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**BINF PRACTICAL 6**

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Protein structure Visualization

Introduction

The main feature of computer visualization programs is interactivity,

which allows users to visually manipulate the structural images through a

graphical user interface. At the touch of a mouse button, a user can move,

rotate, and zoom an atomic model on a computer screen in real time, or

examine any portion of the structure in great detail, as well as draw it in

various forms in different colours. Further manipulations can include

changing the conformation of a structure by protein modelling or matching

a ligand to an enzyme active site through docking exercises.

Because a Protein Data Bank (PDB) data file for a protein structure

contains only x, y, and z coordinates of atoms, the most basic requirement

for a visualization program is to build connectivity between atoms to make

a view of a molecule.

- Protein: E1 domain of the amyloid precursor protein
- Visualization software: Pymol

- **PDB DOI:** 10.2210/pdb4PWQ/pdb

- **Classification: heparin binding protein**
- **Organism(s):** Homo sapiens
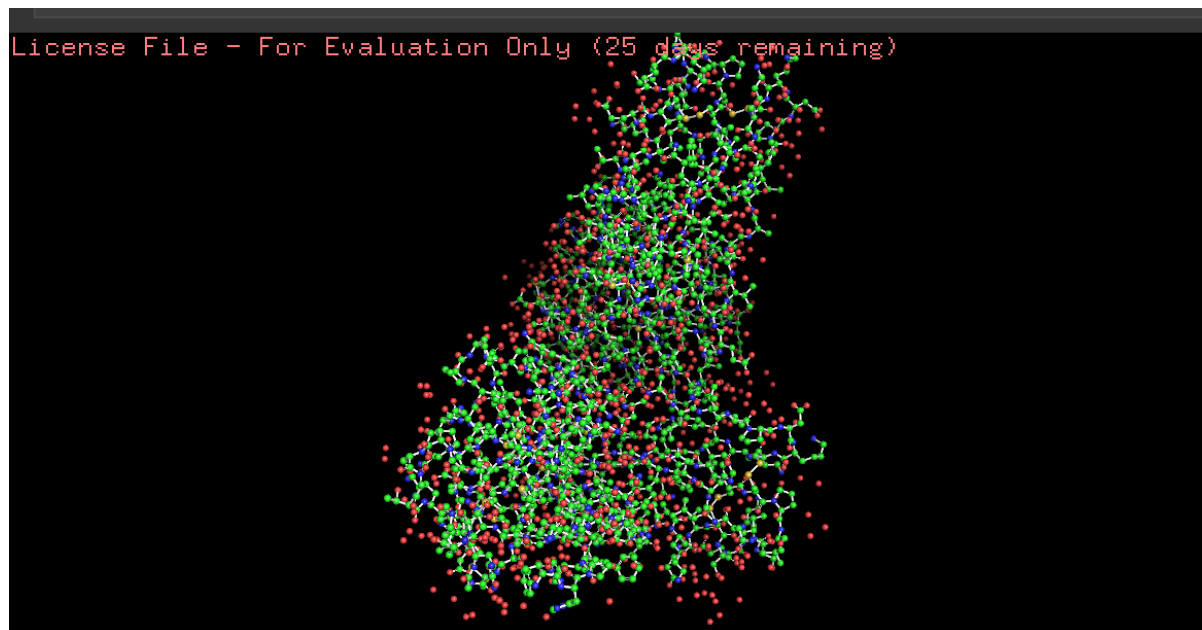- **Expression System:** Escherichia coli
- **Mutation(s):** No
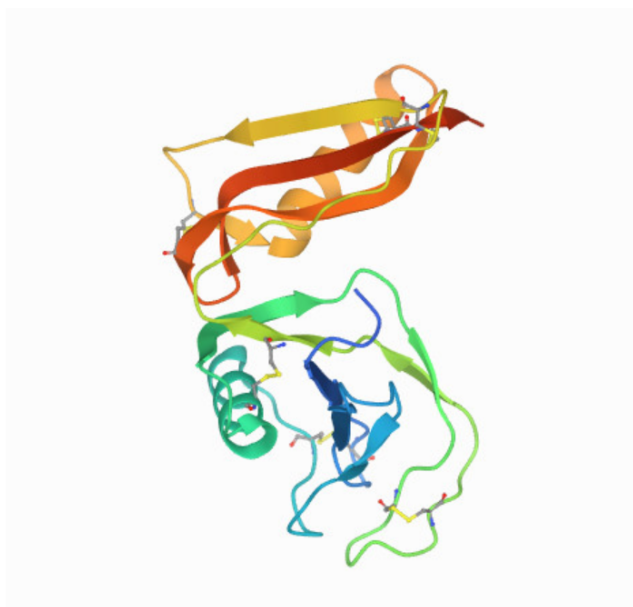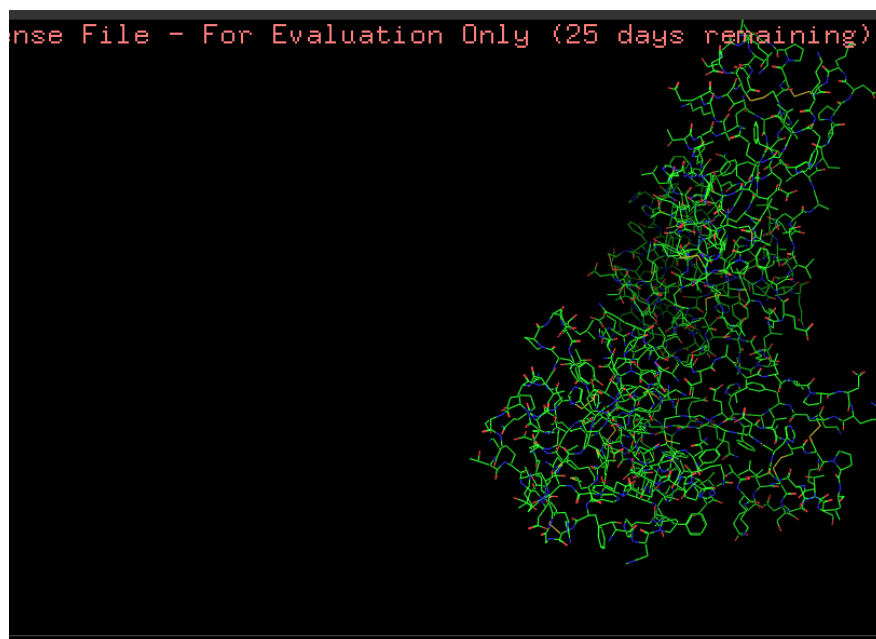
Results:

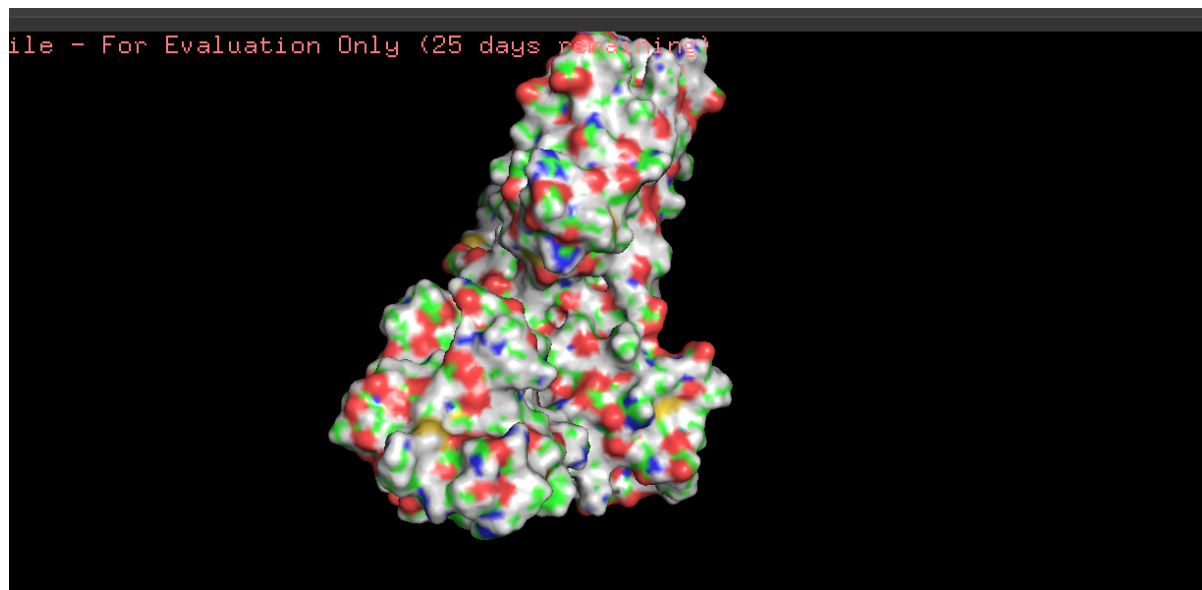<u>visualization state in cartoon:</u>
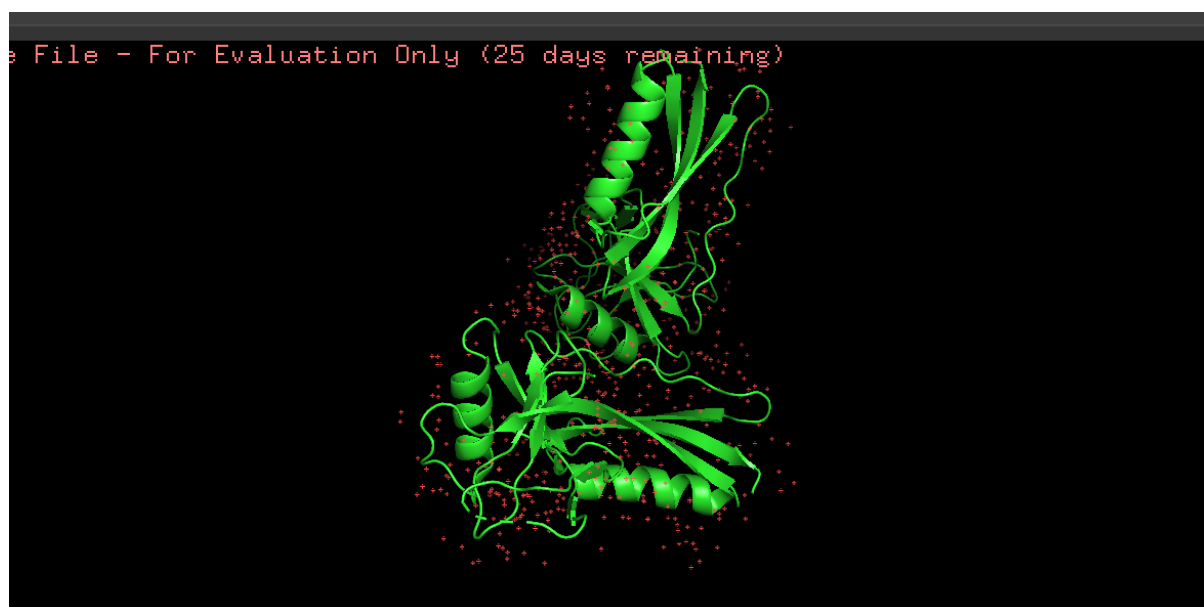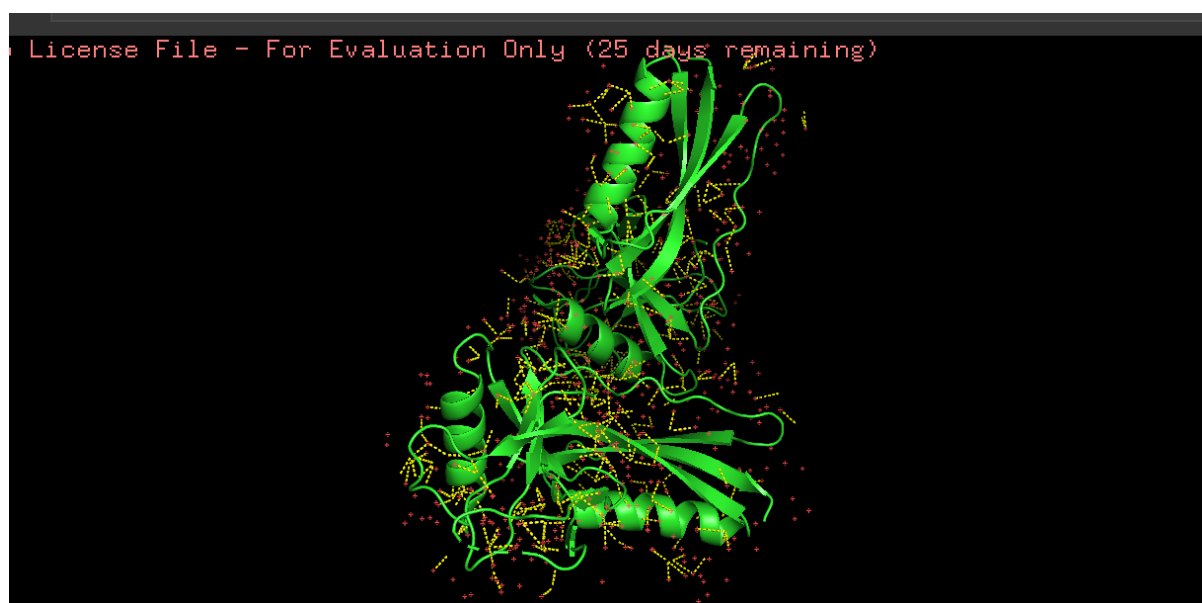

<u>visualization in ball and stick state:</u>

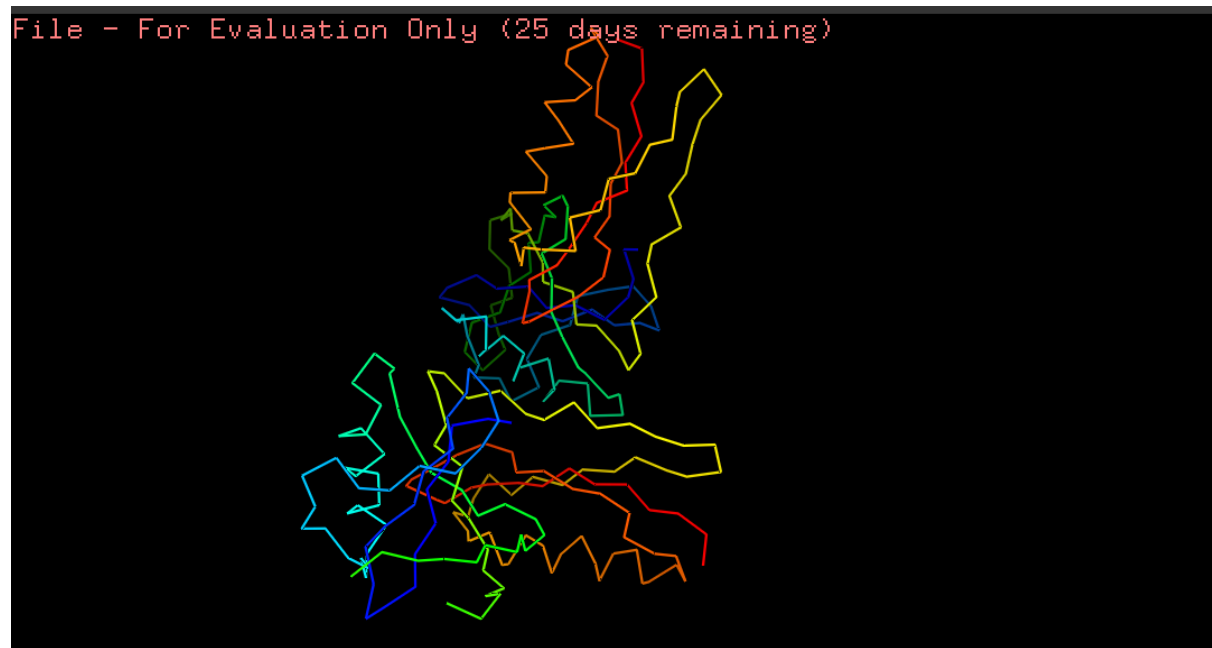visualization state in lines/wire frame representation:

Visualisation state in surface representation:

Visualisation of H bonds involved in protein-protein interactions:

Representation of ligands :

Conclusion: Amyloid precursor protein is taken from rcsb protein data bank to represent its different states like cartoon, surface, ball and stick, ligand sites etc using pymol software tool.