Prerequisites:

1. **Protein structural model**
   (Either predicted using any computational tool or retrieved from PDB or any other databases.)
2. **File format for protein structure:**
   .pdb, .mmdb or .mmcif file is required for structure visualization of a protein.
3. **UCSF Chimera installed on your PC:**

- To download UCSF Chimera on your PC, click on the link below: https://www.cgl.ucsf.edu/chimera/download.html
- After downloading, install the tool on your PC to start the process of protein visualization through it.

Prerequisite terminologies:

In order to have a thorough understanding of our main topic, you should have the basic concept of the following terminologies:

1. **Different types of molecular representations of the protein model.**

Introduction:

CHIMERA is the most commonly used stand-alone tool for protein 3D structure visualization. It is a computational tool for interactive visualization and analysis of molecular structures and related data including density maps, trajectories and sequence alignments. It can be used to generate high quality figures and animations out of the query protein model. It is available for download on any operating system including Mac OS, Windows and Ubuntu, free of cost.

Steps:

- Once you've installed Chimera on your PC, open it.
- **Using CHIMERA as a default program to open the PDB files of your tool:**
    - Right-click on the PDB file of your protein.
    - Click on the 'Open with…' option.
    - Click on 'More Apps' and then click on 'Look for another app from your PC'.
    - Go to the 'Programs' file of your computer.
    - Click on the CHIMERA file and then open the 'bin' folder of Chimera.
    - And then click on 'chimera.exe' file and then open the protein's 3D structure file in PDB format.
- **Opening the 3D protein structure files within Chimera:**
    - Go to 'File' , then select 'Open' and then search for the files containing the protein structure on your PC, using the file directory.
    - Select that particular file of your target protein and click on 'Open'.
- To **change the background color** from Black to White, go to 'Favorites', then 'Preference', then go to 'General', then 'Background', and then set the desired color for the background of Chimera.
  [It is preferable to have a white background on Chimera, due to the reason that most of the publications have a white background.]

- You can **rotate the protein** by holding the left-click button and moving the cursor/mouse. Or with the help of your finger if you're using a touch screen phone, tab or laptop.
- You can open as many protein structures as you want in separate windows as well as in a single window, whatever you want.
- You can also **color the protein** molecule based on different chains. To do so, go to 'Tools', then 'Depiction', and then select the particular option to color your protein model based on chains, amino acid residues, secondary structures of protein, model-wise, and many more.
    - Select the colors and range and then click on 'Apply'.
    - If you've more than 1 protein model in your file, you can color them separately based on different parameters you'll select for that purpose.

Note: To color the protein molecule based on nucleotide residues, you must have the protein nucleotide sequence file along with its structure file.

- Also, you can use this tool to **retrieve the structure** of a particular protein from the PDB, if you have a PDB accession ID of that particular protein. To do so, go to 'File', then 'Fetch by ID' and then select the suitable database having the desired protein structure.
- To **save** your file, go to 'File' then click on 'Save as PDB', then select the suitable folder where you like to save the file on your PC, then enter the name of the file.
  [If there are more than 1 protein structure within the file you're saving, it'll provide you with an option to select which file you want to save, either 1 or all.]
    - Then click on the "save" button, to save the files on your PC.
- To **delete a particular protein chain** or a whole protein molecule, go to 'Select', then 'Chain' and click on 'A' and then select the particular chain or protein model you want to delete.
  [It'll highlight/select the part of the protein you've selected.]
    - Go to 'Action', then 'Atoms' and then click on 'Delete'.
- To **delete a specific ligand** from your protein molecule,

    - Press the ‘Ctrl’ button and ‘up arrow’ button on your keyboard to select that particular ligand.
    - Then go to ‘Actions’, then ‘Atoms’ and then click on ‘Delete’. OR
    - Go to ‘Select’, then ‘Chain’, and click on ‘I’.
      [It’ll select the ligand present on the protein molecule.]
    - To remove that selected ligand, go to ‘Action’, then ‘Atoms’ and then click on ‘Delete’.
- You can go to the ‘Select’ menu and choose any suitable parameter to modify/manipulate the protein structure, based on the ‘chemistry’, ‘structure’, or ‘residues’ of the protein molecule, in Chimera.
- In the ‘Action’ menu, you can apply different sorts of structural modifications to your protein molecule, such as you can visualize the ball-and-stick, rings, wires, and other structures of your protein.
- To **visualize and compare different structural representations** of your protein, go to ‘Presets’ and you can select different parameters that will determine the structural representation of your protein, such as ‘ribbons’, ‘hydrogen surface’, ‘atoms’, etc.
    - After selecting a particular structural representation of your protein you can apply different colors on it by going to the ‘Action’ menu and then click on the ‘Colors’ option to select the color.
    - To add different labels on your protein, go to ‘Action’, then ‘Labels’, and then click on ‘Residues’.
- You can save your file by clicking on the ‘Write PDB’ option in the ‘Actions’ menu.
  [It’ll save the structure in a single file even if you have a complex of proteins in your file.]
- If you know some commands to manipulate or analyze your protein structure, you can go to the ‘Tools’ menu.
- To get the protein’s amino acid sequence, go to ‘Tools’, then click on ‘Sequence’.
  [It’ll provide you the entire length sequence of your protein.]

- Other than these modifications, you can do **‘Structural Comparison’** between different protein molecules from the ‘Tools’ menu.
    - To do so, open 2 or more protein files in the same window and then go to ‘tools’, and then click on ‘Structure comparison’.
    - To align two proteins, go to ‘tools’, and then click on ‘Structure comparison’ and then click on ‘Match Maker’ then select the ‘Reference structure’ and then ‘Structure to match’ and then click on ‘Apply’.

Note: The lower the amount of loops in a protein model, the better the predicted model is.

Summary:

In this tutorial video of UCSF Chimera, we learned to visualize and analyze a protein 3D model using Chimera. We also got to know about different parameters that can be applied on the protein structure to make it visually interactive. Moreover, we learned to compare and analyze more than one protein structure for research purposes.