Universitas Esa Unggul

Smart, Creative and Entrepreneurial

IBT 432 Aplikasi Bioinformatika

Visualisasi protein modelling

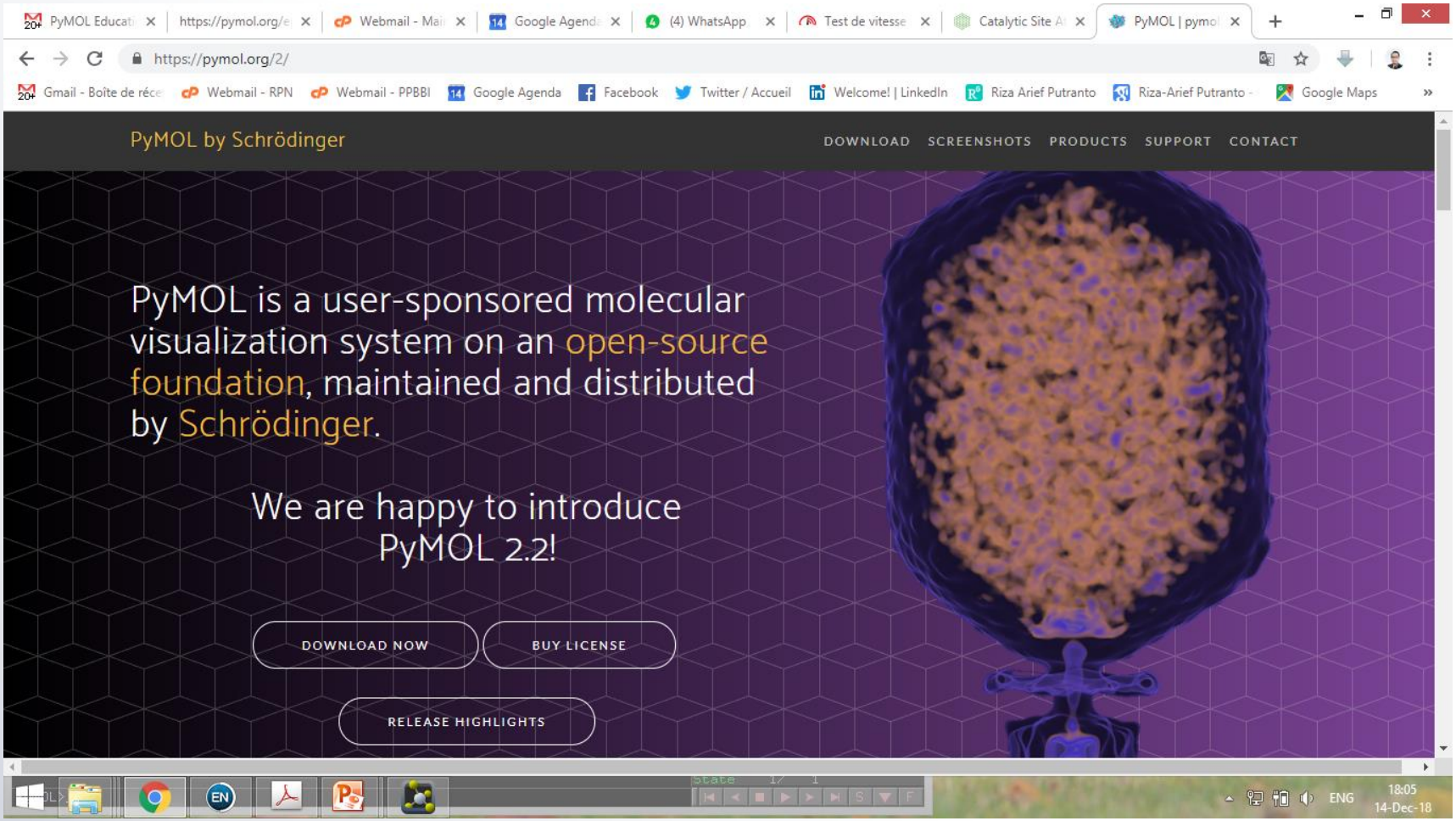
Riza Arief Putranto

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

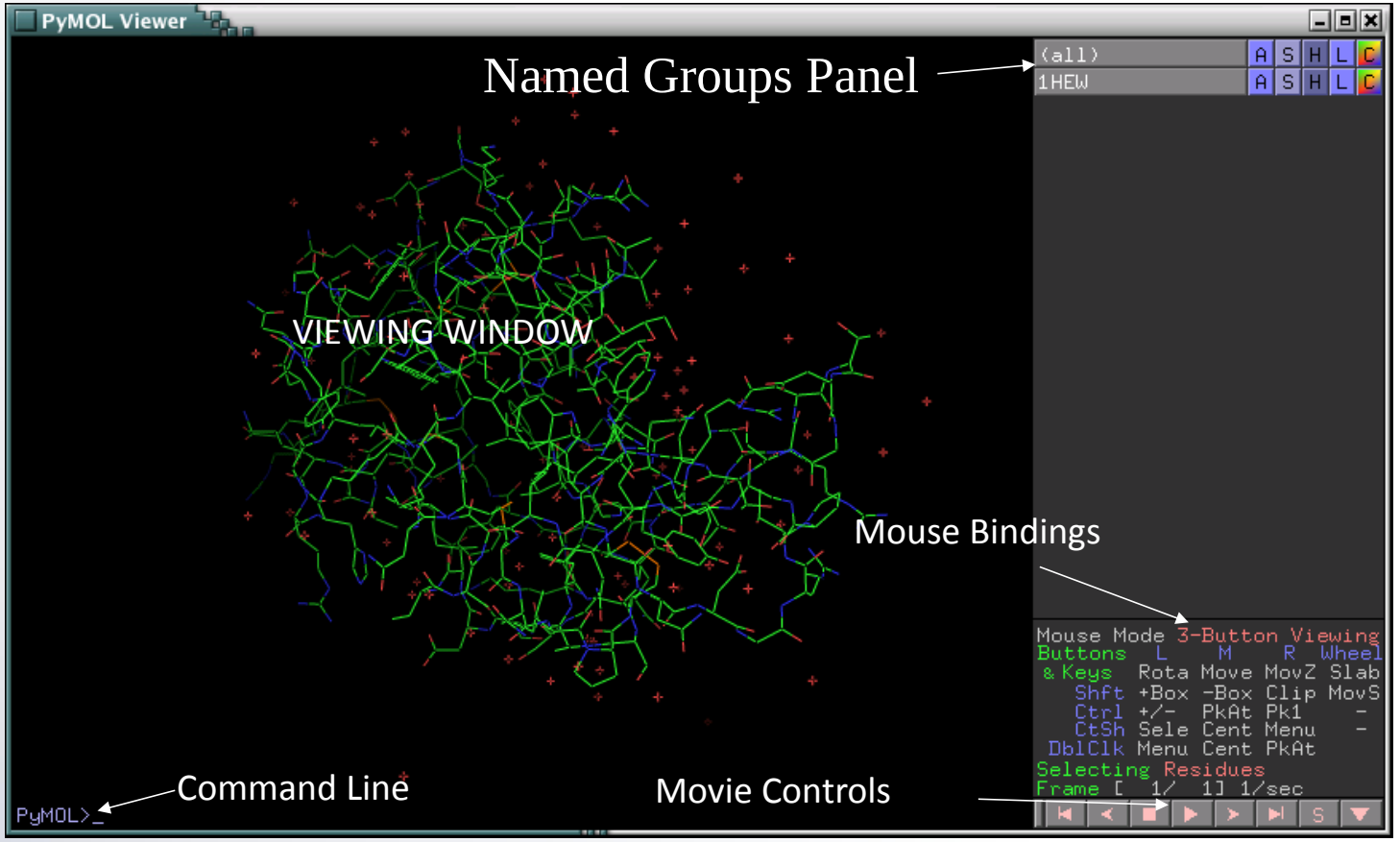
Visualization of protein model: PyMOL

http://www.pymol.org/

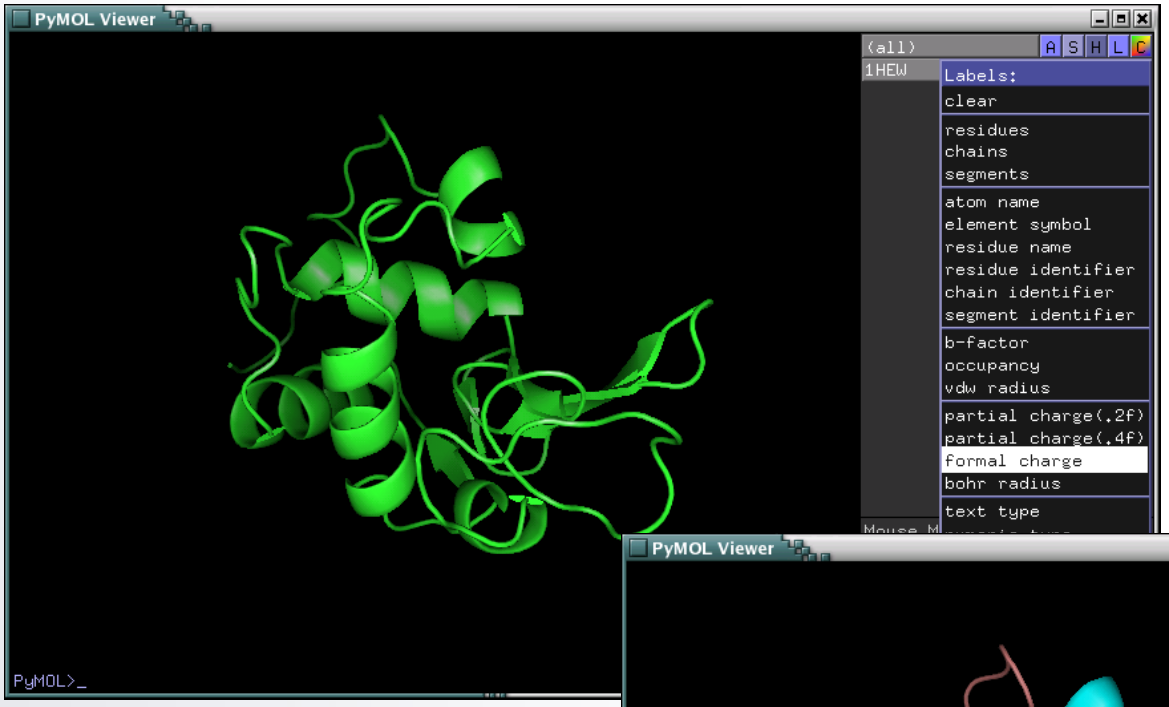


Visualization of protein model: PyMOL

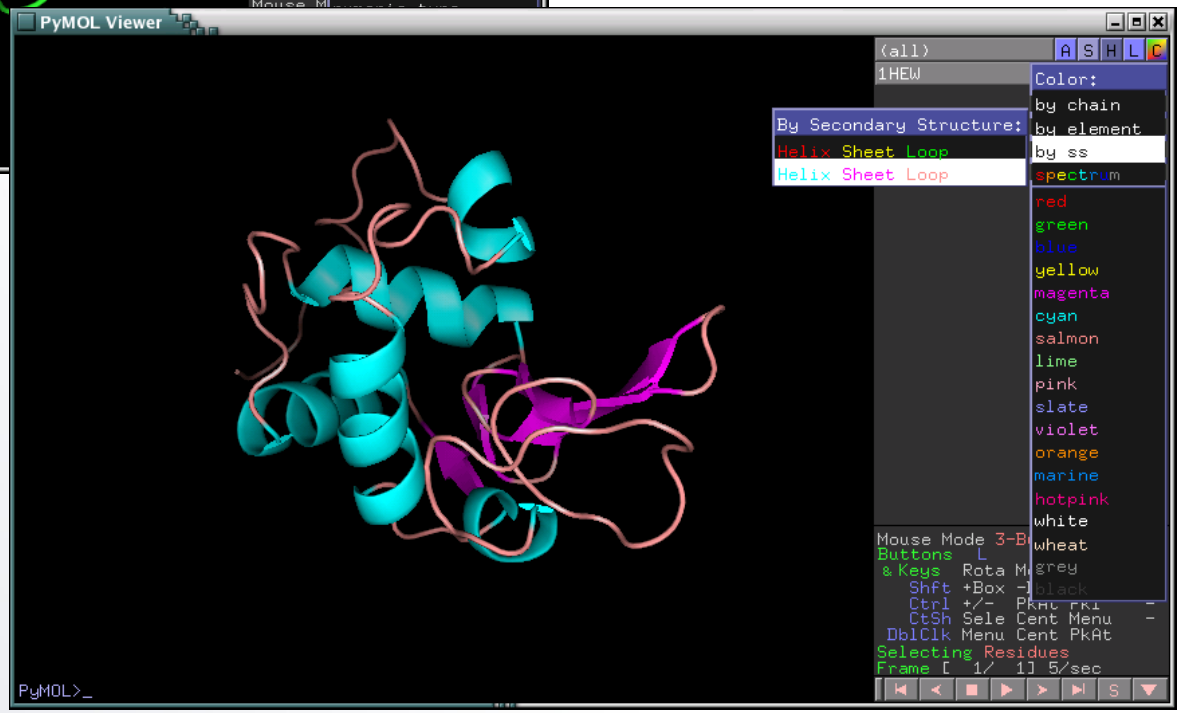
- **PyMOL** is a user-sponsored molecular **visualization system** on an open-source foundation, maintained and distributed by Schrödinger.



Play with PyMOL



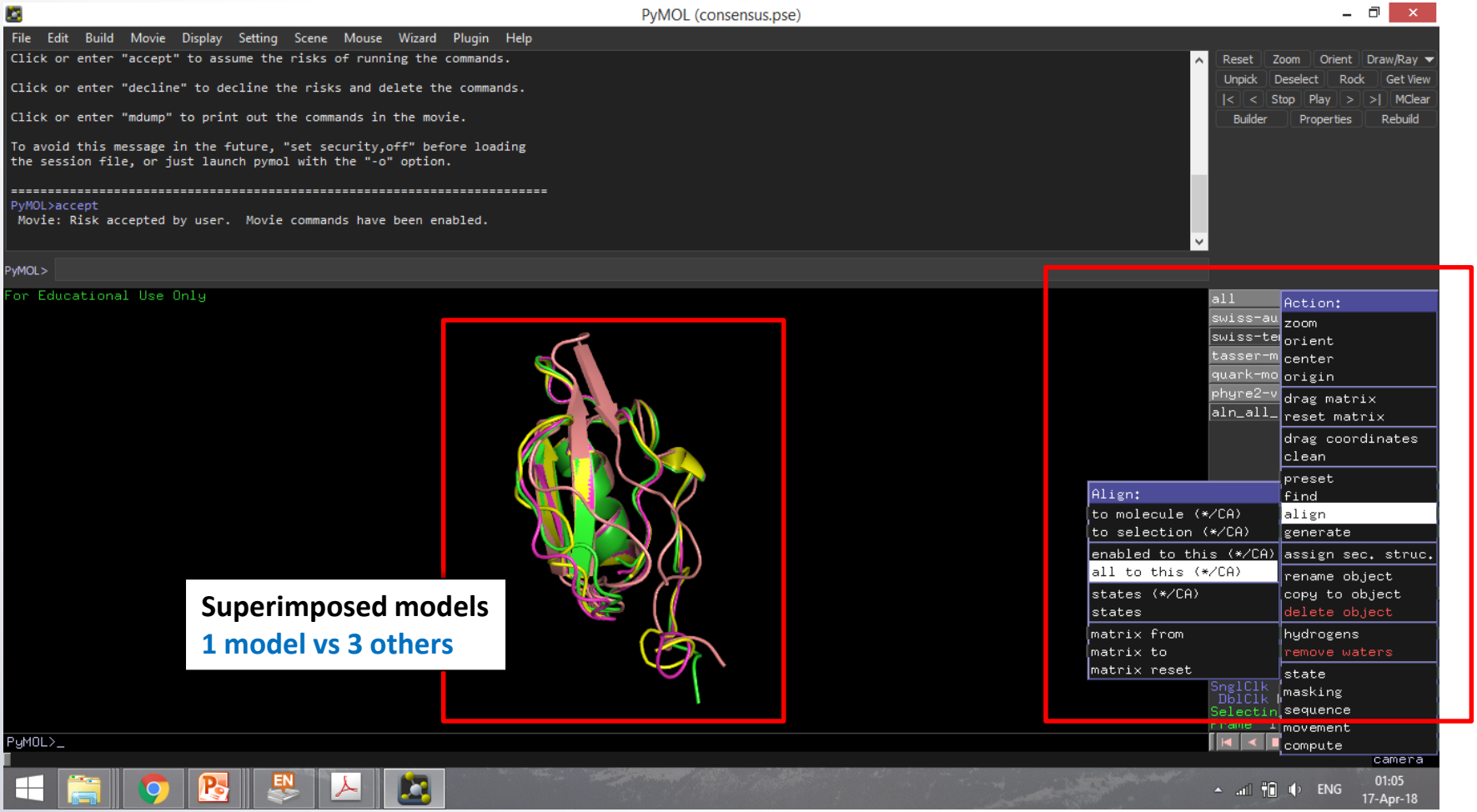
Label panel: residues, chains, segments



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



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.

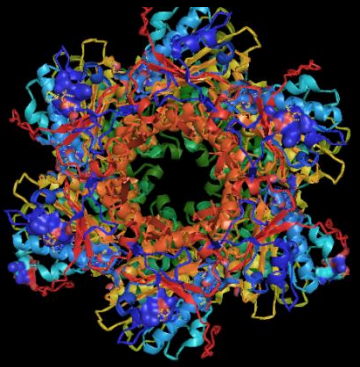
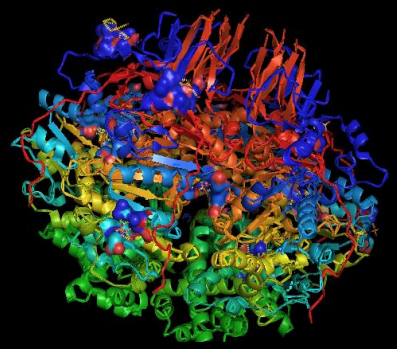
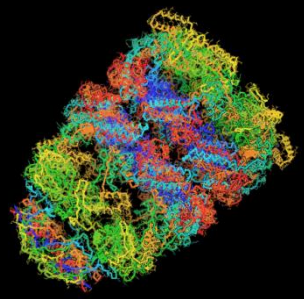
Defining residues and modifying their appearance

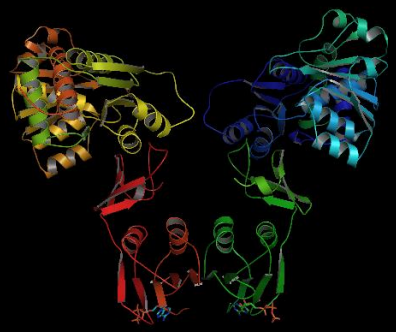
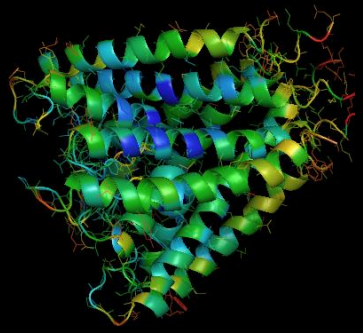
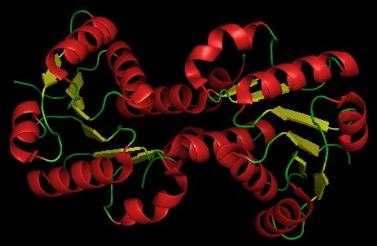
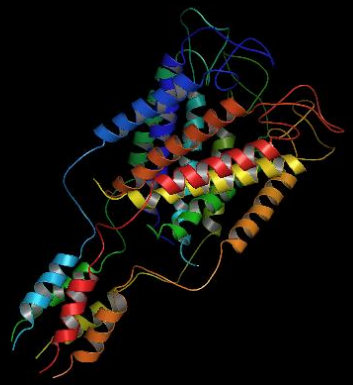
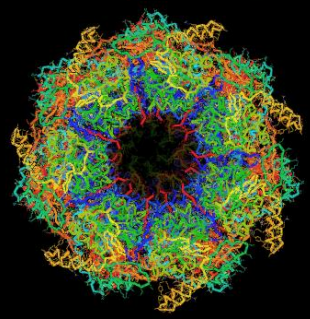
- **If you want to highlight certain residues, try defining them using "Select"**
  - "Select myresidues, resi 17-20,24" or
  - Select myresidues, resi 17+18+19+20+24"
  - The syntax does not allow spaces after commas or after the '+' sign
- **Once you have done this selection, you'll see that item on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

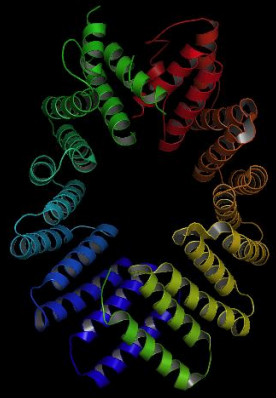
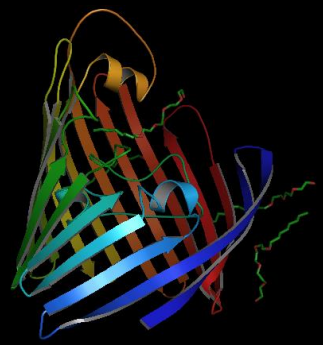
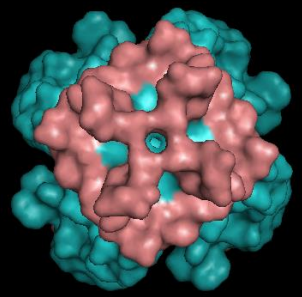
Match up the images to PDB IDs

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

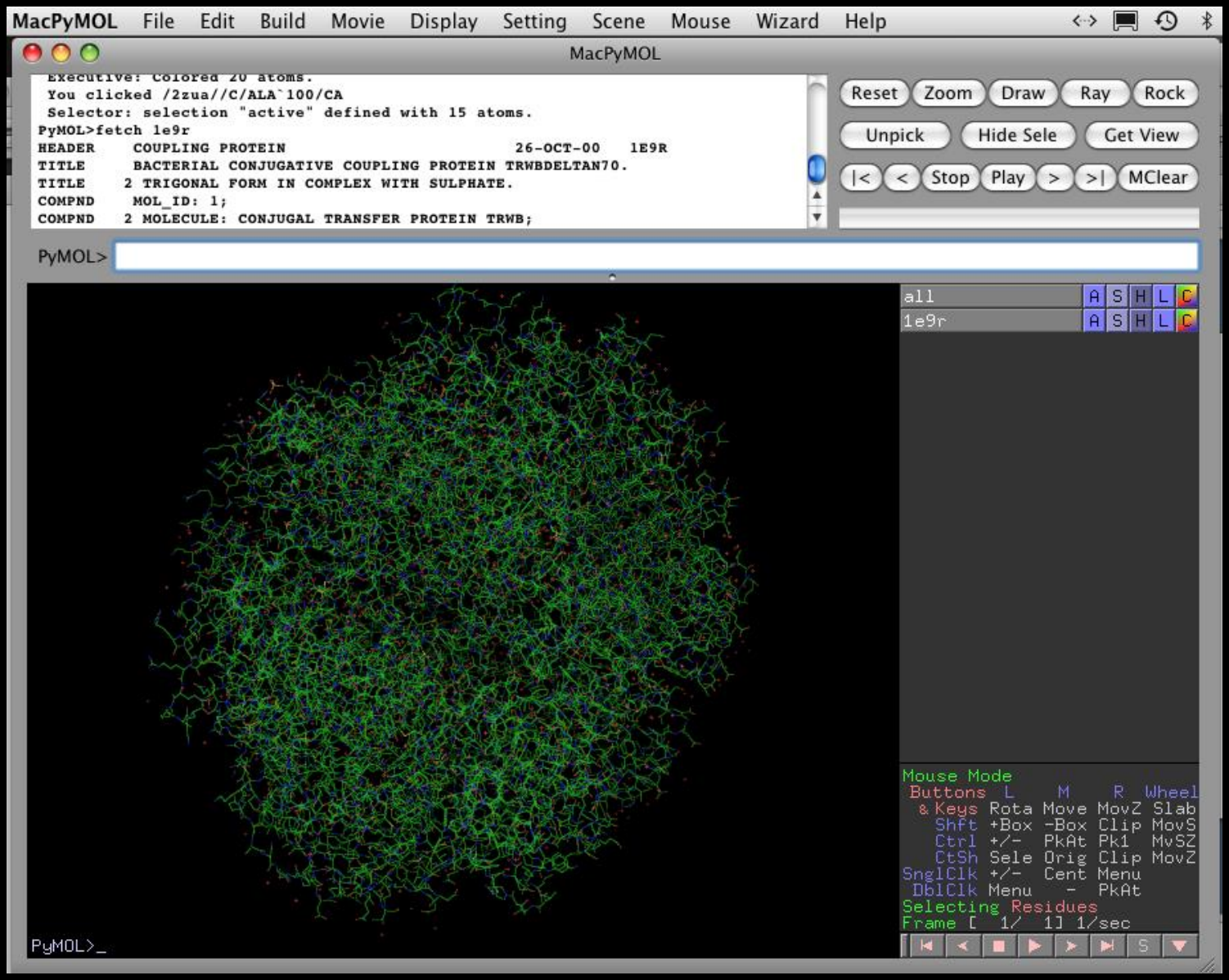
- 1e9ra
- 4at1
- 1aon
- 1bl8
- 1msl
- 2por
- 2jk2
- 1id1
- 2wfh
- 3ceq

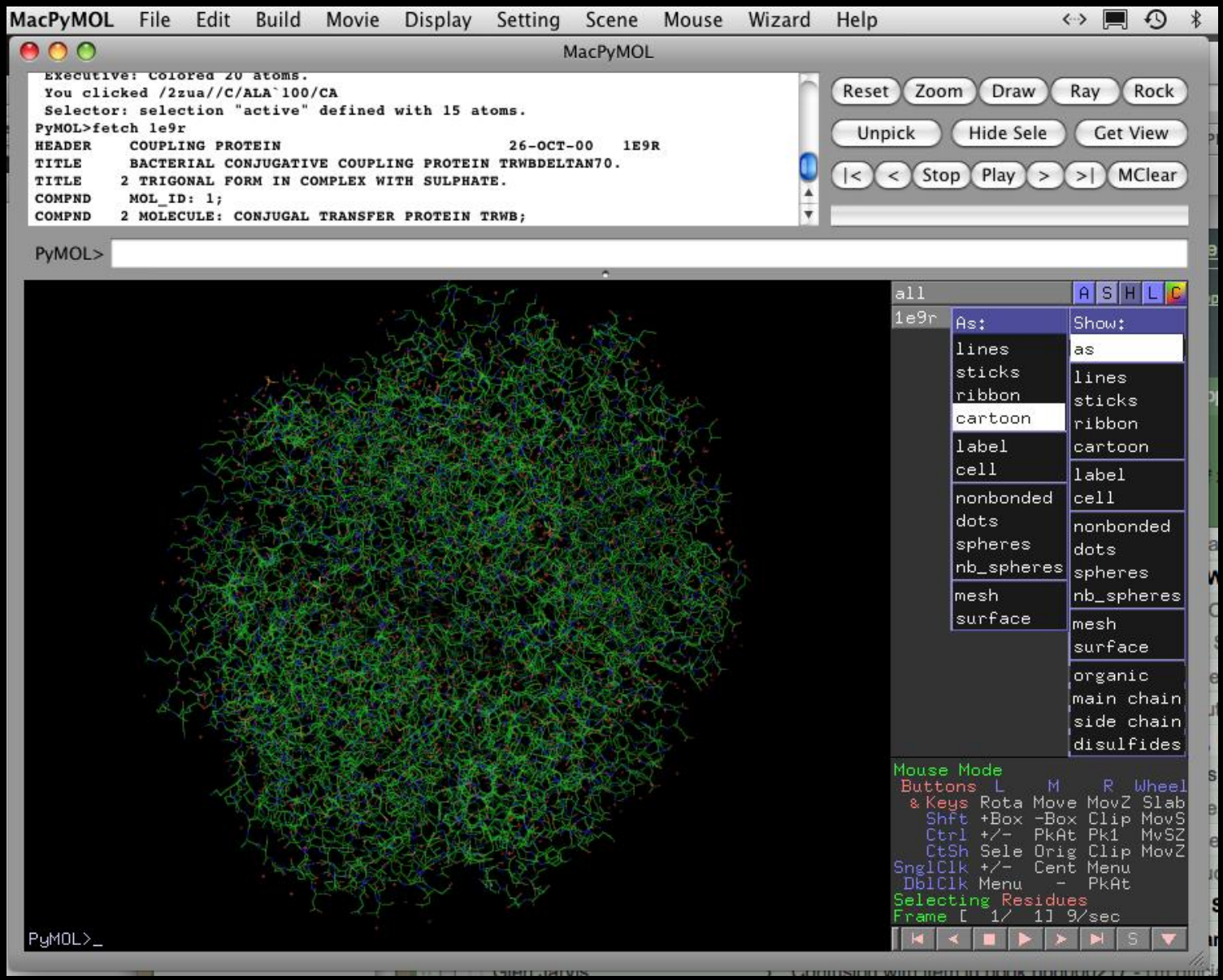






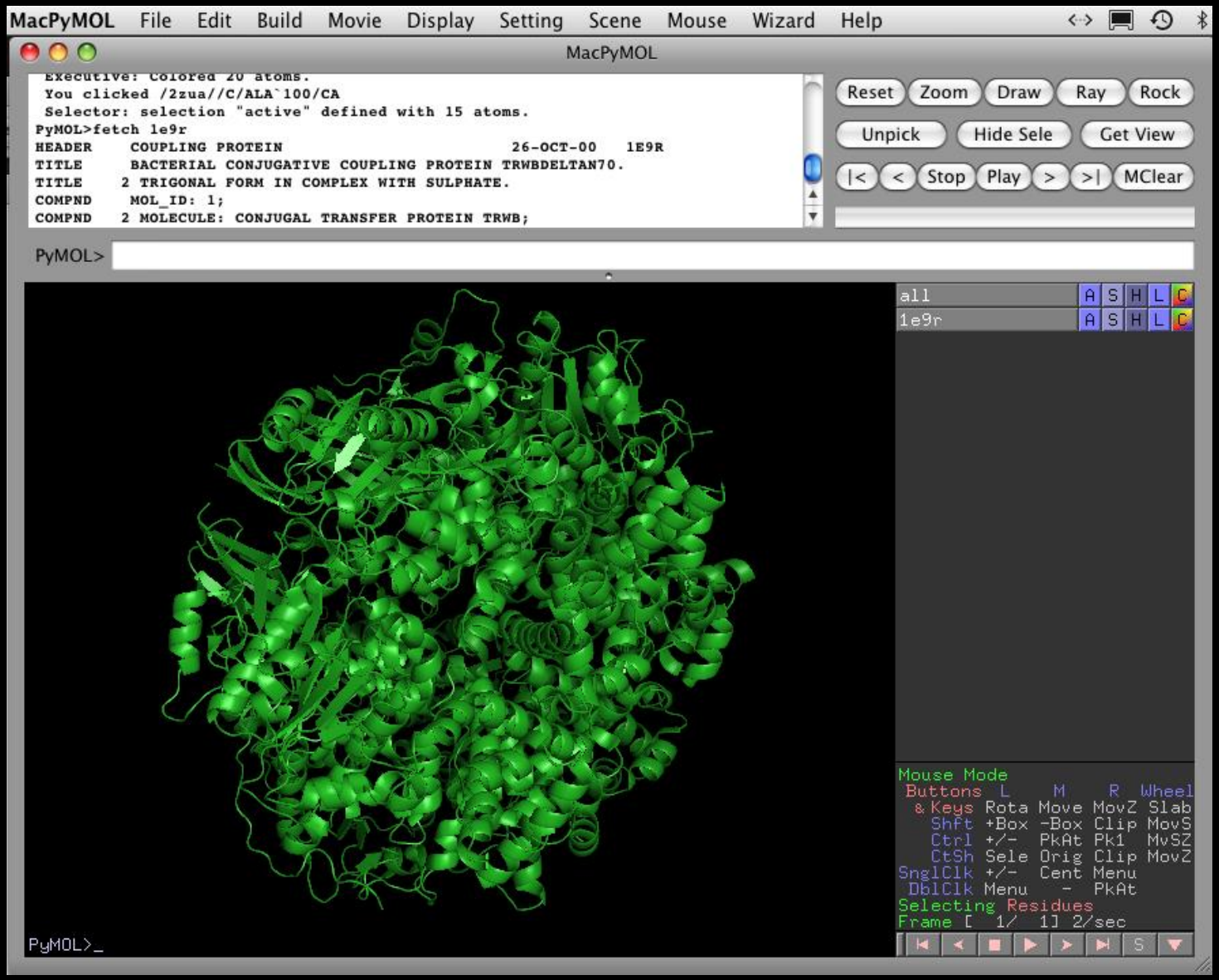
Using “fetch” command to retrieve and load PDB structures



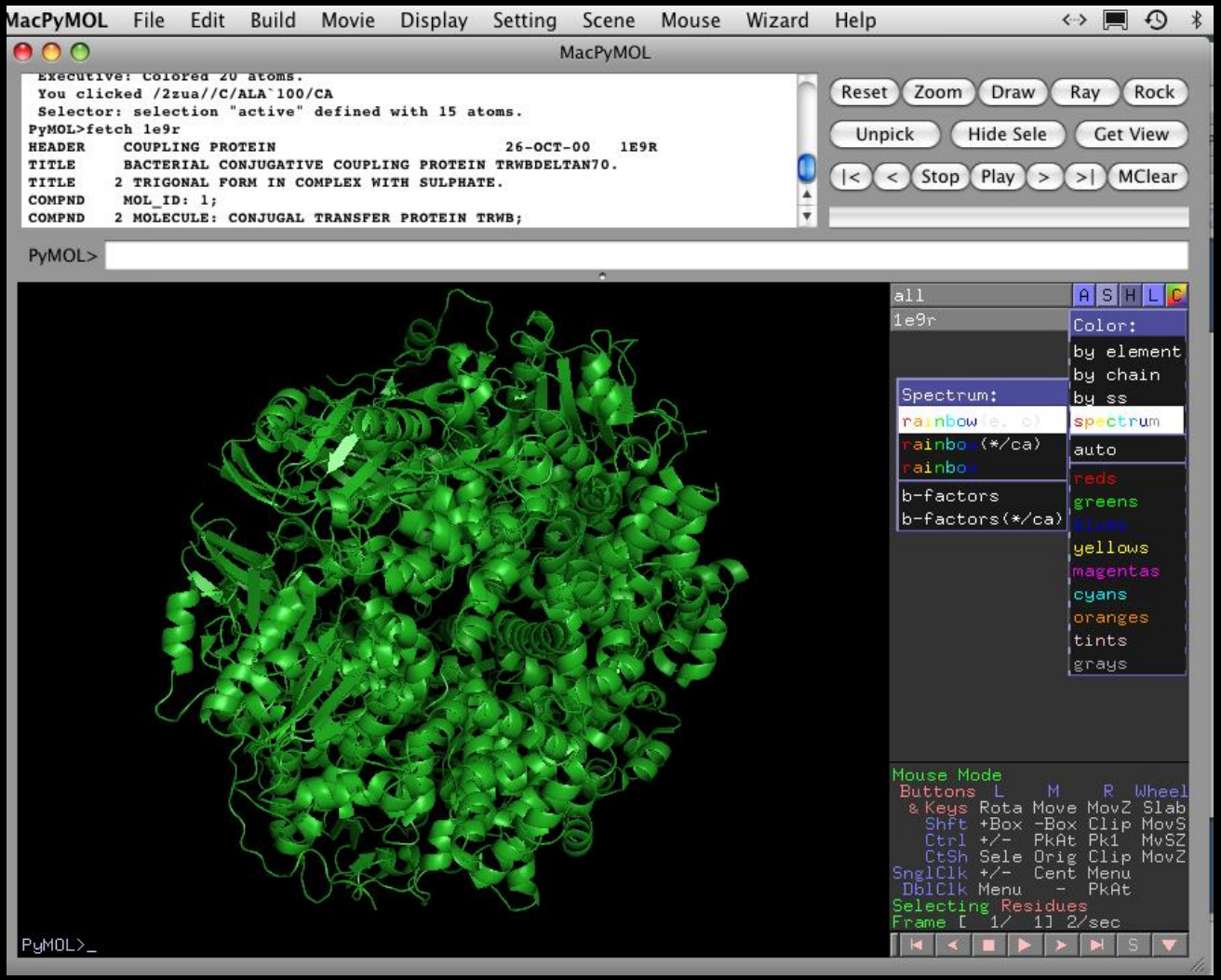
Switching to cartoon view, using Show (S button) as cartoon

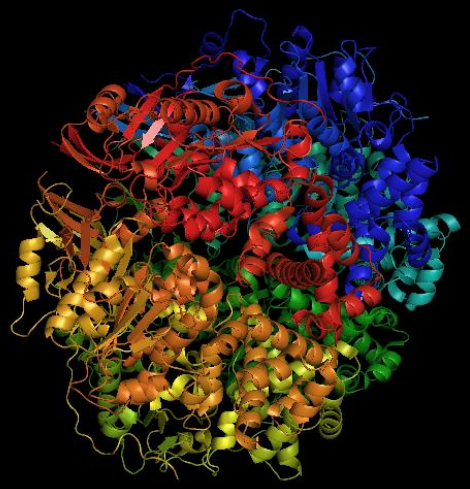


Cartoon view result

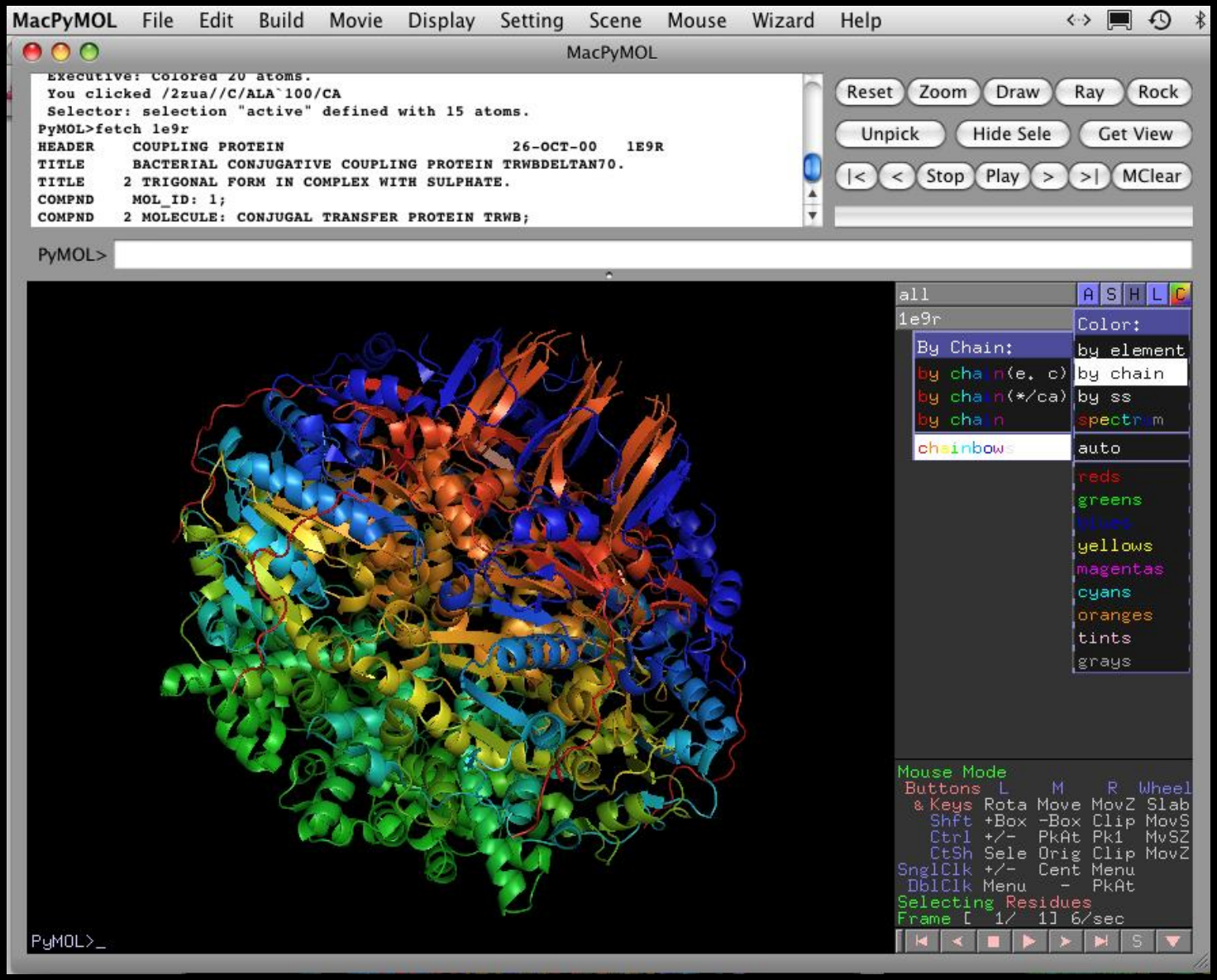


Using Color (C) button

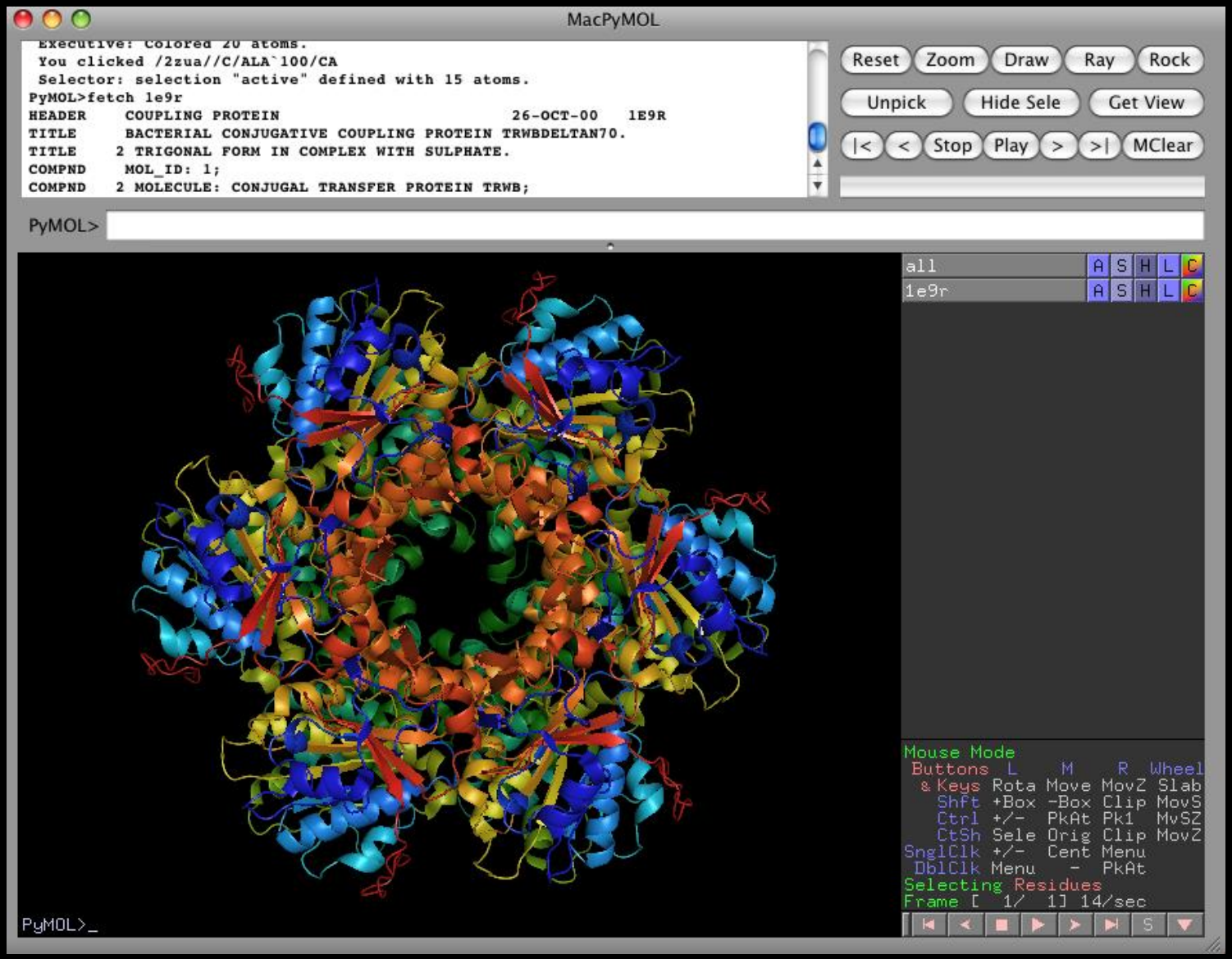




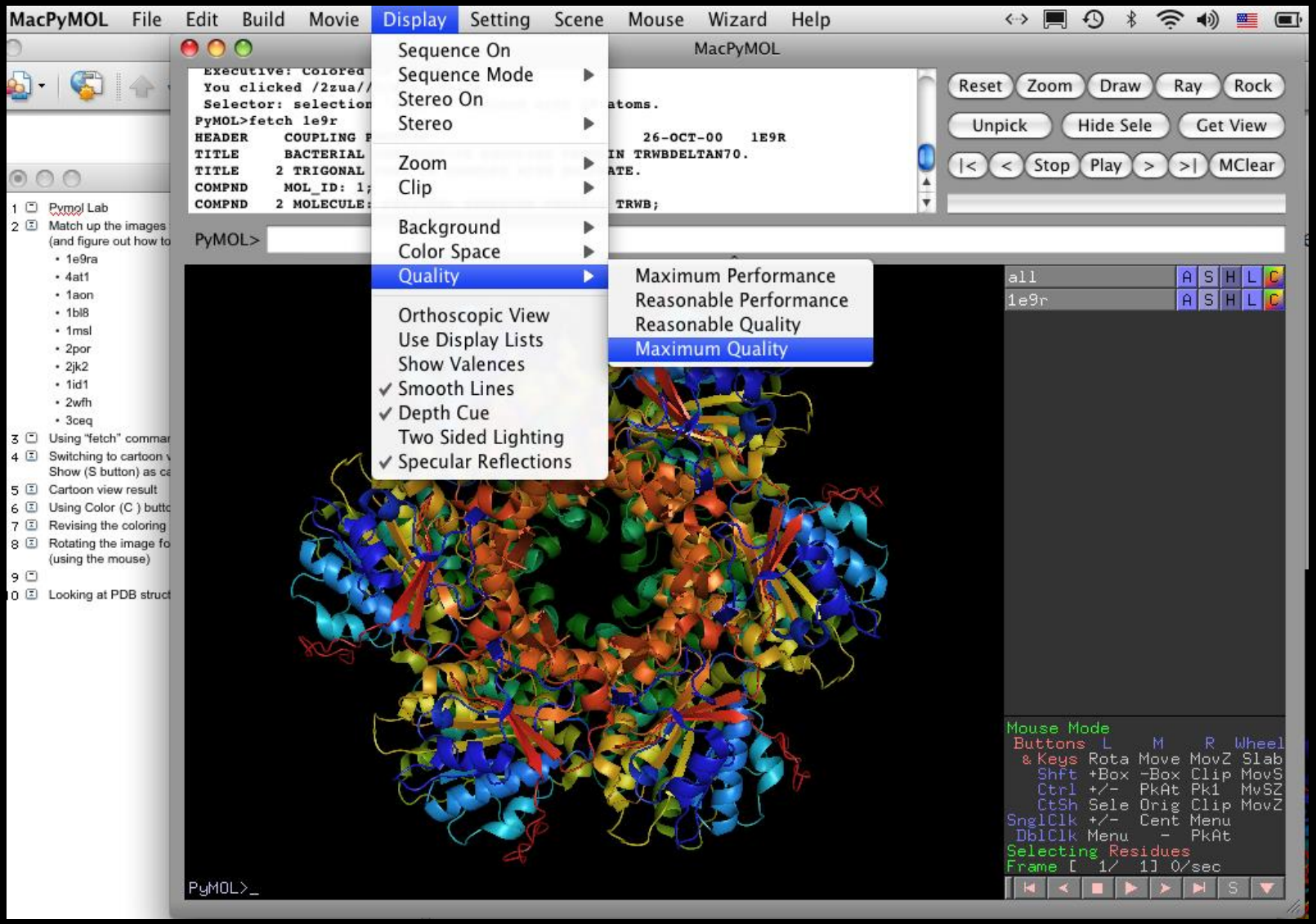
Revising the color



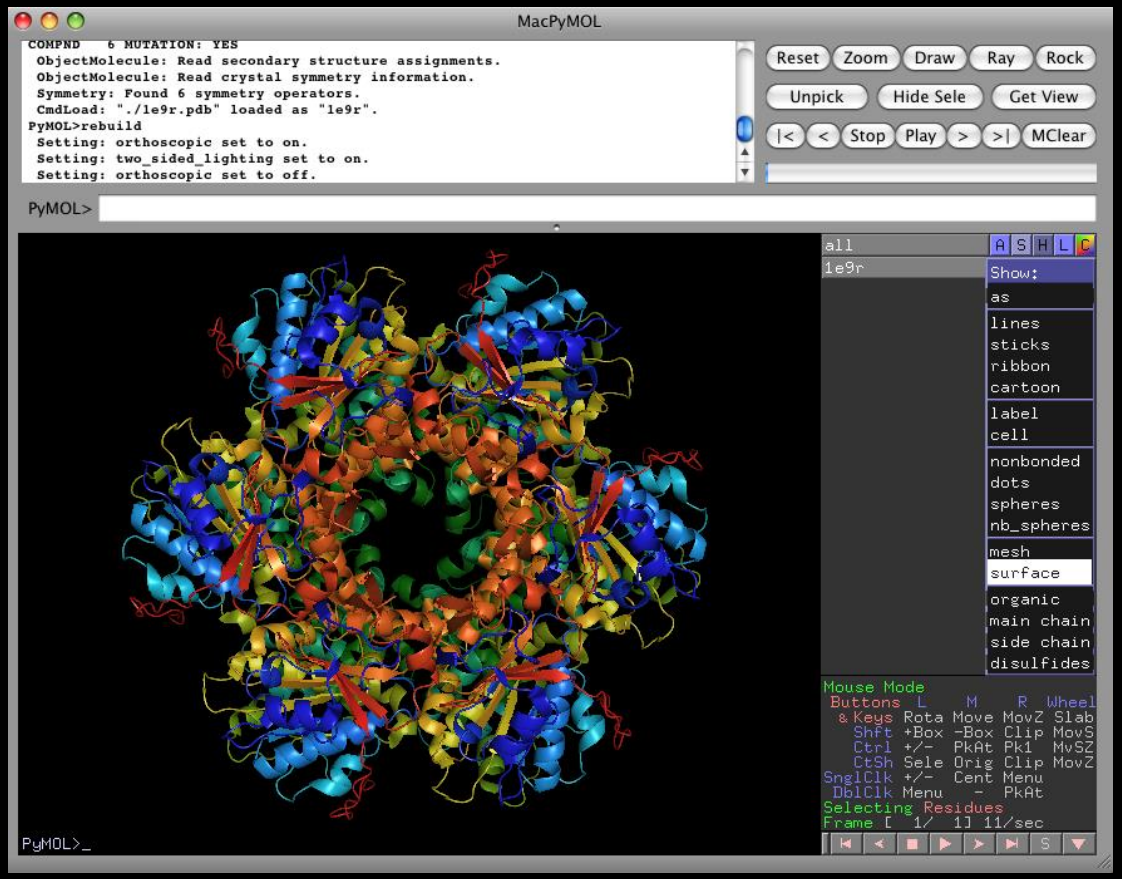
Rotating the image for a different perspective (using the mouse)

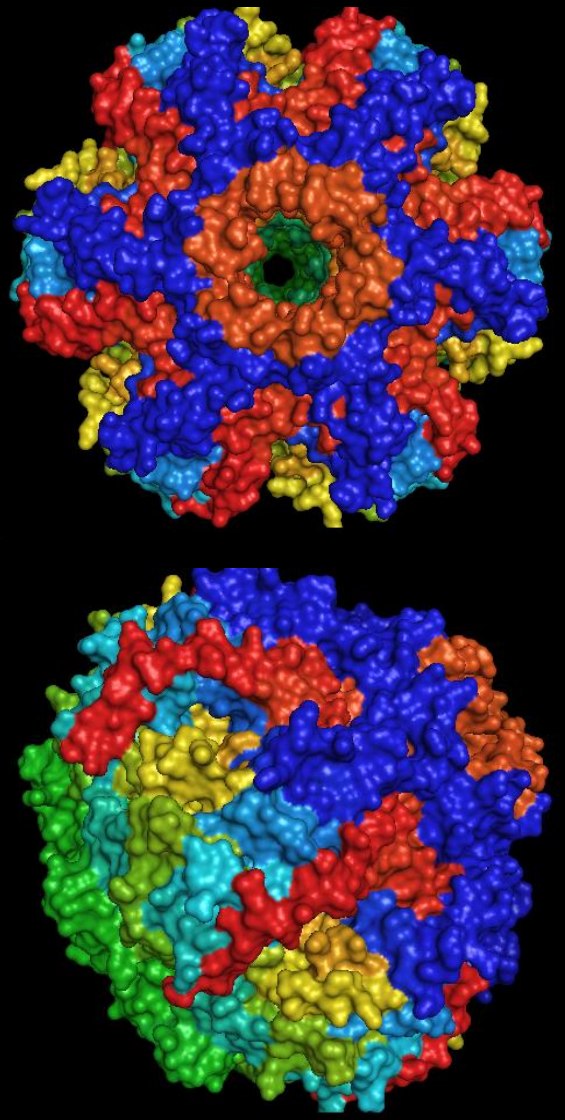


Enhancing image quality

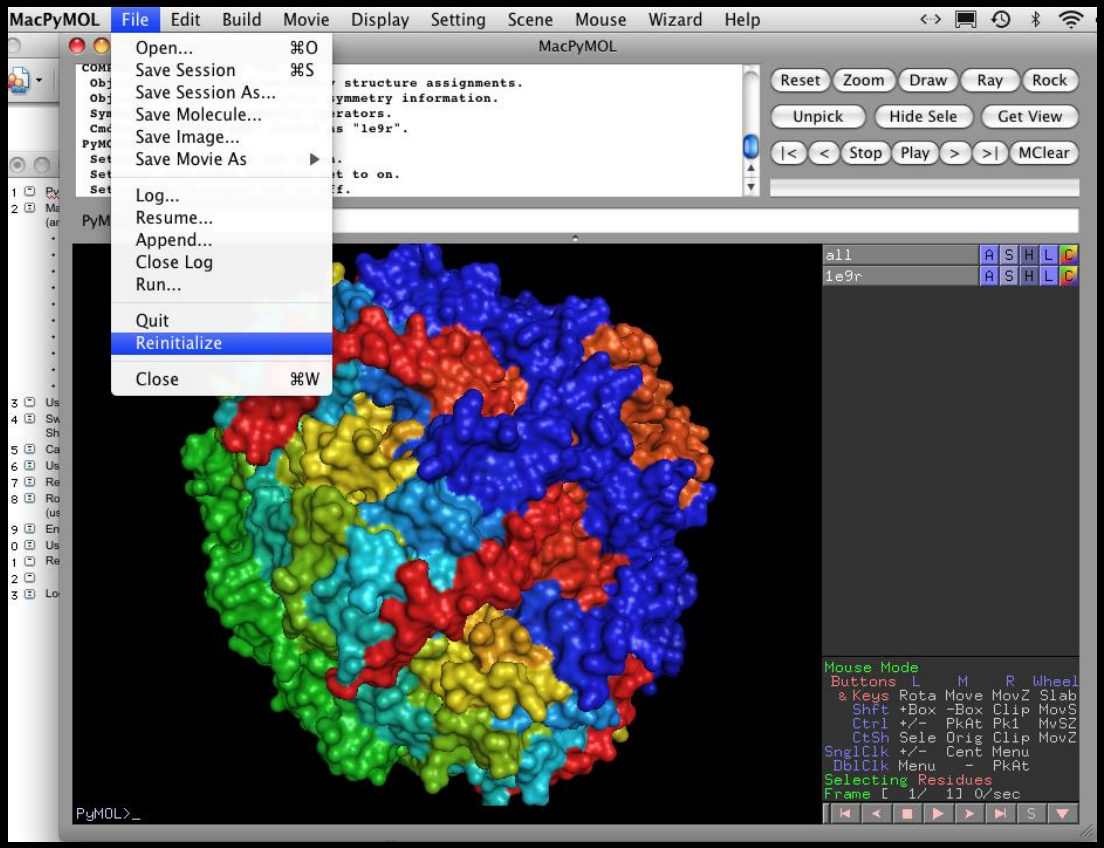


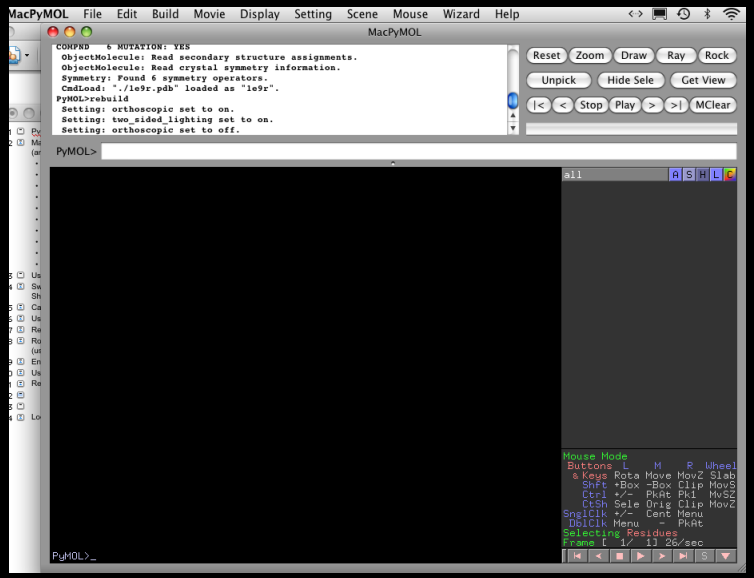
Using the S button to Show surface





Reinitializing to start afresh





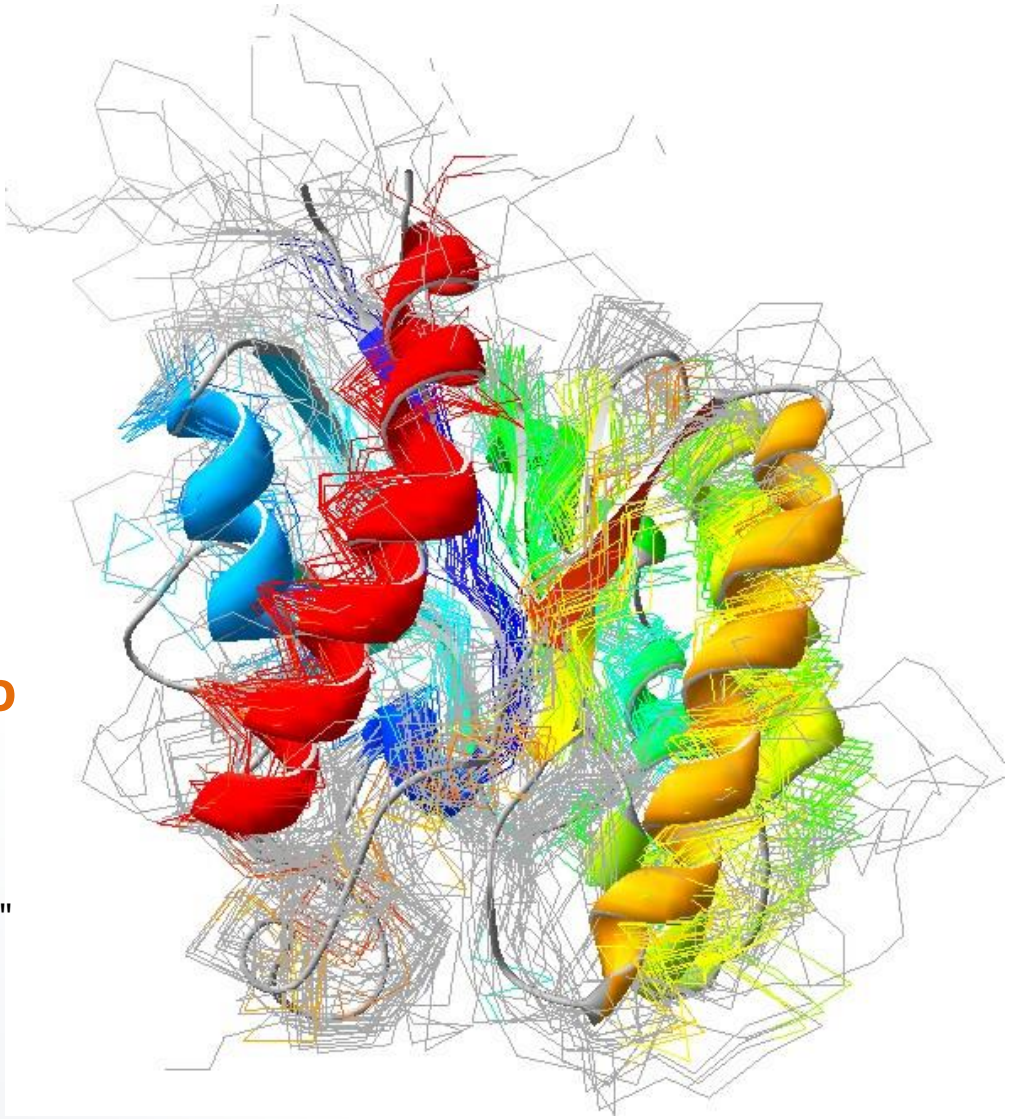
Result

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