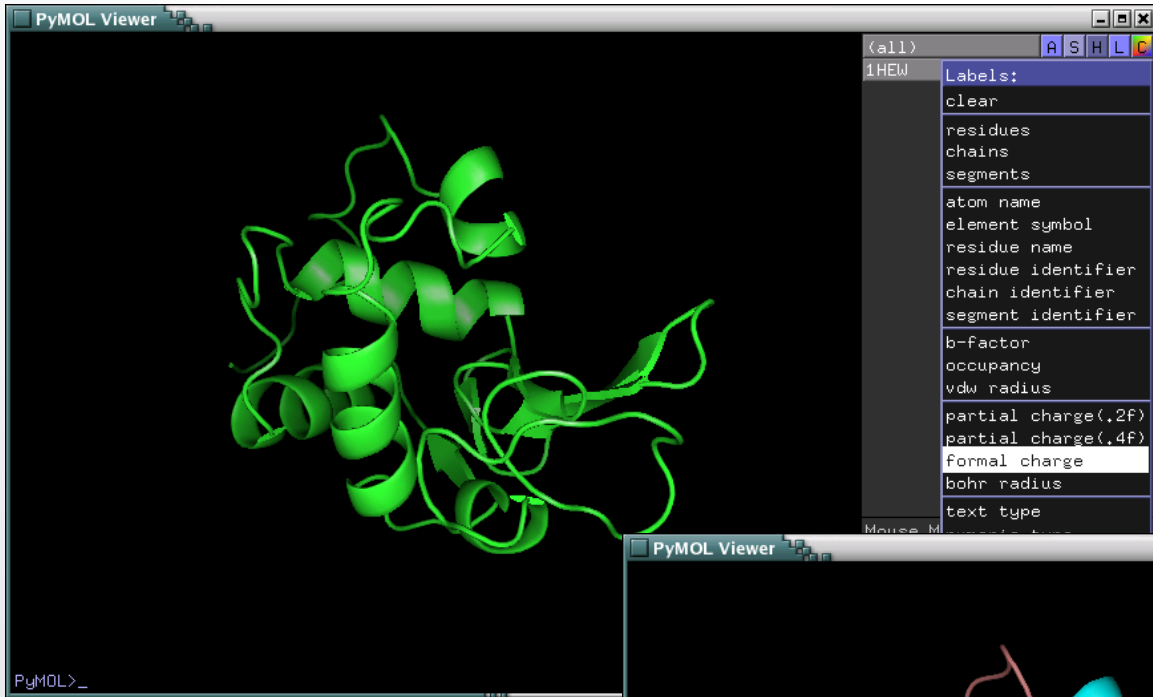
The screenshot shows the PyMOL website homepage. At the top, there is a navigation bar with links for [DOWNLOAD](#), [SCREENSHOTS](#), [PRODUCTS](#), [SUPPORT](#), and [CONTACT](#). The main content area features the text: "PyMOL is a user-sponsored molecular visualization system on an **open-source foundation**, maintained and distributed by **Schrödinger**." Below this, it says "We are happy to introduce PyMOL 2.2!". There are three buttons: "DOWNLOAD NOW", "BUY LICENSE", and "RELEASE HIGHLIGHTS". On the right side, there is a large 3D molecular model of a protein structure, rendered in orange and blue, set against a purple background with a hexagonal grid pattern. The browser's address bar shows the URL <https://pymol.org/2/>. The Windows taskbar at the bottom shows various application icons and the system clock indicating 18:05 on 14-Dec-18.

# Visualization of protein model: PyMOL

- **PyMOL** is a user-sponsored molecular **visualization system** on an open-source foundation, maintained and distributed by Schrödinger.

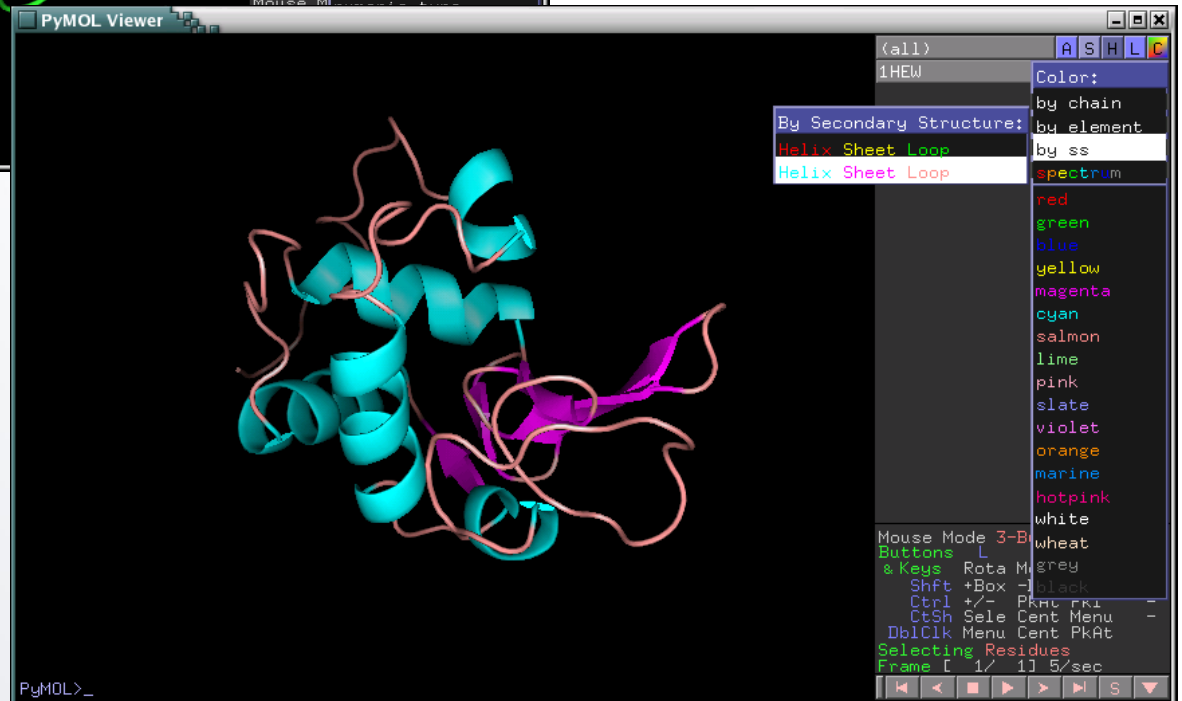


# Play with PyMOL



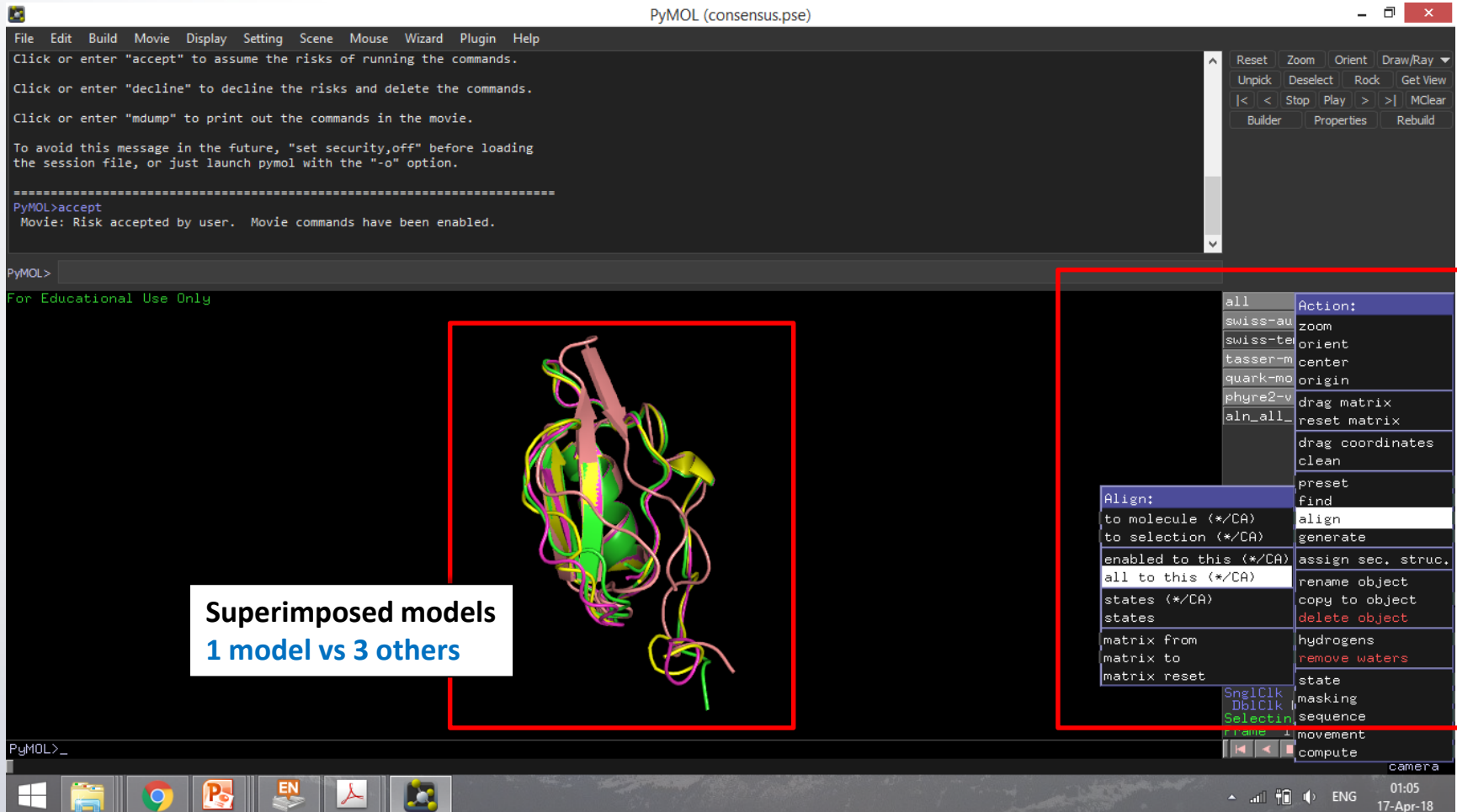
**Label panel:** residues, chains, segments

**Color panel:** by chain, by element, by secondary structure, by spectrum



# Super[imposition] with PyMOL

- Take on protein model and **align with molecule or all models** viewed in PyMOL



The screenshot displays the PyMOL interface. The main window shows a protein structure with four different models superimposed: one in green, one in yellow, one in pink, and one in light blue. A red box highlights this 3D view. A white text box with a blue border is overlaid on the bottom left of the 3D view, containing the text: "Superimposed models 1 model vs 3 others". On the right side, a command menu is open, listing various actions. A sub-menu titled "Align:" is also visible, listing alignment options. The PyMOL command line at the bottom left shows "PyMOL>accept" and "Movie: Risk accepted by user. Movie commands have been enabled." The Windows taskbar at the bottom shows the system tray with the date "17-Apr-18" and time "01:05".

PyMOL (consensus.pse)

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

Click or enter "accept" to assume the risks of running the commands.

Click or enter "decline" to decline the risks and delete the commands.

Click or enter "mdump" to print out the commands in the movie.

To avoid this message in the future, "set security,off" before loading the session file, or just launch pymol with the "-o" option.

=====

PyMOL>accept

Movie: Risk accepted by user. Movie commands have been enabled.

PyMOL>

For Educational Use Only

all Action:  
swiss-au zoom  
swiss-te orient  
tasser-m center  
quark-mo origin  
phyre2-v drag matrix  
aln\_all\_ reset matrix  
drag coordinates  
clean  
preset  
find  
Align:  
to molecule (\*CA) align  
to selection (\*CA) generate  
enabled to this (\*CA) assign sec. struc.  
all to this (\*CA) rename object  
states (\*CA) copy to object  
states delete object  
matrix from hydrogens  
matrix to remove waters  
matrix reset state  
Sng1C1k masking  
Db1C1k sequence  
Selectin movement  
Frame compute

camera

01:05  
17-Apr-18

# Interacting with PyMOL

- **Command-line (fetch, select, color)**
  - d.g., “fetch 1e9r” to retrieve and load the PDB structure with identifier 1e9r
- **Use A, S, H, L and C buttons**
  - for Action, Show, Hide, Label and Color
  - Try the Action->preset options
- **Pull-down menu options from Display**
  - Sequence On (to show sequence)
  - Change color of background
  - Change quality
  - Stereo view
  - Etc.



# Defining residues and modifying their appearance

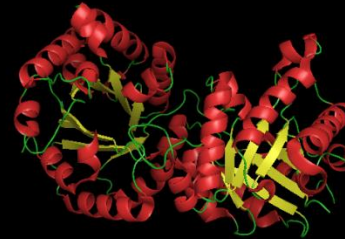
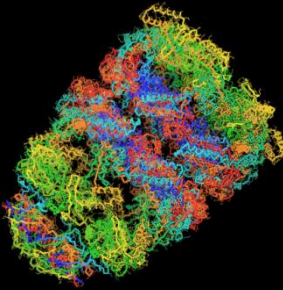
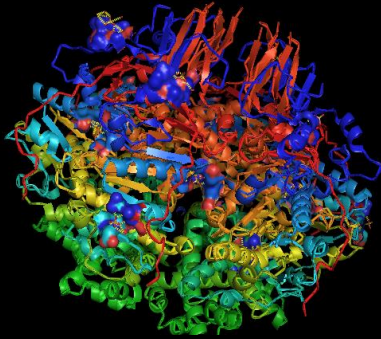
- **If you want to highlight certain residues, try defining them using “Select”**
  - “Select myresidues, resi 17-20,24” or
  - Select myresidues, resi 17+18+19+20+24”
  - The syntax does not allow spaces after commas or after the ‘+’ sign
- **Once you have done this selection, you’ll see that item on the GUI**
- **You can then modify the display using the GUI or on the command-line**
  - “Color red, myresidues”



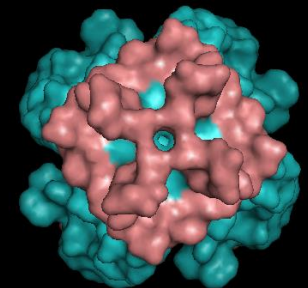
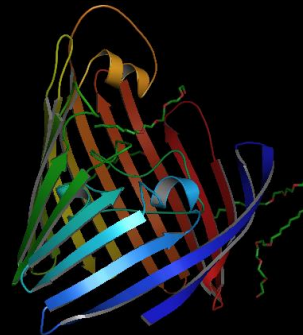
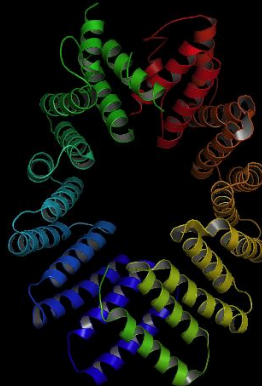
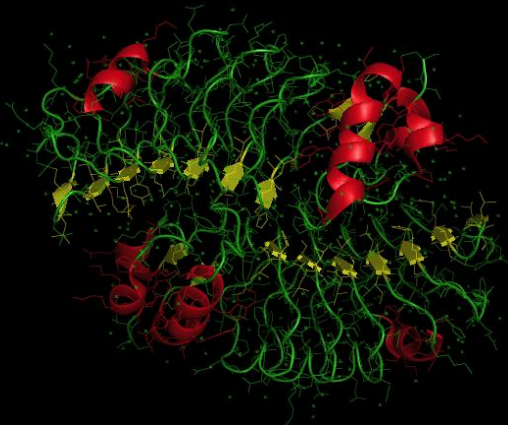
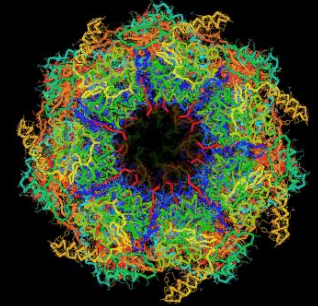
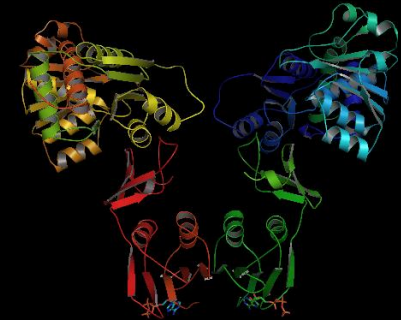
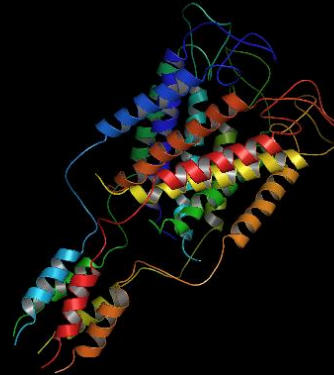
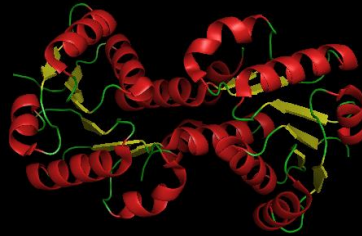
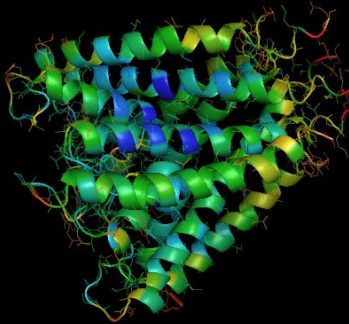
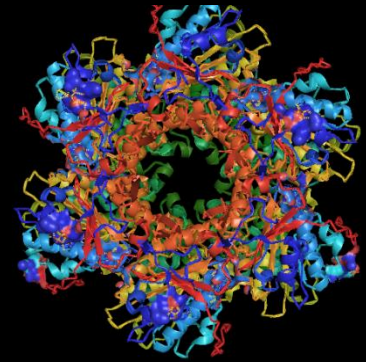
# Match up the images to PDB IDs

(and figure out how to make them, or something similar)

- 1e9ra
- 4at1
- 1aon
- 1bl8
- 1msl
- 2por
- 2jk2
- 1id1
- 2wfh
- 3ceq



1e9ra



# Using "fetch" command to retrieve and load PDB structures

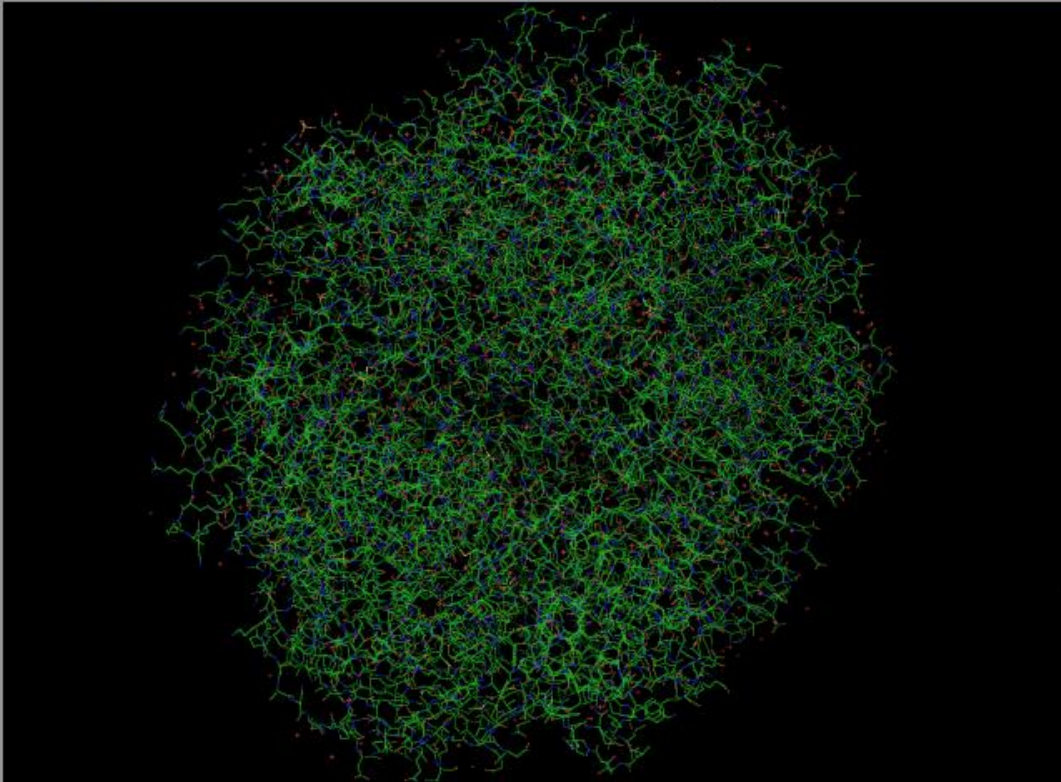
MacPyMOL File Edit Build Movie Display Setting Scene Mouse Wizard Help

MacPyMOL

Executive: Colored 20 atoms.  
You clicked /2zua//C/ALA`100/CA  
Selector: selection "active" defined with 15 atoms.  
PyMOL>fetch 1e9r

```
HEADER    COUPLING PROTEIN                26-OCT-00   1E9R
TITLE     BACTERIAL CONJUGATIVE COUPLING PROTEIN TRWBDELTA70.
TITLE     2 TRIGONAL FORM IN COMPLEX WITH SULPHATE.
COMPND    MOL_ID: 1;
COMPND    2 MOLECULE: CONJUGAL TRANSFER PROTEIN TRWB;
```

PyMOL> \_\_\_\_\_



all A S H L C  
1e9r A S H L C

Mouse Mode  
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  
Frame [ 1/ 11] 1/sec

PyMOL>\_



# Switching to cartoon view, using Show (S button) as cartoon

MacPyMOL File Edit Build Movie Display Setting Scene Mouse Wizard Help

MacPyMOL

Executive: Colored 20 atoms.  
You clicked /2zua//C/ALA`100/CA  
Selector: selection "active" defined with 15 atoms.  
PyMOL>fetch 1e9r  
HEADER COUPLING PROTEIN 26-OCT-00 1E9R  
TITLE BACTERIAL CONJUGATIVE COUPLING PROTEIN TRWBDELTA70.  
TITLE 2 TRIGONAL FORM IN COMPLEX WITH SULPHATE.  
COMPND MOL\_ID: 1;  
COMPND 2 MOLECULE: CONJUGAL TRANSFER PROTEIN TRWB;

PyMOL>

all A S H L C  
1e9r As: Show:  
lines as  
sticks lines  
ribbon sticks  
cartoon ribbon  
label cartoon  
cell label  
nonbonded cell  
dots nonbonded  
spheres dots  
nb\_spheres spheres  
mesh nb\_spheres  
surface mesh  
surface  
organic  
main chain  
side chain  
disulfides

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

Selecting Residues  
Frame [ 1 / 11 9/sec

# Cartoon view result

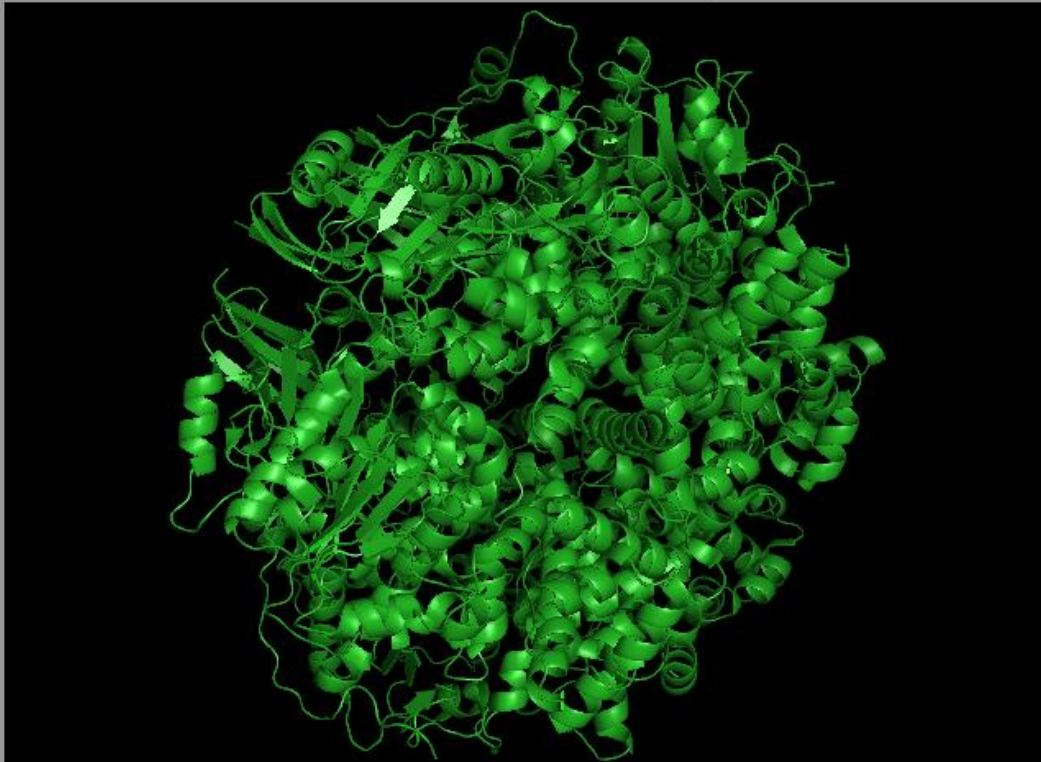
MacPyMOL File Edit Build Movie Display Setting Scene Mouse Wizard Help

MacPyMOL

Executive: Colored 20 atoms.  
You clicked /2zua//C/ALA`100/CA  
Selector: selection "active" defined with 15 atoms.  
PyMOL>fetch 1e9r

```
HEADER    COUPLING PROTEIN                26-OCT-00   1E9R
TITLE     BACTERIAL CONJUGATIVE COUPLING PROTEIN TRWBDELTA70.
TITLE     2 TRIGONAL FORM IN COMPLEX WITH SULPHATE.
COMPND    MOL_ID: 1;
COMPND    2 MOLECULE: CONJUGAL TRANSFER PROTEIN TRWB;
```

PyMOL> \_\_\_\_\_



all A S H L C  
1e9r A S H L C

Mouse Mode  
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  
Frame [ 1 / 11 ] 2/sec

PyMOL>\_

# Using Color (C) button

MacPyMOL File Edit Build Movie Display Setting Scene Mouse Wizard Help

MacPyMOL

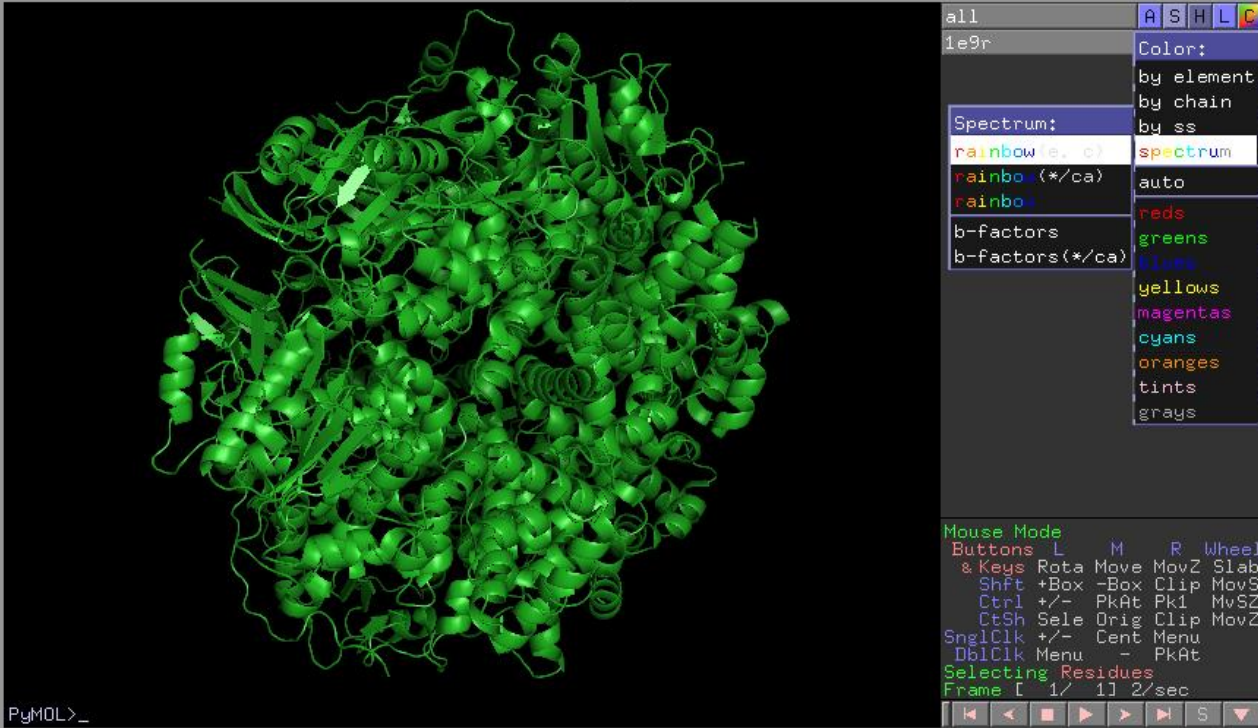
Executive: Colored 20 atoms.  
You clicked /2zua//C/ALA`100/CA  
Selector: selection "active" defined with 15 atoms.

PyMOL>fetch 1e9r  
HEADER COUPLING PROTEIN 26-OCT-00 1E9R  
TITLE BACTERIAL CONJUGATIVE COUPLING PROTEIN TRWBDELTA70.  
TITLE 2 TRIGONAL FORM IN COMPLEX WITH SULPHATE.  
COMPND MOL\_ID: 1;  
COMPND 2 MOLECULE: CONJUGAL TRANSFER PROTEIN TRWB;

PyMOL>

all A S H L C  
1e9r Color:  
by element  
by chain  
by ss  
Spectrum:  
rainbow(s, c) spectrum  
rainbow(\*/\*ca) auto  
rainbow reds  
b-factors greens  
b-factors(\*/\*ca) blues  
yellows  
magentas  
cyans  
oranges  
tints  
grays

Mouse Mode  
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  
Frame [ 1 / 1 ] 2/sec





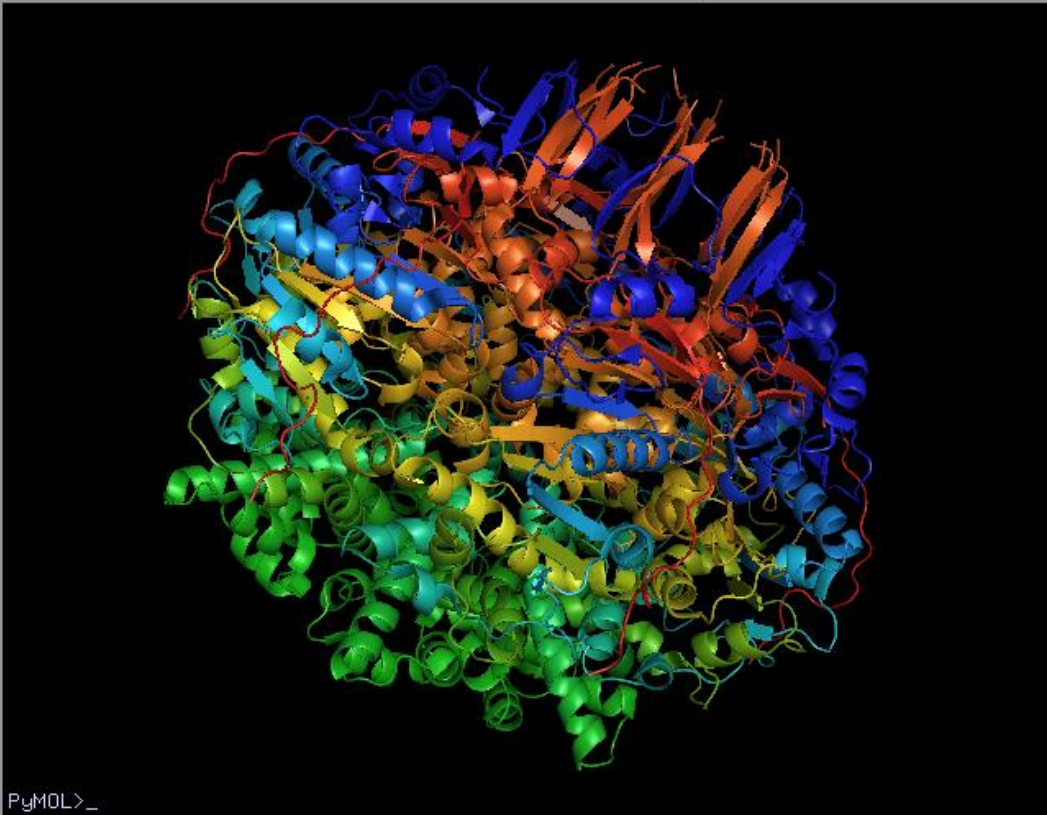
# Revising the color

MacPyMOL File Edit Build Movie Display Setting Scene Mouse Wizard Help

MacPyMOL

Executive: Colored 20 atoms.  
You clicked /2zua//C/ALA`100/CA  
Selector: selection "active" defined with 15 atoms.  
PyMOL>fetch 1e9r  
HEADER COUPLING PROTEIN 26-OCT-00 1E9R  
TITLE BACTERIAL CONJUGATIVE COUPLING PROTEIN TRWBDELTA70.  
TITLE 2 TRIGONAL FORM IN COMPLEX WITH SULPHATE.  
COMPND MOL\_ID: 1;  
COMPND 2 MOLECULE: CONJUGAL TRANSFER PROTEIN TRWB;

PyMOL>



The image shows a 3D ribbon representation of a protein structure. The protein is composed of two chains, each colored differently to distinguish them. The left chain is primarily blue and green, while the right chain is primarily orange and red. The structure is complex, with many loops and helices. The background is black.

all A S H L C  
1e9r Color:  
By Chain: by element  
by chain(e, c) by chain  
by chain(\*/\*ca) by ss  
by chain spectrum  
chainbows auto  
reds  
greens  
blues  
yellows  
magentas  
cyans  
oranges  
tints  
grays

Mouse Mode  
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  
Frame [ 1 / 1 ] 6/sec

PyMOL>\_

# Rotating the image for a different perspective (using the mouse)

MacPyMOL

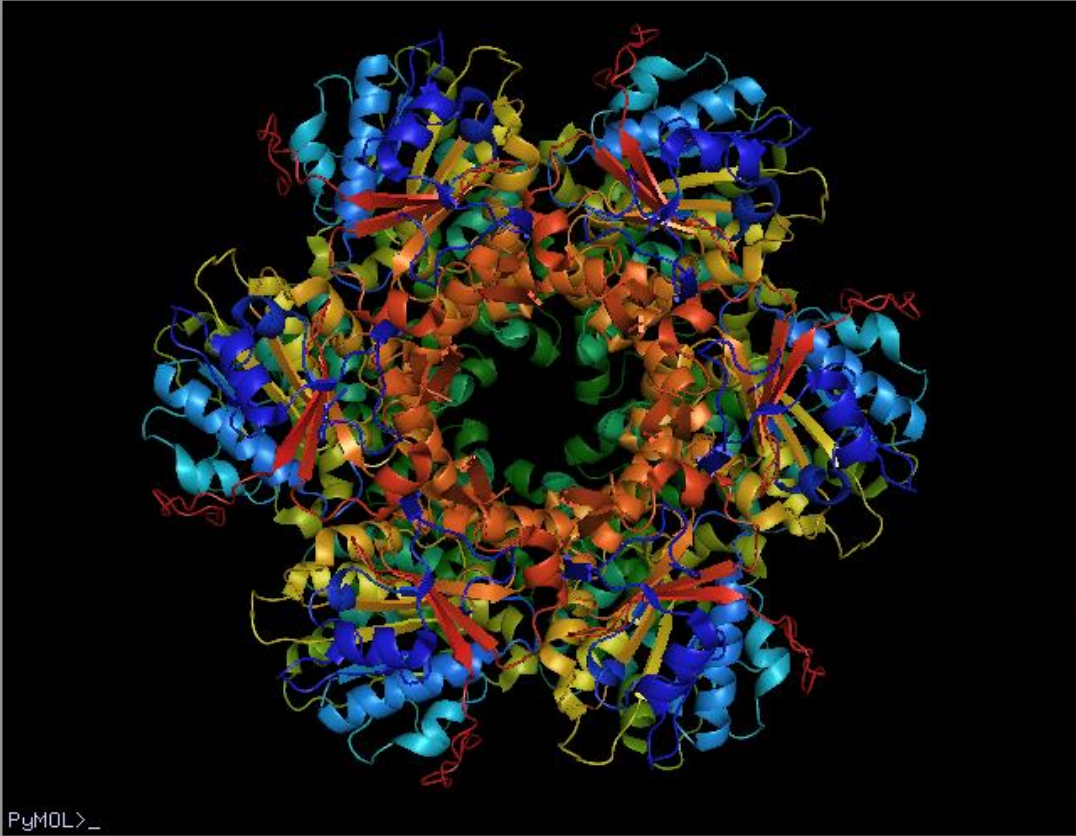
Executive: Colored 20 atoms.  
You clicked /2zua//C/ALA`100/CA  
Selector: selection "active" defined with 15 atoms.

PyMOL>fetch 1e9r

```
HEADER    COUPLING PROTEIN                               26-OCT-00   1E9R
TITLE     BACTERIAL CONJUGATIVE COUPLING PROTEIN TRWBDELTA70.
TITLE     2 TRIGONAL FORM IN COMPLEX WITH SULPHATE.
COMPND    MOL_ID: 1;
COMPND    2 MOLECULE: CONJUGAL TRANSFER PROTEIN TRWB;
```

PyMOL> \_\_\_\_\_

all A S H L C  
1e9r A S H L C



Mouse Mode  
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  
Frame [ 1/ 1] 14/sec

PyMOL>\_



# Enhancing image quality

The screenshot shows the MacPyMOL application window. The 'Display' menu is open, showing various options. The 'Quality' submenu is also open, highlighting 'Maximum Quality'. The main window displays a 3D ribbon model of a protein structure, colored by residue type (blue, orange, green, red). The interface includes a menu bar at the top, a toolbar with buttons like 'Reset', 'Zoom', 'Draw', 'Ray', 'Rock', 'Unpick', 'Hide Sele', 'Get View', and 'MClear'. A command line at the bottom shows 'PyMOL>'. The right side of the window has a list of loaded files and a 'Mouse Mode' section with keyboard shortcuts.

MacPyMOL File Edit Build Movie **Display** Setting Scene Mouse Wizard Help

Sequence On  
Sequence Mode  
Stereo On  
Stereo  
Zoom  
Clip  
Background  
Color Space  
**Quality**  
Orthoscopic View  
Use Display Lists  
Show Valences  
✓ Smooth Lines  
✓ Depth Cue  
Two Sided Lighting  
✓ Specular Reflections

Maximum Performance  
Reasonable Performance  
Reasonable Quality  
**Maximum Quality**

PyMOL> fetch 1e9r  
HEADER COUPLING P  
TITLE BACTERIAL  
TITLE 2 TRIGONAL  
COMPND MOL\_ID: 1;  
COMPND 2 MOLECULE:  
TRWB;

all A S H L C  
1e9r A S H L C

Mouse Mode  
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

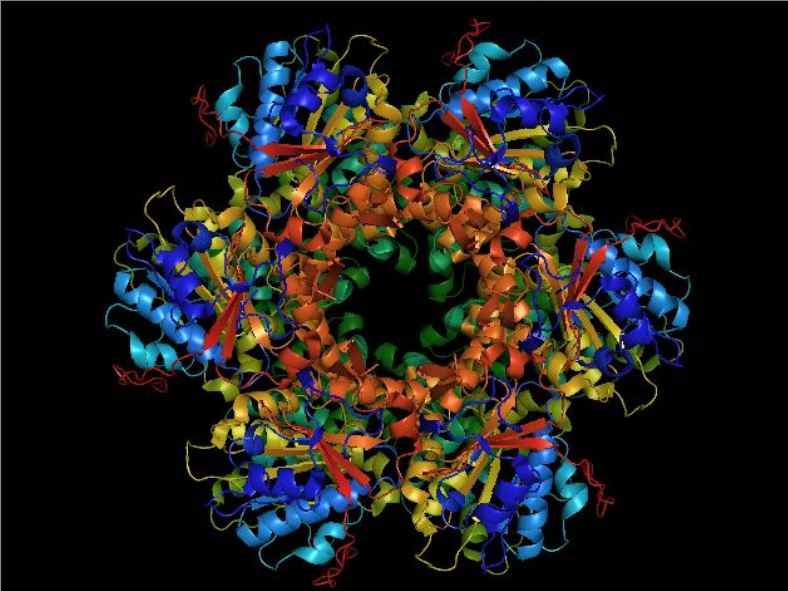
Selecting Residues  
Frame [ 1 / 11 0/sec

# Using the S button to Show surface

MacPyMOL

COMPND 6 MUTATION: YES  
ObjectMolecule: Read secondary structure assignments.  
ObjectMolecule: Read crystal symmetry information.  
Symmetry: Found 6 symmetry operators.  
CmdLoad: "/1e9r.pdb" loaded as "1e9r".  
PyMOL>rebuild  
Setting: orthoscopic set to on.  
Setting: two\_sided\_lighting set to on.  
Setting: orthoscopic set to off.

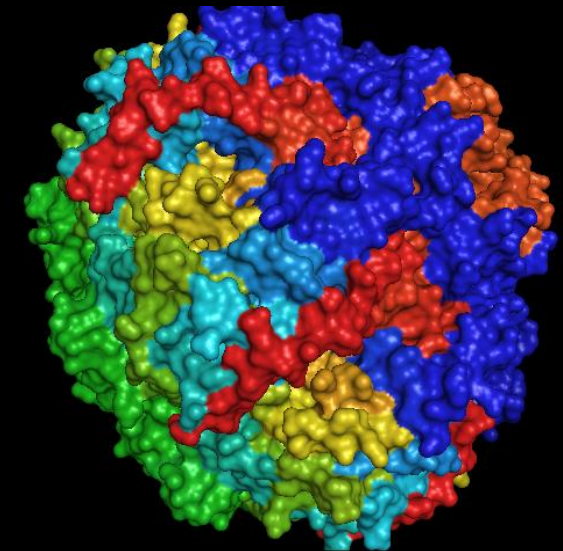
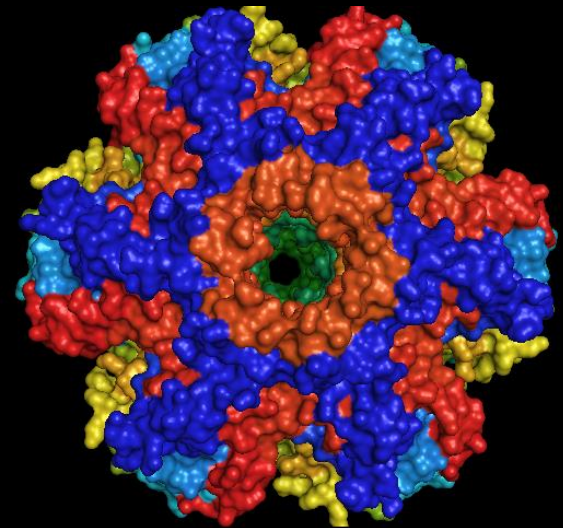
PyMOL>



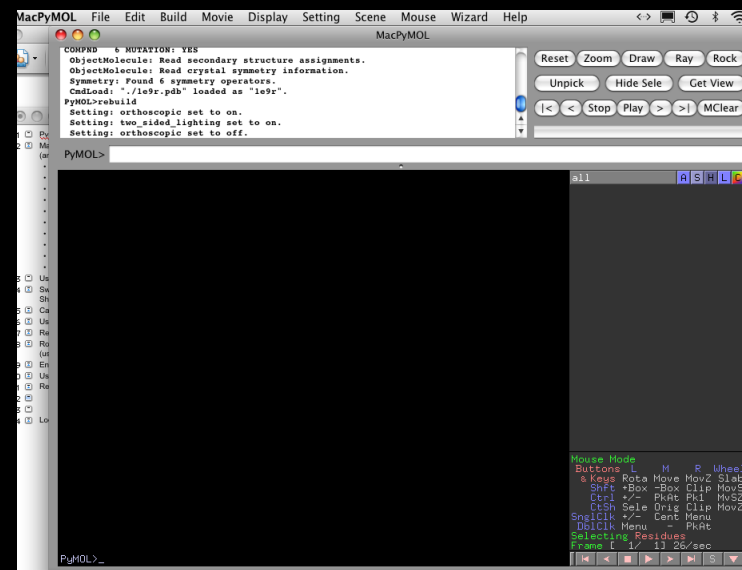
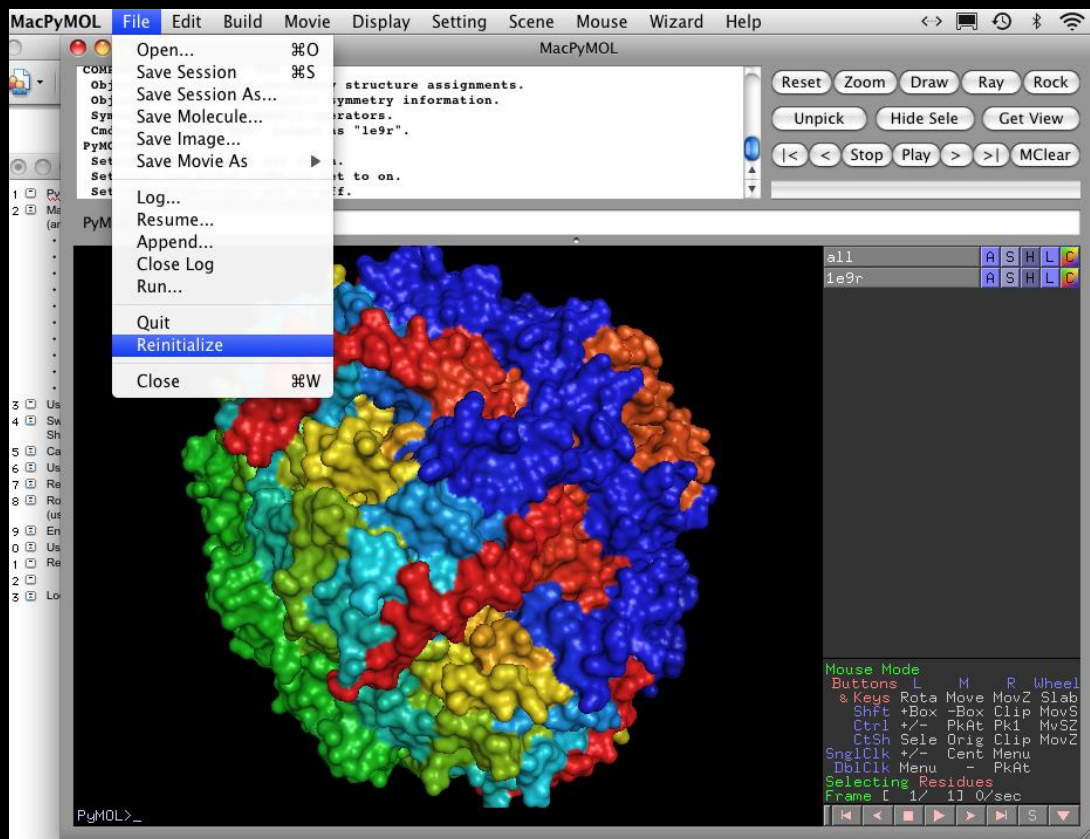
all | A S H L C  
1e9r | Show:  
as  
lines  
sticks  
ribbon  
cartoon  
label  
cell  
nonbonded  
dots  
spheres  
nb\_spheres  
mesh  
surface  
organic  
main chain  
side chain  
disulfides

Mouse Mode  
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  
Frame 1 1/ 11 11/sec

PyMOL>



# Reinitializing to start afresh



Result



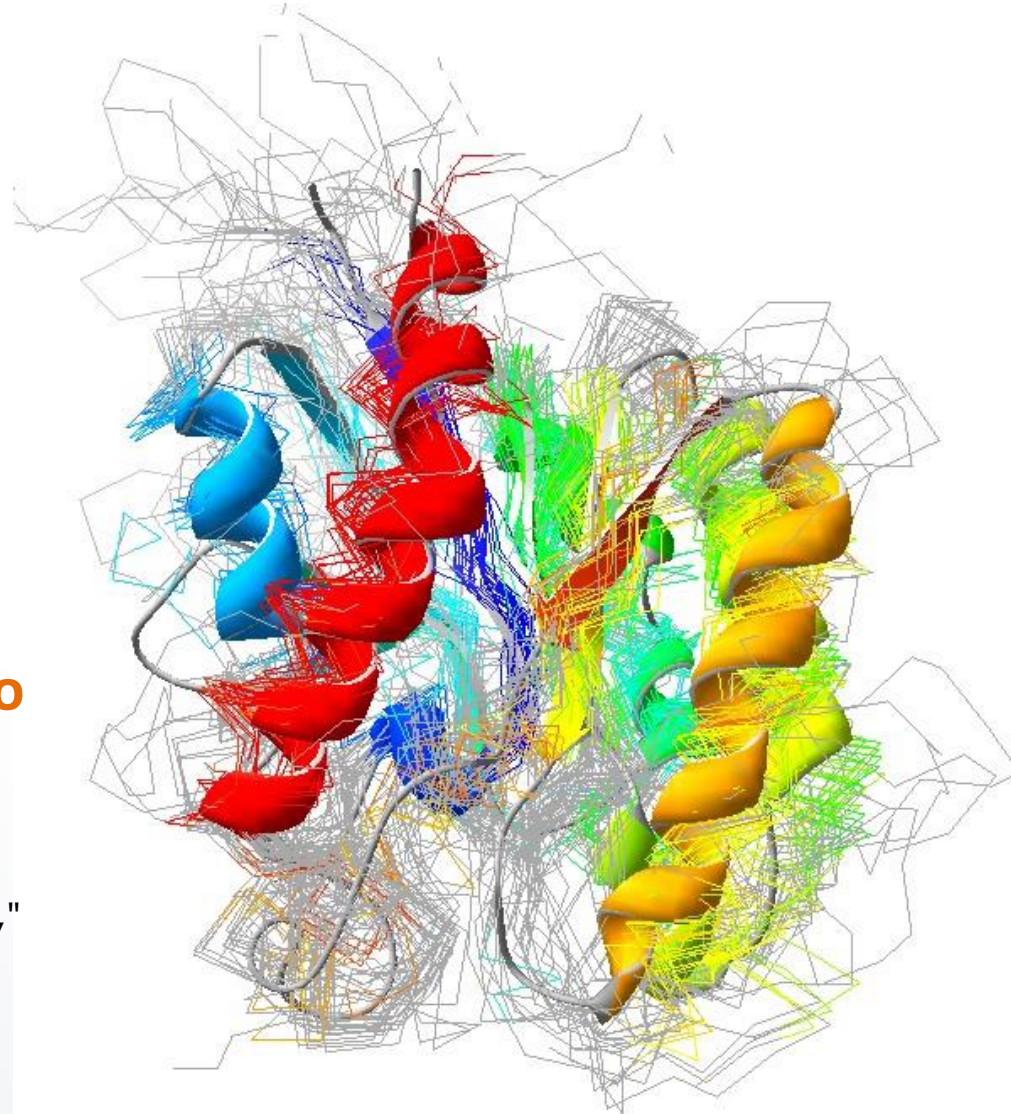
# Paradox: modeling is not a real protein

**Ceci n'est pas une protéine.**

“... a model must be **wrong**, in some respects --- else it would be the thing itself. The trick is **to see ... where it is right.**”

**Henry A. Bent**

"Uses (and Abuses) of Models in Teaching Chemistry,"  
J. Chem. Ed. 1984 61, 774.



It was still the twelfth course,  
don't get dizzy yet

