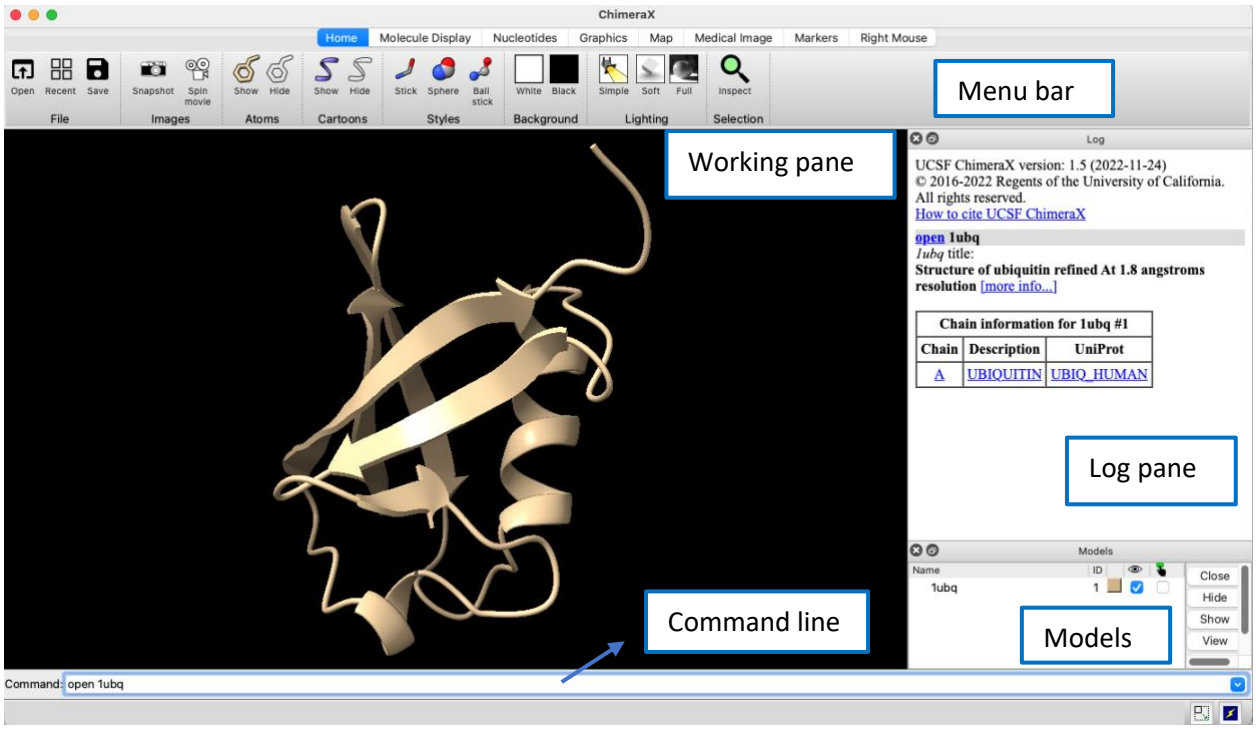
Example protein: Ubiquitin

To fetch the protein directly from the PDB databank by typing `open 1ubq` in the command line. After you load the file you should see something like this:



You can change the color of the background in Graphics tab. To change the color of the protein chain go to **Actions → Color →All Options**.

Mouse controls:

- Holding the protein with right-click allows you to move the protein about the horizontal and vertical axis.
- Holding the black region with right-click allow syou to rotate the protein clockwise or counter clockwise.
- Holding the protein with left-click allows you to change the pose of the protein you see on the screen.
- If you wish to select a part of the protein, press ctrl and left-click and drag the mouse over that part. To let go of the selection, press ctrl and click anywhere on the black region.

Practicing different representations of a protein:

- Click **Molecule Display** on menu bar. From this tab, you can display the protein surface by clicking **Surfaces → Show** and color it based on electrostatics, hydrophobicity and b-factor. If you have more than one chain, you can color each chain differently. You can also locate one or more residues by clicking **Sequence** on the analysis tab and selecting the residue that you want to display.

- Residue selection is also done by command line. Let's select the first amino acid by typing `select #1:1` . Display the side chain atoms by clicking **Atoms → Show**. Label the residue by typing `label #1:1` . Increase label size by typing `label height 1.4`. It is a Methionine, as in all encoded proteins ! Color the selected residue in **Actions → Color →All Options** by selecting Atoms/bonds and By Heteroatom**.** You should see that the sulfur atom in methionine side chain colored differently than the carbons.

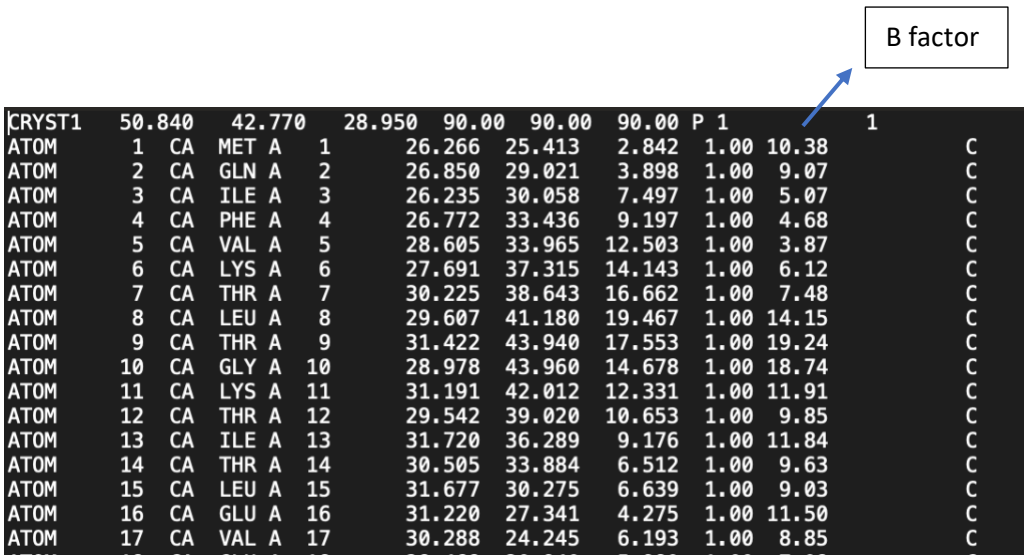
- You can change the thickness and transparency of the ribbon using the command line. Try out following commands:

```
cartoon style helix width 1.0
cartoon style strand width 1.0
transparency 40 cartoon
```

- To save a high resolution figure of the protein with a transparent background, type in;
`save 1ubq.png transparentBackground true pixelSize 0.02`

Measured experimental flexibility of a protein and its secondary structure content

- We will now learn more about our molecule; every PDB structure has a column dedicated to the flexibility of each atom as measured from the Debye–Waller factors (also called B-factors; this is only physically meaningful for PDB files whose experimental method is X-ray crystallography). Color the protein by the *b-factor* coloring method. What can you say about the new colors?



Measuring distances and angles:

Now let's focus on the molecular geometry of the first residue. Zoom in and select a covalently bonded sulfur and carbon atom by pressing ctrl+shift and left click. Label the atoms by clicking **Actions→ Label → Atoms → Name**. Now go to **Tools → Structure Analysis →Distances** and click **Create**. Select one more carbon atom and go to **Angles/Torsions** and measure the angle between three atoms.

How big is the protein ? Select two atoms on two residues that seem to be the farthest apart and click **Create** on **Distances** tab.

Learning more about your molecule - PDBsum

PDBsum is a database that collects information on deposited PDB structures. Go to the PDBsum web, and type in your pdb ID (and chain info, if any).

From the Protein tab, get the secondary structure diagrams and CATH codes. You can also get conservation scores from ConSurf Database. Predicted tunnels for ligand entry-exit are also provided along with a plethora of other information.