BINF PRACTCAL -6

PROTEIN STRUCTURE VISUALIZATION

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 STRUCTURE:

Protein structure is the three-dimensional arrangement of atoms in an amino acid-chain molecule. Proteins are polymers – specifically polypeptides – formed from sequences of amino acids, the monomers of the polymer. A single amino acid monomer may also be called a residue indicating a repeating unit of a polymer. Most generally used visualization softwares include: PYMOL, RASMOL, JMOL etc.

Here we are using PYMOL software to visualize the structure of a protein SARS-CoV-2 S Omicron Spike B.1.1.529

- **PDB DOI:** 10.2210/pdb7QO7/pdb
- **EM Map EMD-14086:** EMDB EMDataResource

- **Classification: VIRAL PROTEIN**
- **Organism(s):** Severe acute respiratory syndrome coronavirus 2
- **Expression System:** Cricetulus griseus
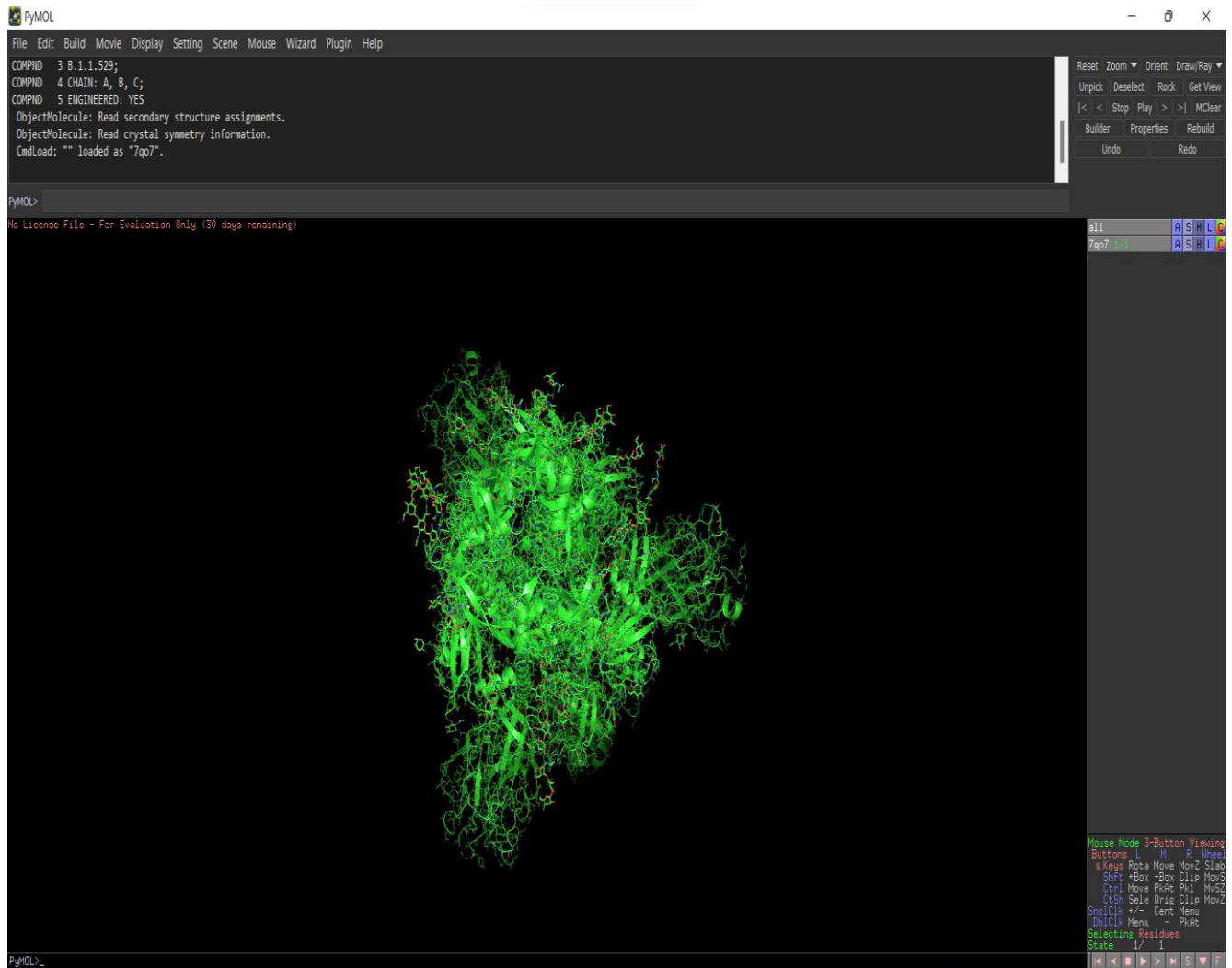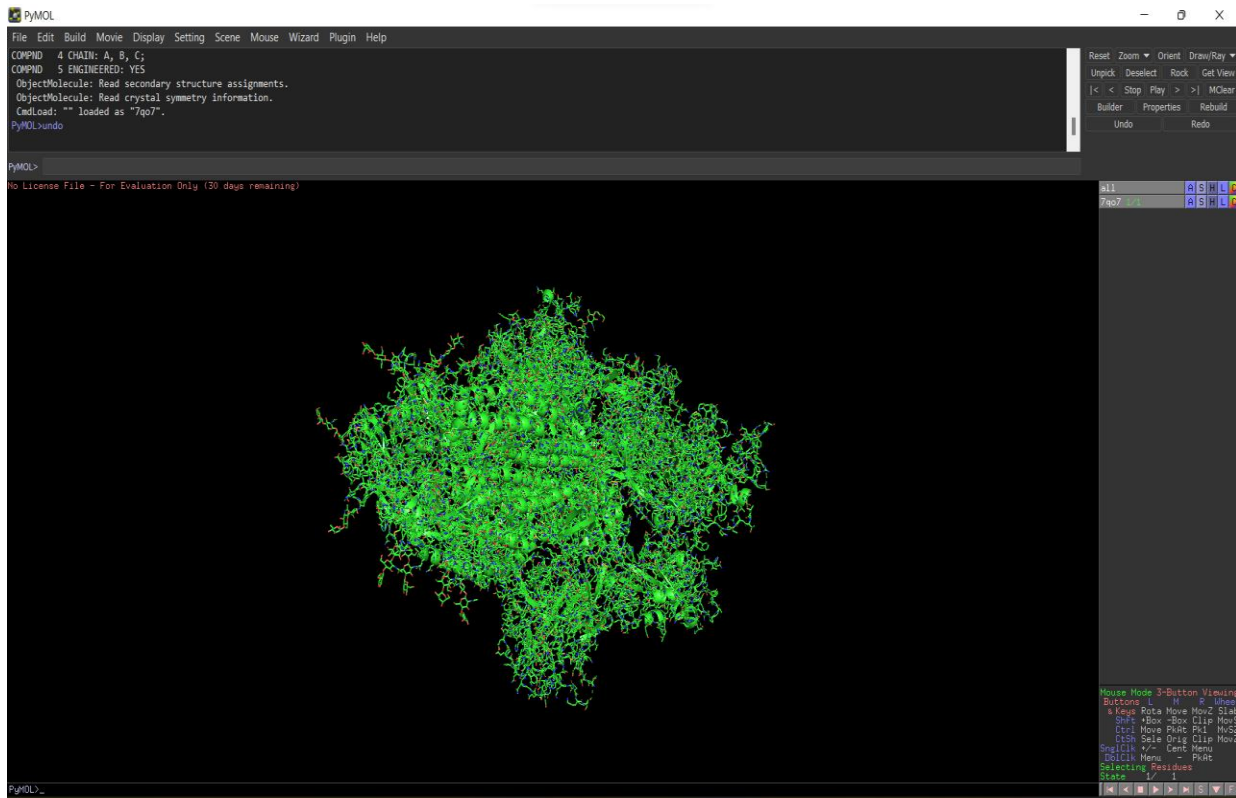- **Mutation(s):** No

Result:

Fig:Wire Representation
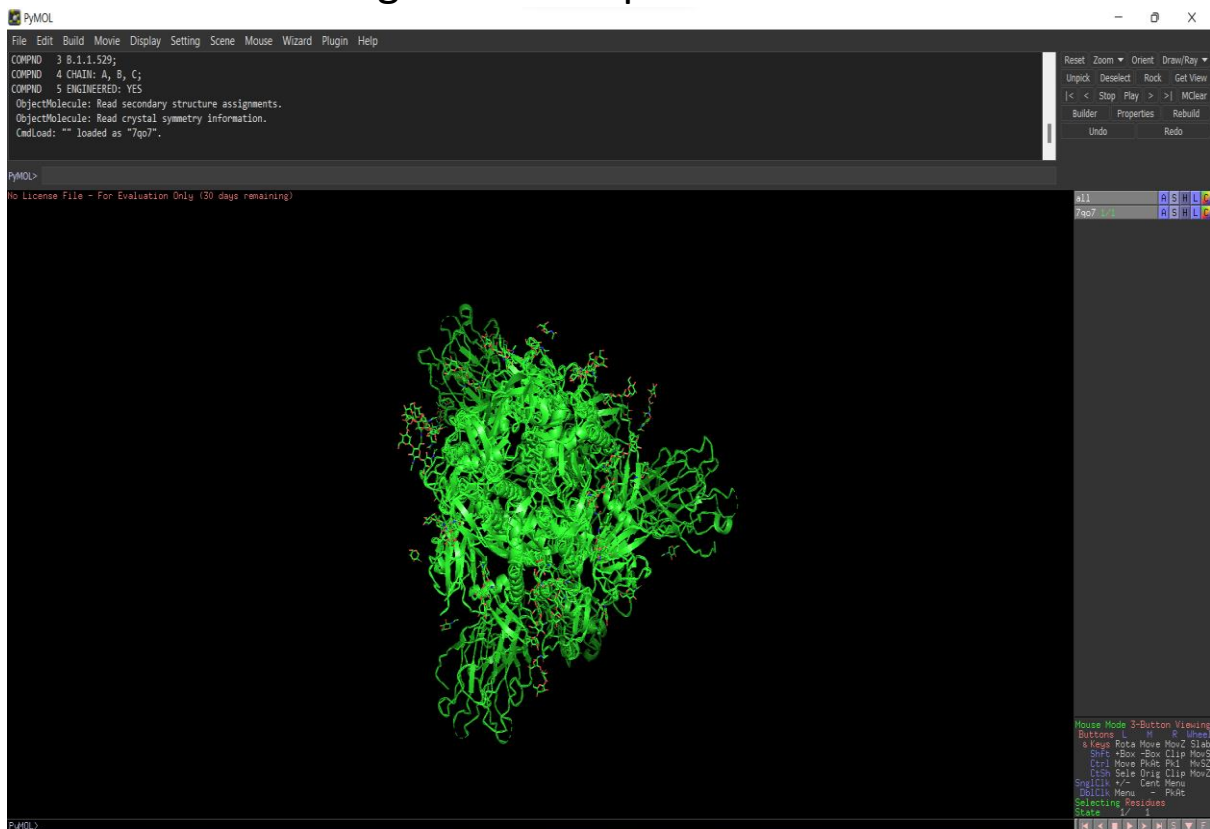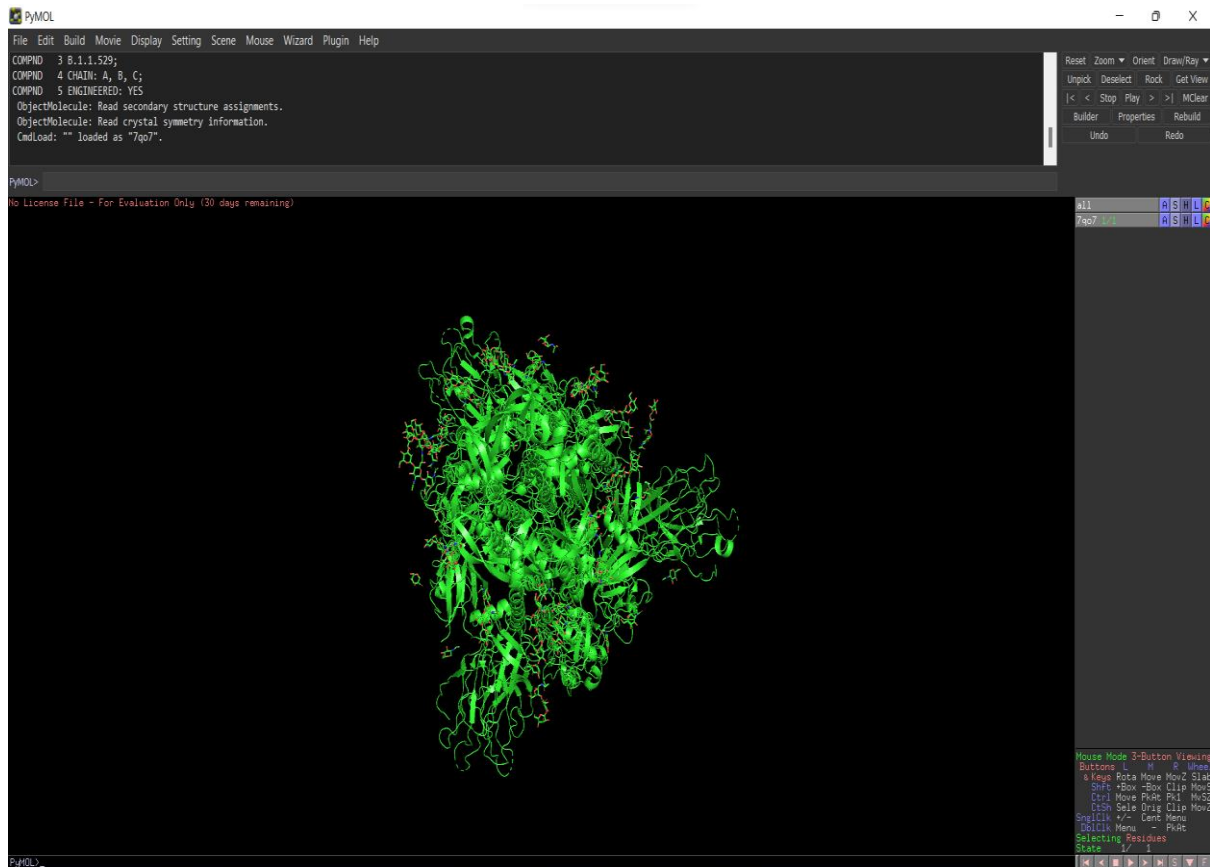
Fig:Licorice Representation

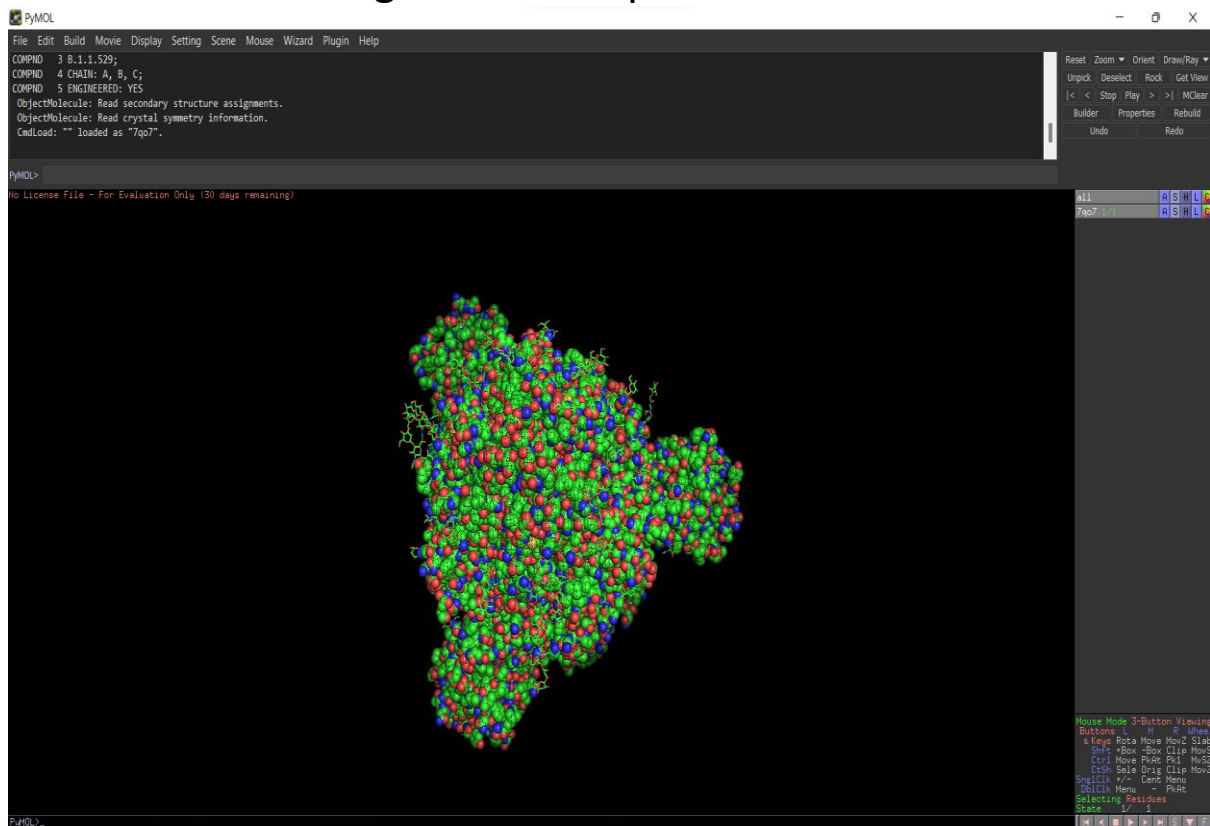

Fig:Ribbon Representation

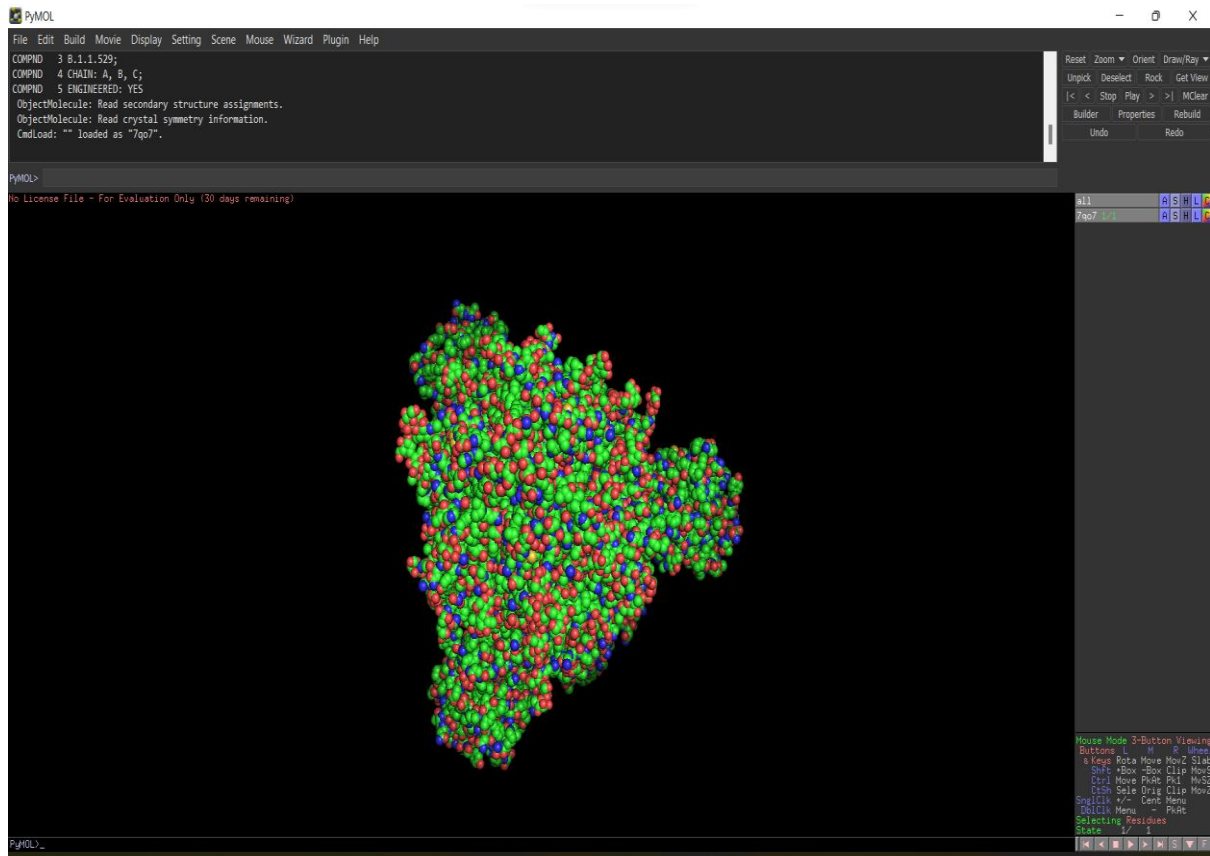Fig:Cartoon Representation

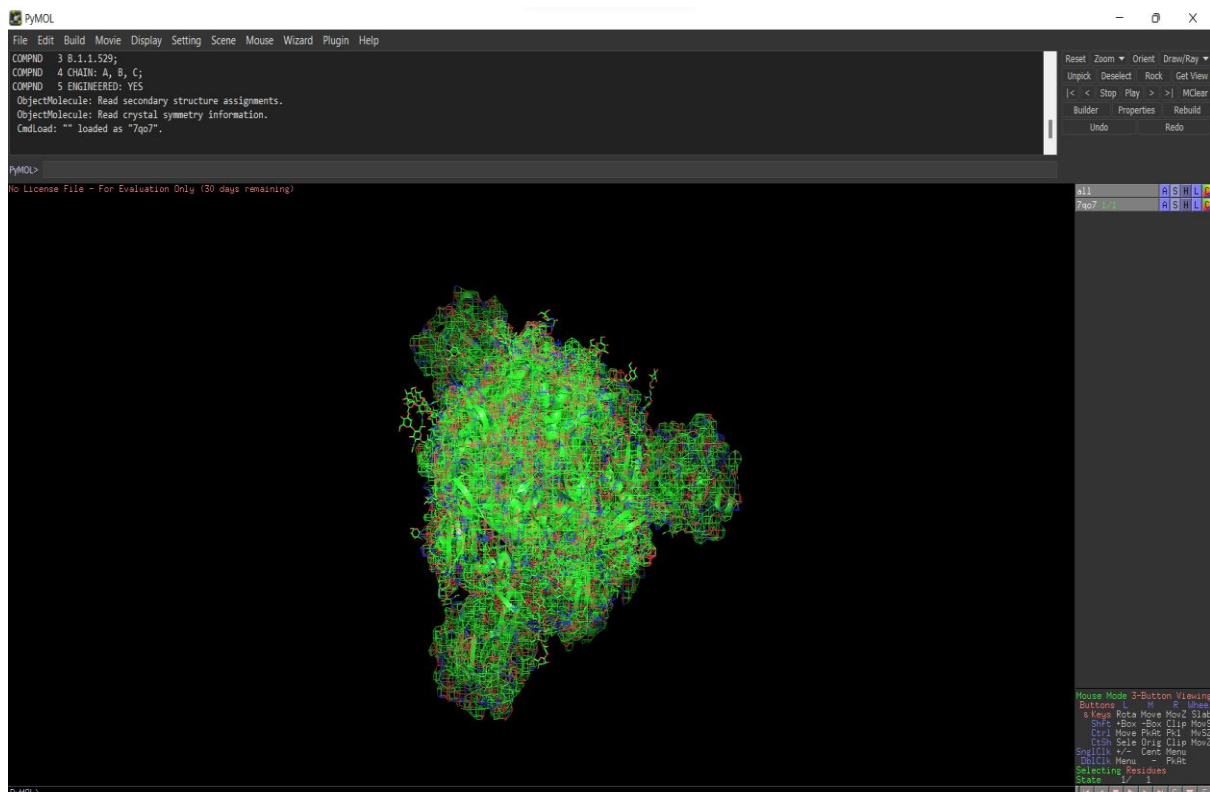Fig:Dots Representation

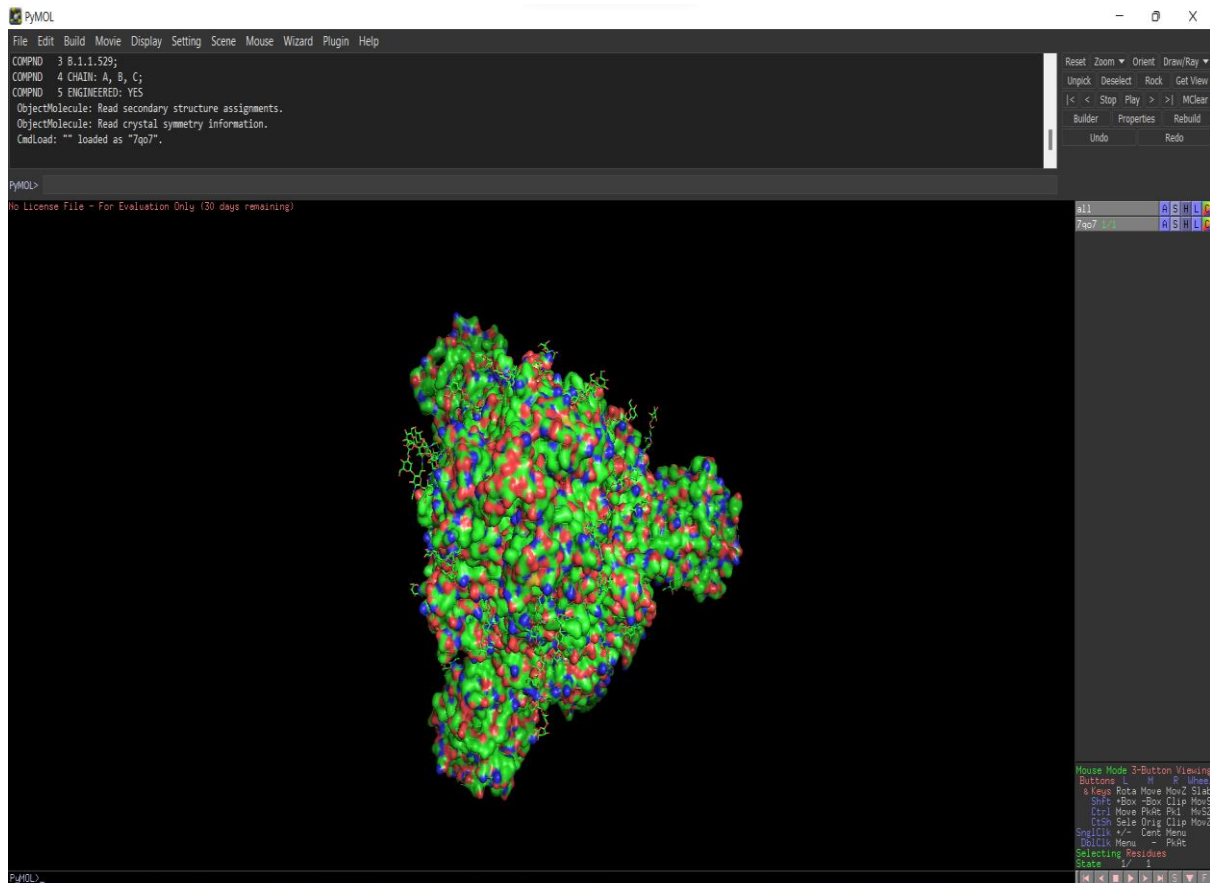Fig:Sphere Representation

Fig:Mesh Representation

Fig:Surface Representation

Conclusion:

SARS-CoV-2 S Omicron Spike B.1.1.529

was visualized using PyMOL and the images in the document were a result of exports from PyMOL. We have visualized the cartoon, surface, licorice, wire, mesh ribbon and spherical representation of the crystallographic protein structure. was visualized using PyMOL and the images in the document were a result of exports from PyMOL. We have visualized the cartoon, surface, licorice, wire, mesh ribbon and spherical representation of the crystallographic protein structure.