

Project III: Protein Structures and Chimera

Lu Zhicong

January 19, 2023

1 Exercise 1

- (a) Load the structure with ID 1HEW into Chimera.



Figure 1: 1.a

- (b) What is this structure? Look for basic information.

REFINEMENT OF AN ENZYME COMPLEX WITH INHIBITOR BOUND AT PARTIAL OCCUPANCY. HEN EGG-WHITE LYSOZYME AND TRI-N-ACETYLCHITOTRIOSE AT 1.75 ANGSTROMS RESOLUTION

PDB DOI: 10.2210/pdb1HEW/pdb

Classification: HYDROLASE(O-GLYCOSYL)

Organism(s): Gallus gallus

Mutation(s): No

Deposited: 1992-01-20 Released: 1994-01-31

Deposition Author(s): Cheetham, J.C., Artymiuk, P.J., Phillips, D.C.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 1.75 Å

R-Value Observed: 0.229

(c) Select and display all water molecules. How many are there?
Color them blue.

103 atoms.

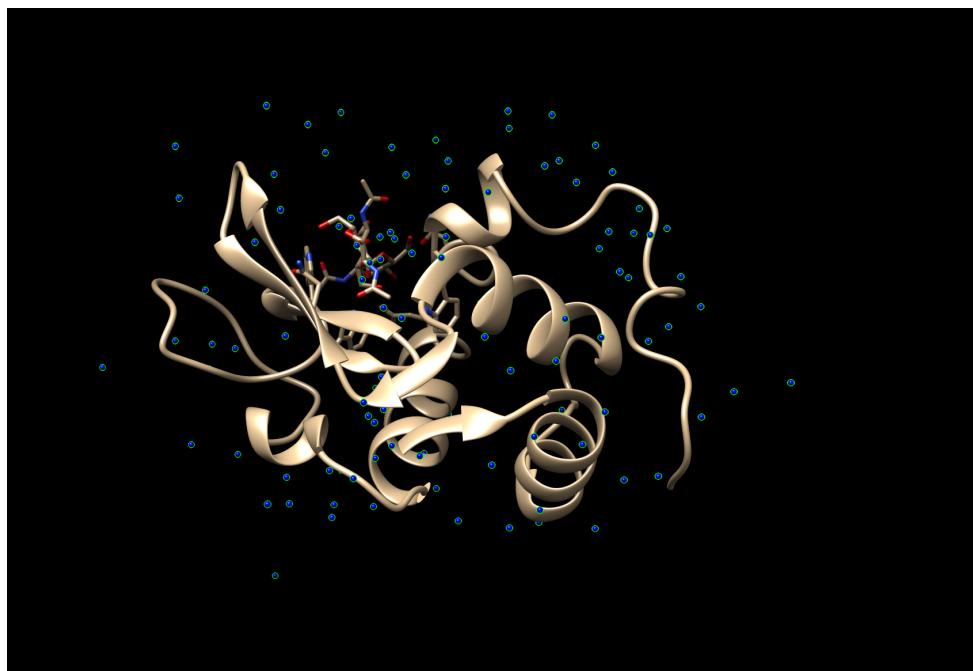


Figure 2: 1.c

(d) Find and mark the ligand. How many atoms does it consist of?

43 atoms. (and 45 bonds)

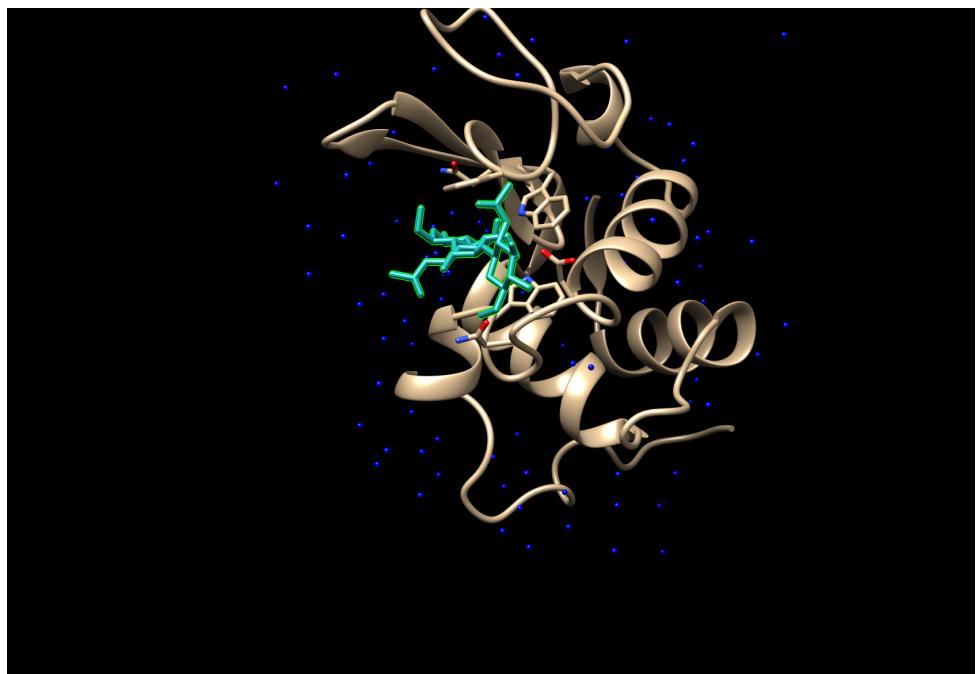


Figure 3: 1.d

(e) Color the protein chain and the ligand in different colors.

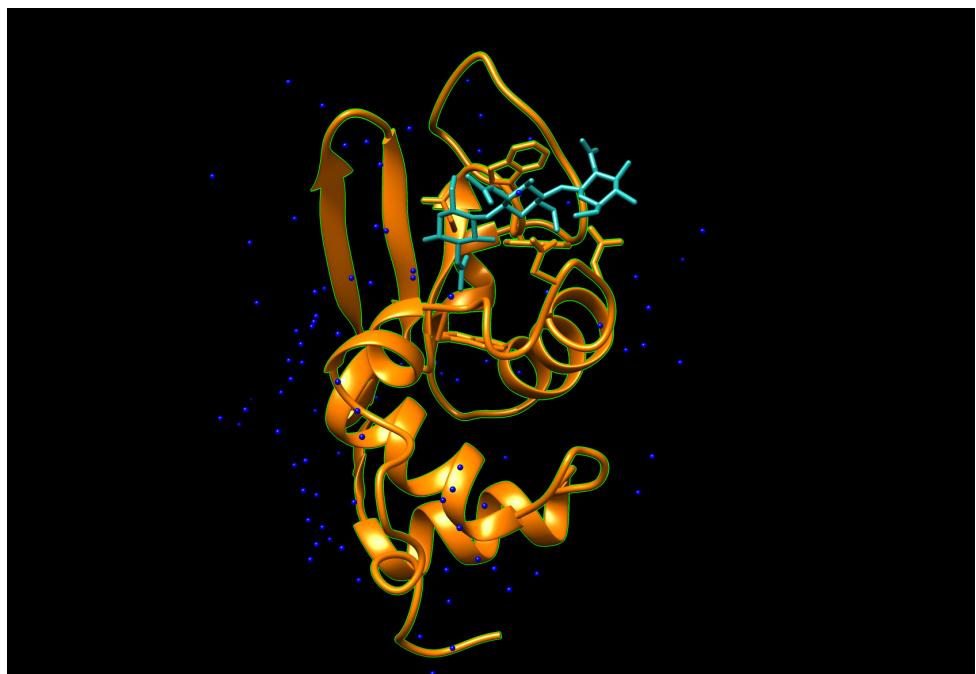


Figure 4: 1.e

(f) Color all the helices the same color.



Figure 5: 1.f

(g) Display the surface of the protein chain (only) and set its transparency to 75%.

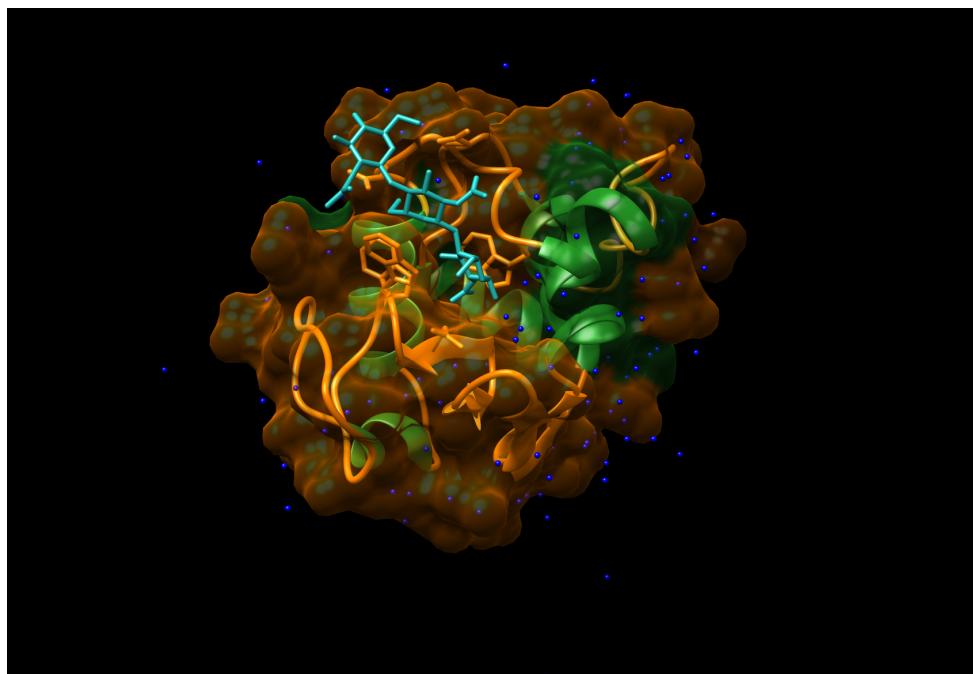


Figure 6: 1.g

(h) Record a video of the rotating structure and attach to the resulting files.

(i) Save the Chimera sessions (File > Save Session As > .py) and append to the resulting files as well.

2 Exercise 2

(a) Load the 1BMF structure into Chimera.

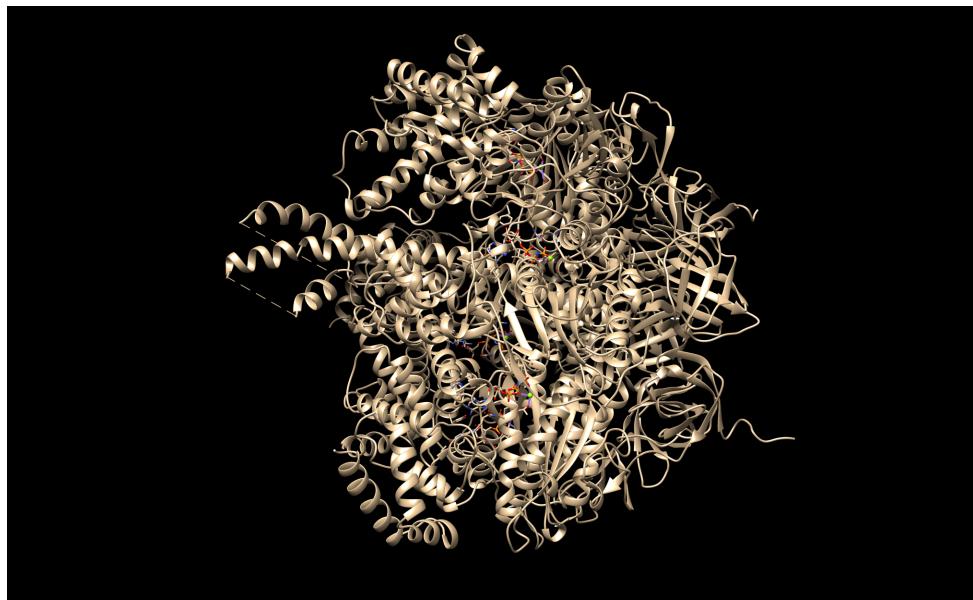


Figure 7: 2.a

(b) What protein are you analyzing?

BOVINE MITOCHONDRIAL F1-ATPASE

PDB DOI: 10.2210/pdb1BMF/pdb

Classification: ATP PHOSPHORYLASE

Organism(s): Bos taurus

Mutation(s): Yes

Membrane Protein: Yes mpstruc

Deposited: 1996-03-13 Released: 1996-12-07

Deposition Author(s): Abrahams, J.P., Leslie, A.G.W., Lutter, R., Walker, J.E.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 2.85 Å

(c) How many chains does this protein have? Color each of them a different color with Rainbow.

7 chains.



Figure 8: 2.c

(d) How many ligands are in this protein? Display the surface of each of them.

5 ligands.

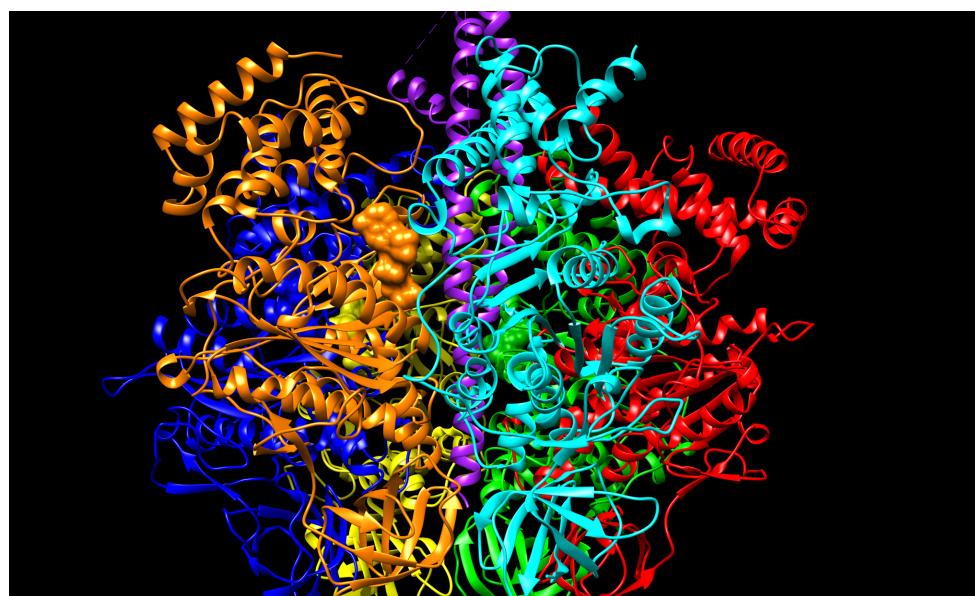


Figure 9: 2.d

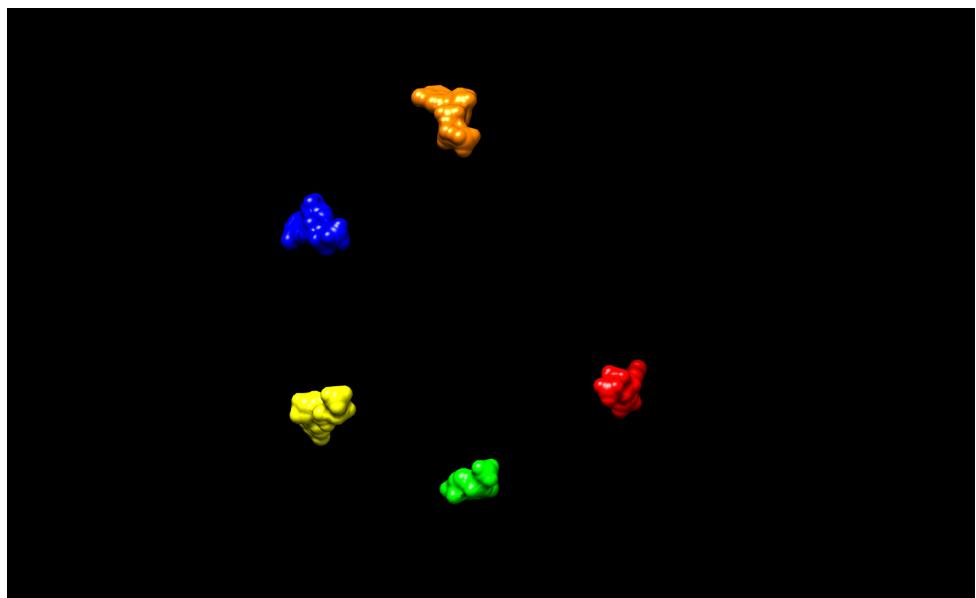


Figure 10: 2.d2

(e) Display all hydrogen bonds in a protein.



Figure 11: 2.e

(f) Display the surface of all chains. Which hydrogen bonds cross it?

There are HOH molecules outside the surface.

The hydrogen bonds could cross the surface if one end of the bond is a HOH molecule outside the surface and the other end inside the surface.

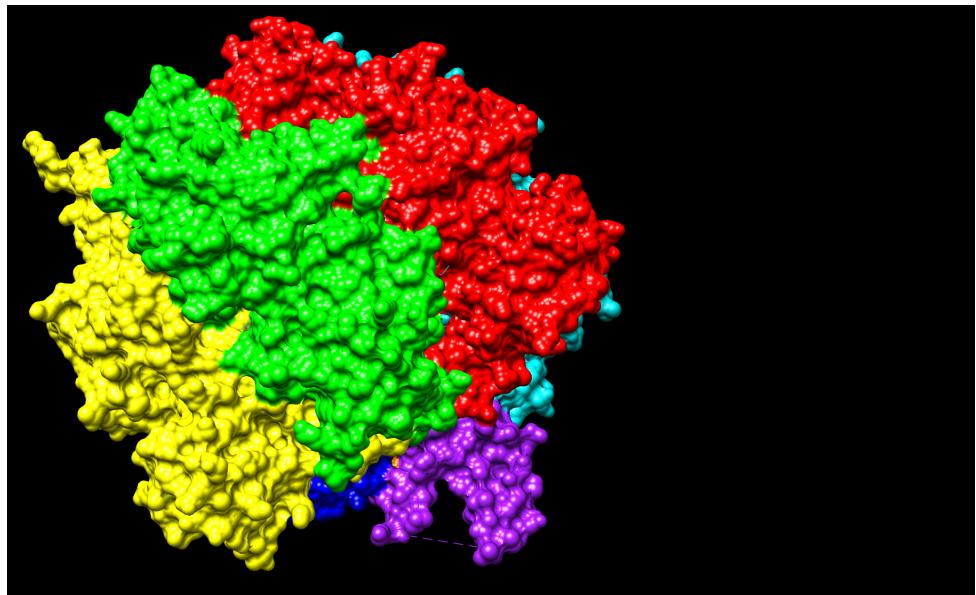


Figure 12: 2.f

(g) Remove the chain that is in the middle of the protein.

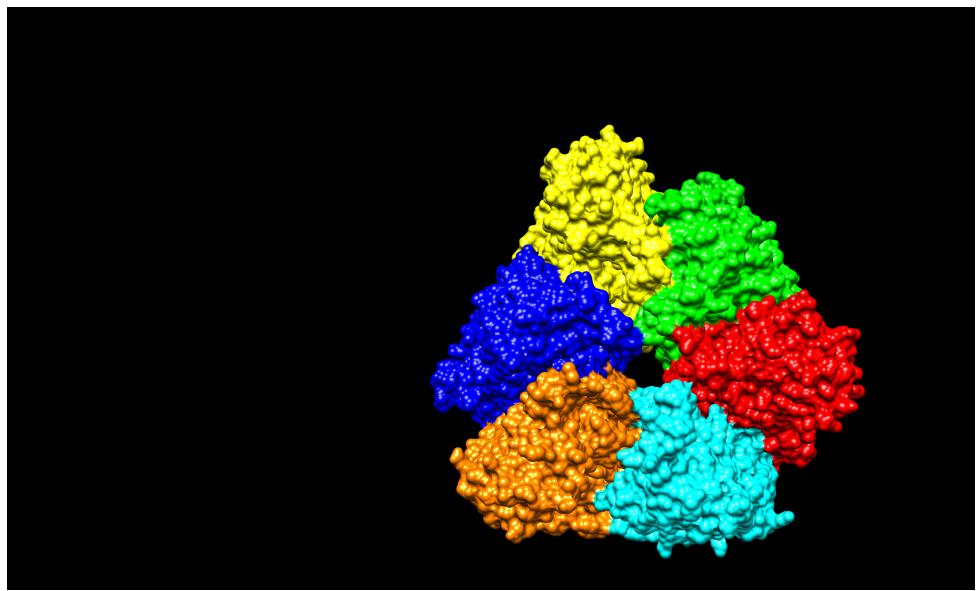


Figure 13: 2.g

(h) Remove all water particles. Has there been any change in hydrogen bonding?

There are no more hydrogen bonding across the surface, because the HOH molecules are removed.



Figure 14: 2.h

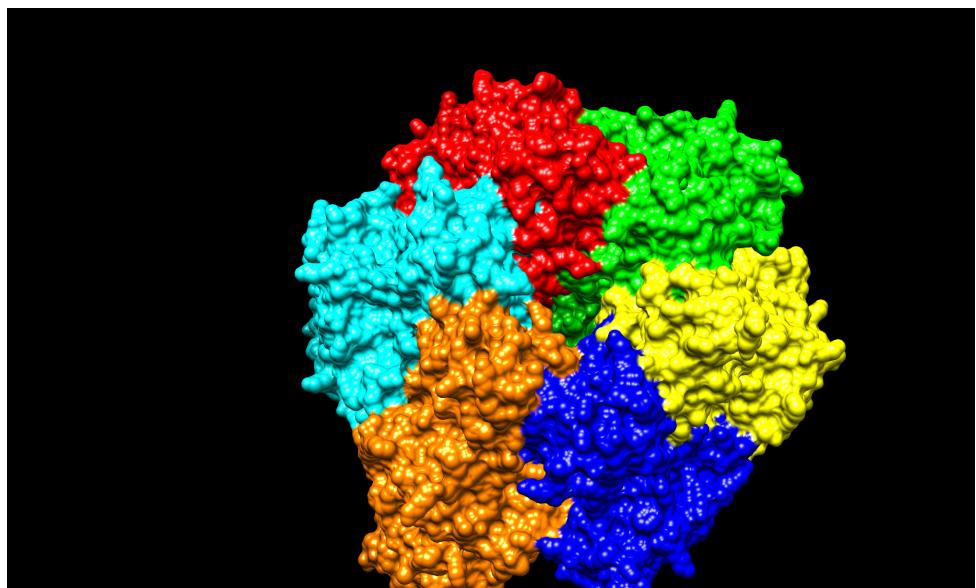


Figure 15: 2.h2

(i) Select all the lysines (how many?), color them white and display the side chains

153 lysines

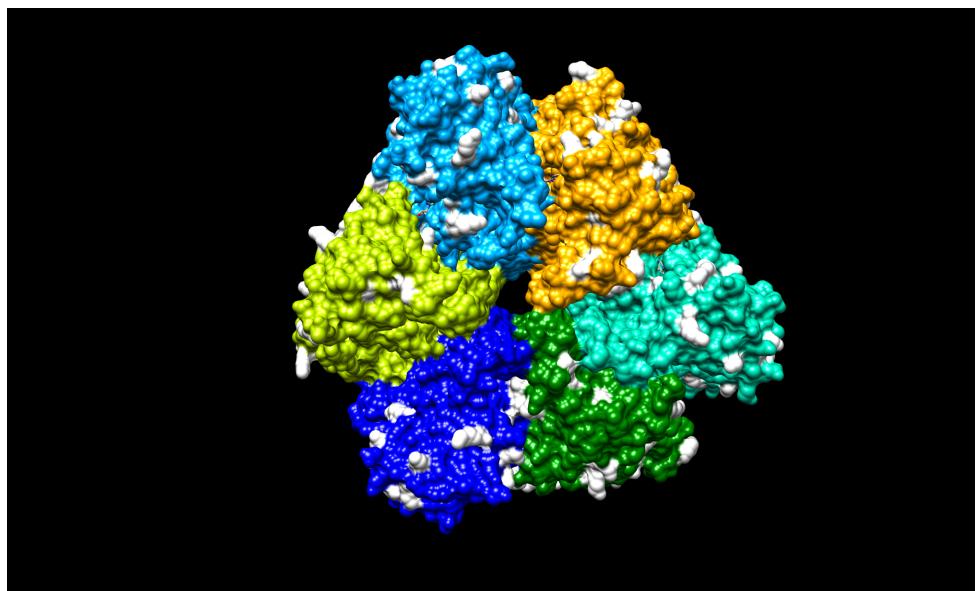


Figure 16: 2.i

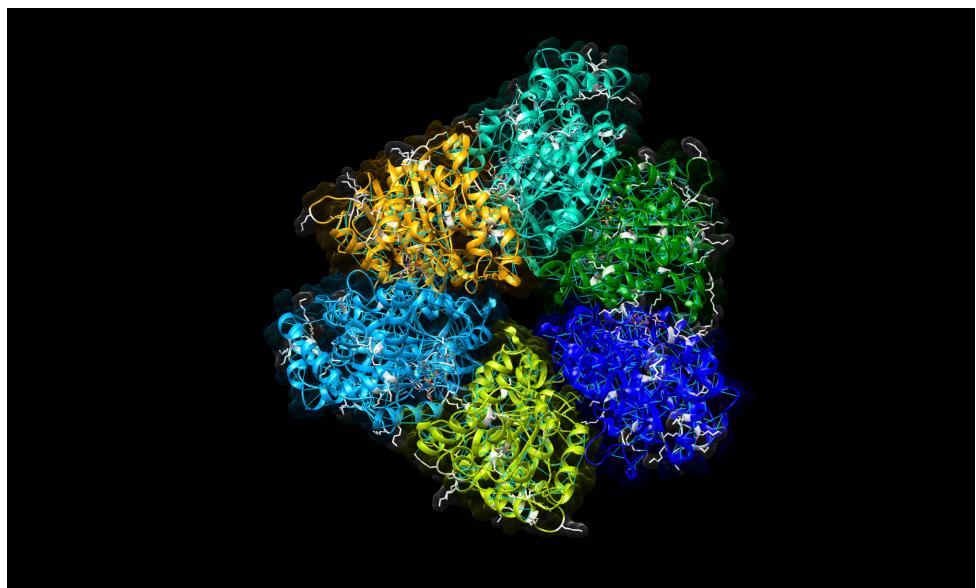


Figure 17: 2.i2

(j) Record a video with the rotating structure and join the resulting files.