

# **Introduction to Bioinformatics**

## **Project 3: 3D Protein Structure**

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### **Exercise 1:**

**b) What is this structure(1HEW)? Look for basic information.**

Refining an Enzyme Complex with Inhibitor Bound at Partial Occupancy:  
Hen egg-white HEW Lysozyme and Tri-N-Acetylchitotriose at 1.75  
Angstrom Resolution.

Classification: HYDROLASE

Organism: Gallus Gallus

**c) How many water molecules are in there?**

103

**d) How many ligand atoms does it consist of?**

43 atoms, 45 bonds

### **Exercise 2:**

**b) What protein are you analyzing in 1BMF?**

Bovine mitochondrial F1-atpase

Classification: ATP PHOSPHORYLASE

Organism: Bos taurus

**c) How many chains does this protein have?**

7 protein chains

**d) How many ligands are in this protein?**

5 ligands

151 atoms

161 bonds

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

I able to display the surface of all chains. But issues regarding visualization due to slow and hang of software etc.

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

Yes, there is a change in hydrogen bonding when I remove all water particles. The bonds that connected the water particles with the chains disappeared/removed.

**i) How many lysines?**

Before removing the middle of the chain of protein:

1503 atoms, 1345 bonds in lysines

After removing the middle of the chain of protein:

1377 atoms, 1233 bonds in lysines

24 molecules of lysines