BioInformatics: Algorithms and Applications
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Lecture – 16b
Protein Tertiary Structure II

Then these PDB structures they have one more term. So, I will show you here.

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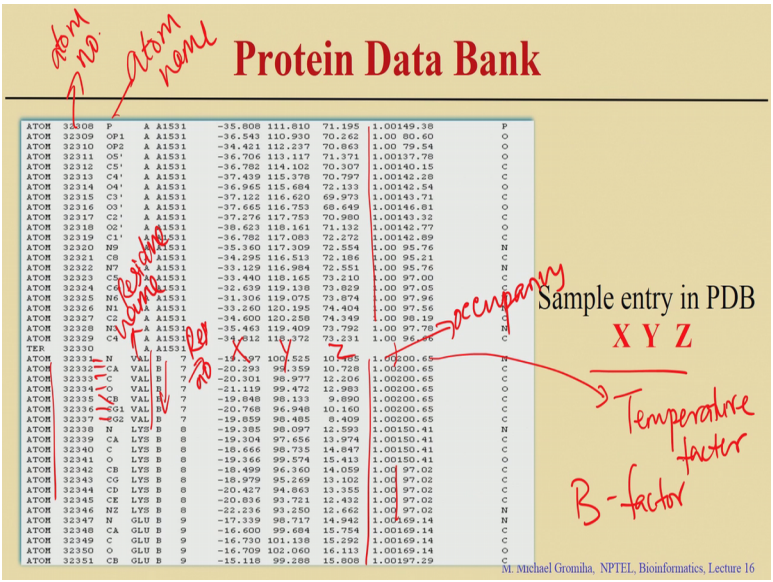

So, if you have the XYZ coordinates, this is the occupancy right then we have another one term here right this is called a temperature factor, also we can call this as the B-factor. This will tell you the flexibility of each atom how to get this one.

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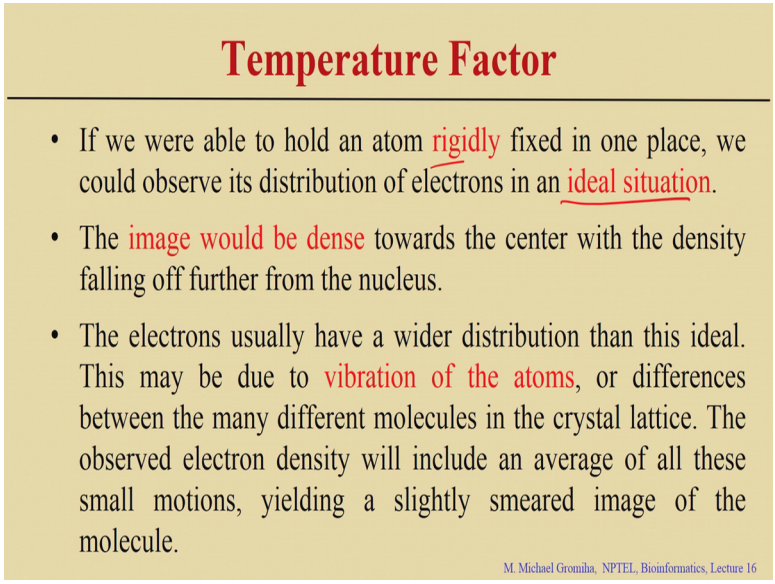

So, if you are able to fix the atom within the electron density map, if you fix the atom within that space right. So, they are rigid, and in this case they do not disturb these electrons. So, in this they become an ideal situation.

In this case you can get the dense distribution right within that particular conformation, then they are very rigid. But usually the electrons are wide distribution right because the right then they vibrate because the vibration of these atoms, they have the different molecules. In the crystal lattice in this case you can see the electron density, they will include all the average of the motions if they vibrate more, then you can see the deviation is very high. If you can occupy the same residue or same atom within that rigid position, then this is very small; if not then they fluctuate very much in this case you can see the variation of these fluctuations there this is what they give in terms of temperature factor ok.

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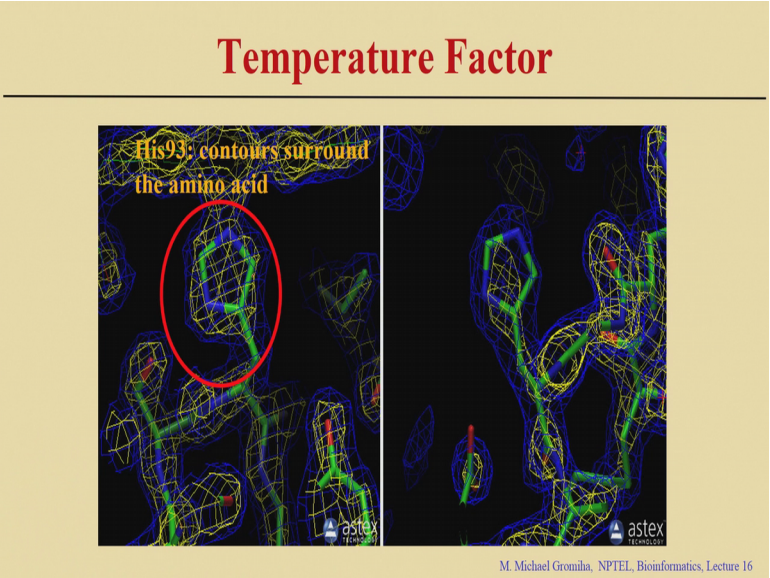

We see this this case right you can see the histidine 93 you can see you this contour can accommodate this particular residue, and some case the contour is not able to accommodate the full residue because it is vibrating more inside this map.

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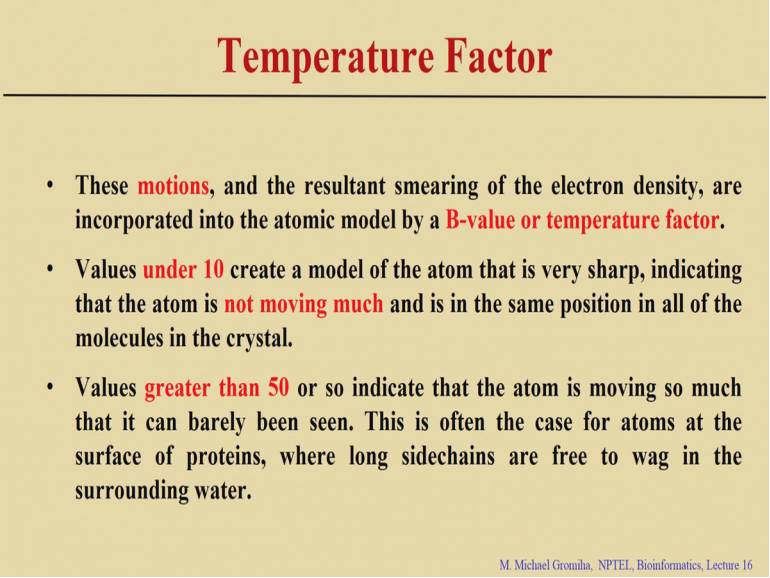

So, you can get this information right and account these motions in the PDB structures right this is what they give you the data B-factor or the temperature factor. Essentially if the number is less than 10 and less than 20, then you can said that the vibration is less and they are rigid right and then they have the particular position in the structure.

If it is more than 50, then the atom is moving here and there and the fluctuations are more, in this case the temperature factor or B-factor is high in this case.

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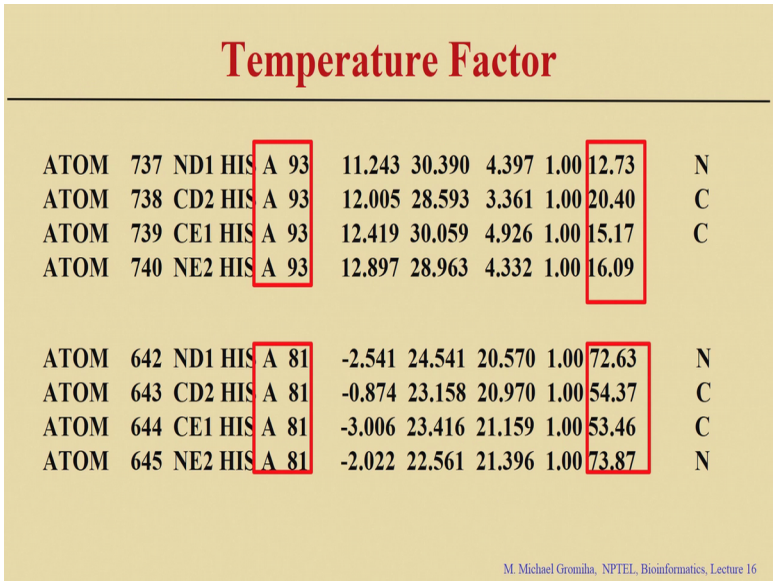

So, this is one example. So, here you can see the histidine 93 ND1 and the CD2, the value is around 12 or 15 or 16, and you can see these atoms they are rigid. On the same case if you see the histidine 81 right ND1 and CD2 right here you can see the values are more than 50, say 72 or 73, and this case we can see that these atoms they are highly flexible and this is why the B-factors are very high.

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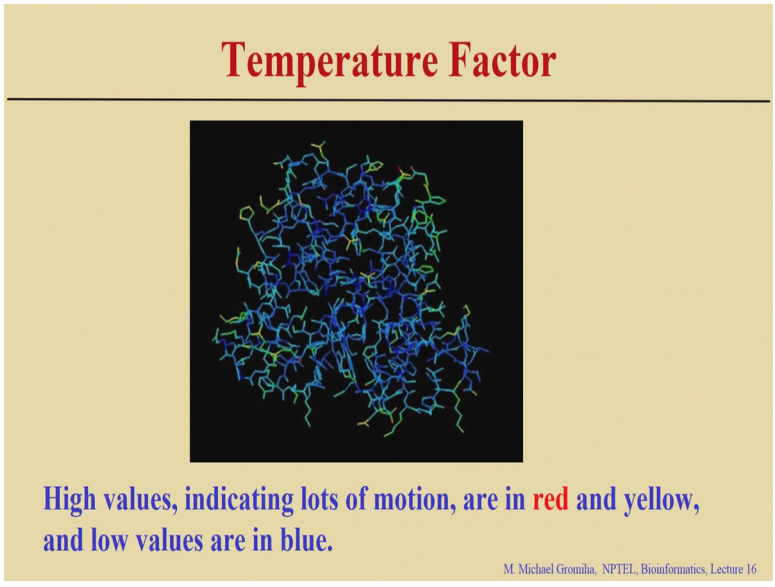

So, here I show the picture, in this case you can see a different colors for example, which is a blue color or some of them are in yellow and the red; is the blue color ones right they are having low values right low values means what is the meaning of low values.

Student: Rigid (blue).

They are rigid that is lower flexibility they are rigid. So, some cases if it is yellow or it is in the red, in this case they have a lot of motions right and in this case they are highly flexible. So, if you see this data right for example, I show the structure right here. So, if you see they are highly flexible because the values are very high in this case, because this is from the DNA and this is from the protein side.

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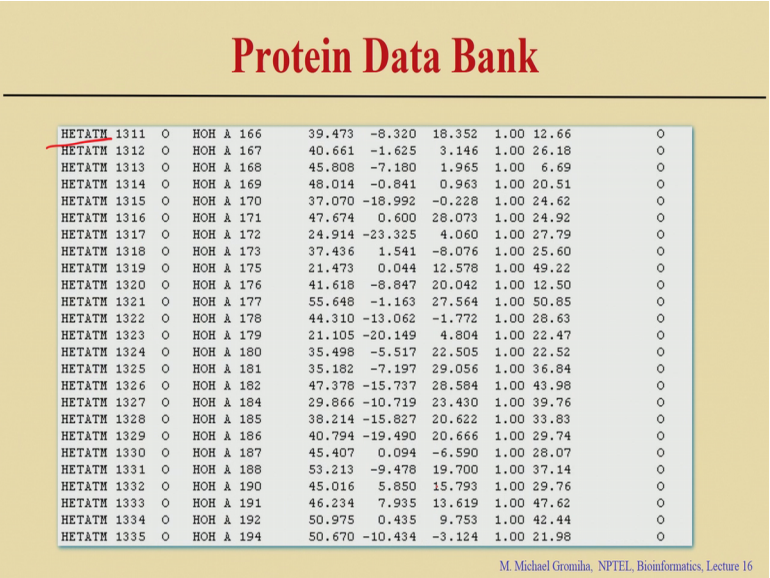

And some cases if you see here and many case to these right. So, here there are less then this case these atoms are rigid.

So, now we get the 3D coordinates, right now I will explain about the various options available in Protein Data Bank.

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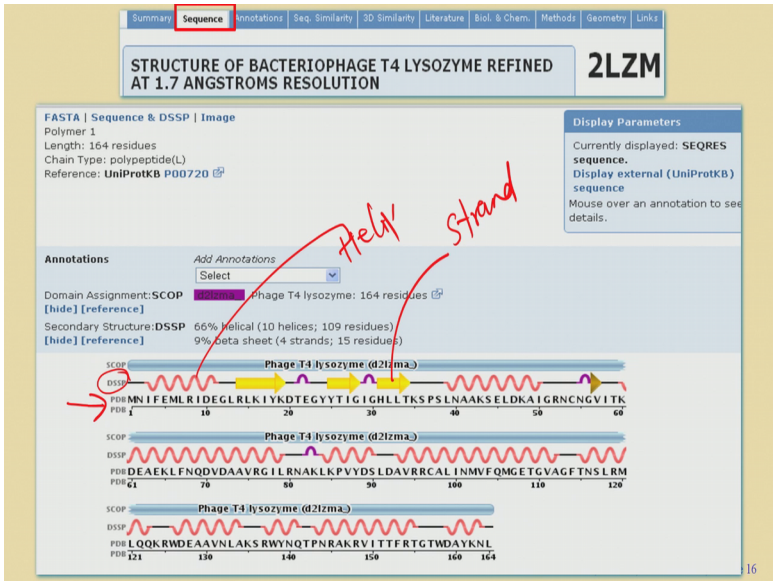

So, first we have the sequence, when we get the sequence information right you can see the amino acid sequence here right. Earlier I showed the fasta format, you can see the PDB here as well as you can see the second structure assignments; what is the meaning of this spiral ones.

Student: Helix

This is helix and this is strand right this is based on the DSSP. What is DSSP? Dictionary of secondary structures of protein. So, they take the PDB structures and based on the hydrogen bonding pattern it will assign the secondary structures right. So, here given the amino acid sequence you can see the helix strands and so on, different secondary structures.

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So, now go to these different annotations, the proteins are classified in different groups, I will explain the details maybe in the next class right in some cases which are dominated by helical regions.

In this case we can say the proteins as helical proteins, and some cases you can see the protein is dominated by beta strands. These proteins we call as beta proteins and some proteins we have both alpha helixes in beta strands, they are called alpha beta proteins or alpha plus beta proteins or mixture proteins. So, there are some databases which have this information right.

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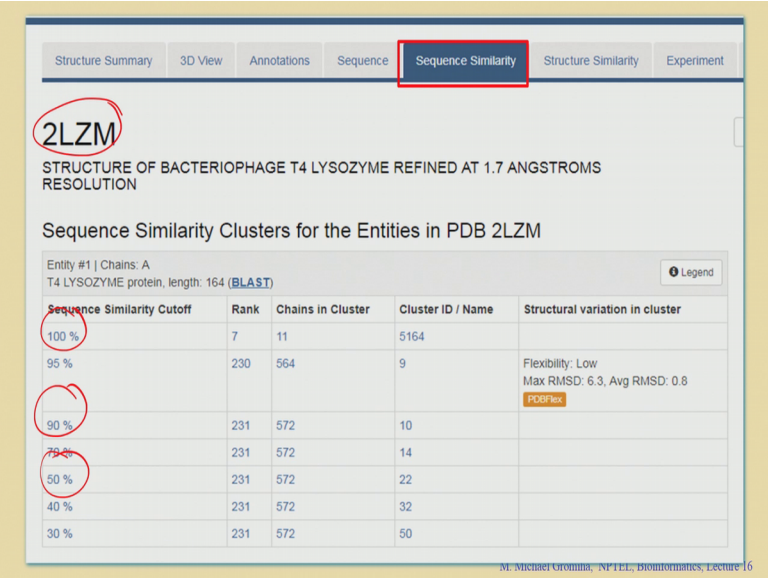

If you see the annotations you will get the information regarding that, that I will explain more detail in next classes.

So, you can see the sequence similarity right the PDB recently revised the page. So, for each similarity for example, 100 percent or 90 percent or 50 percent, they developed several clusters right we discussed about the clustering method right which cluster method we discuss.

Student: CD HIT.

Right will be which clustering method.

Student: k-means.

k-means clustering right. So, it uses the different clusters they keep all the sequences together and they put the similar sequences in one cluster. So, they can make different clusters depending upon the threshold any threshold right. So, we clustered various clusters right with respect to the identity and we can see from these clusters they take the non-redundant sequences, they have the sequence similarity you can get for each a protein right in the PDB.

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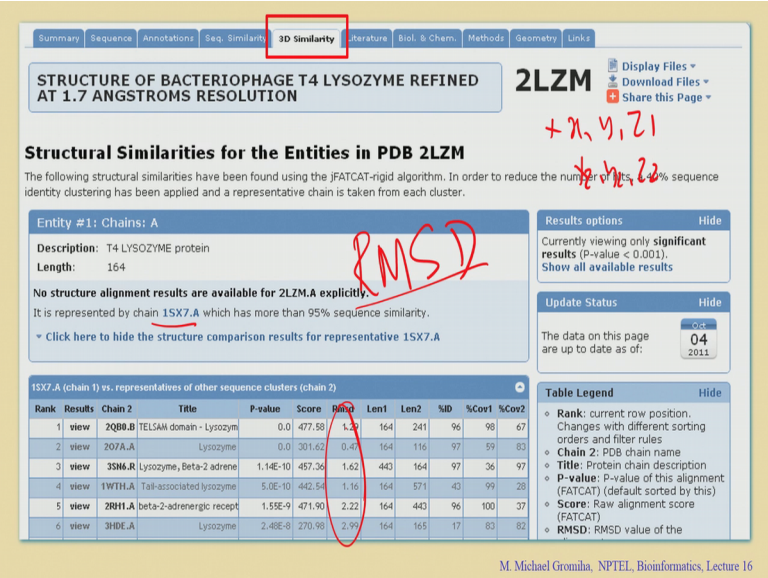

Then you go with the 3D similarity what is 3D similarity? The similarity in the structures.

So, now we discussed about the sequence similarity, in this case we have a sequence align the sequence one which is aligned with sequence two and see why are they are similar. In the case of a 3D similarity, they take ones protein structure and they superimpose this protein with the other protein structures right we will discuss the details later and see how far they are different.

Depending upon a Cα position or all atoms right they define based on the term RMSD that is root mean square deviation. So, here we have the coordinate x1, y1, z1 and x2, y2, z2 they can get the distance when they assigned to superimpose the structures there are several atoms right or several Cα atoms for each way case we calculate the distance and finally, they get the root mean square deviation right this will tell you how far these 2 structures are similar. If the structure are similar then the RMSD is less or high.

Student: Low.

Low right if it is less you can say the structures are similar, if it is very high then we say that they are not similar fine. So, you can have the values right these are the structures right, which you can have the similar structures right. So, in this case they are they align

with the another chain, 1SX7 and to give this root mean square deviation right this 0.47 or 1.29 right they are very close to each other right.

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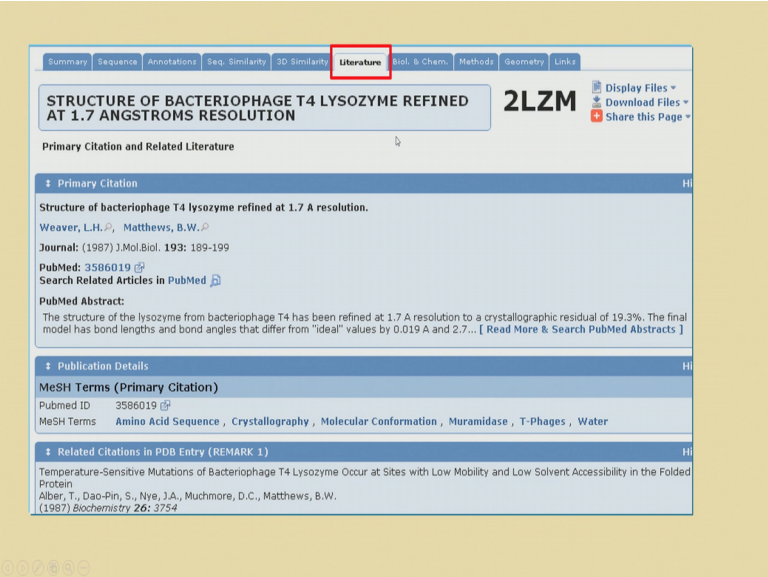

Then we go the literature, literature will give you the information on the papers which have been published.

So, based on different techniques or different stability or different information right in the literature for example, for the structure to T4 lysozyme right there are various papers published on this aspect so, the listed of the primary citations for that particular paper.

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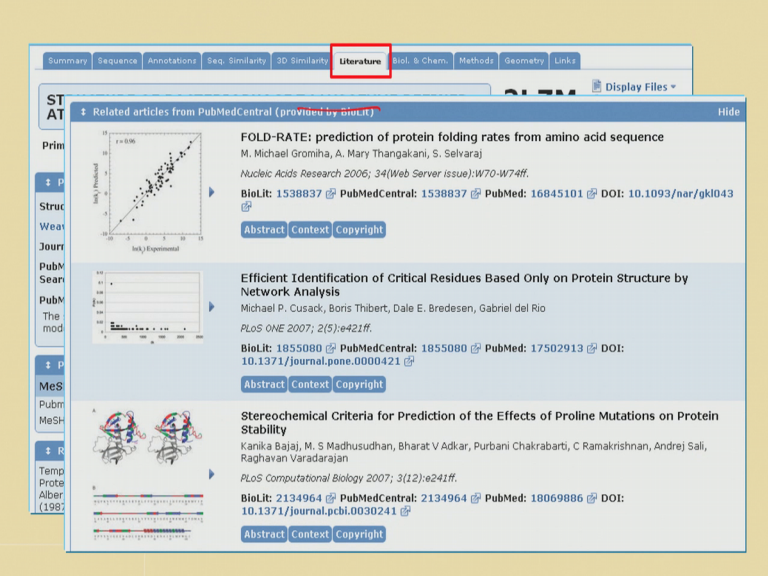

So, then if you see they also linked with the other papers which used the PDB structures for example, there are several other methods right so, for example this fold rate, and getting critical residues and the effect of proline mutations and stability right.

So, there are various methods, these papers they use the PDB structures for developing a model right. So, there are several papers they use the structural information right further analysis, the listed of all the papers in the side.

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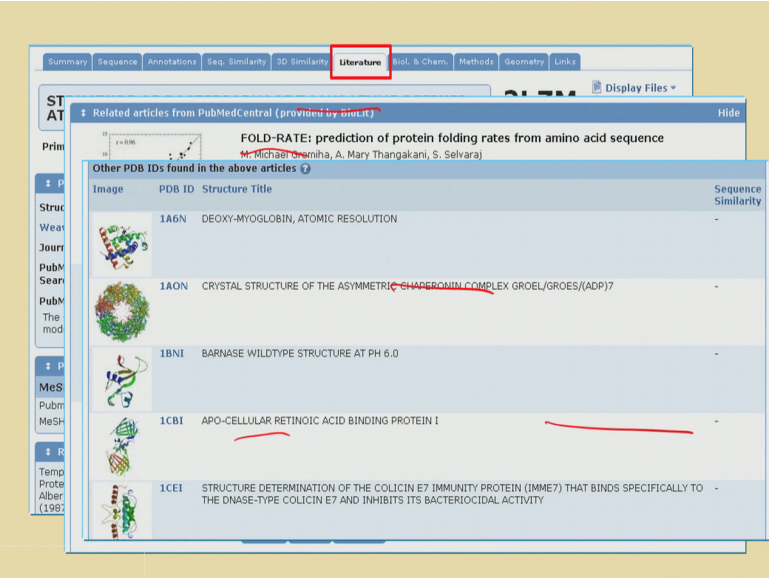

So, if you click on this one right then if you see these are the structures which are used in the paper. They also give the data about the structures they used in a particular paper right. So, this will give you the PDB is important; PDB structures are important and the PDB structures are widely used for the analysis as well as for developing prediction methods.

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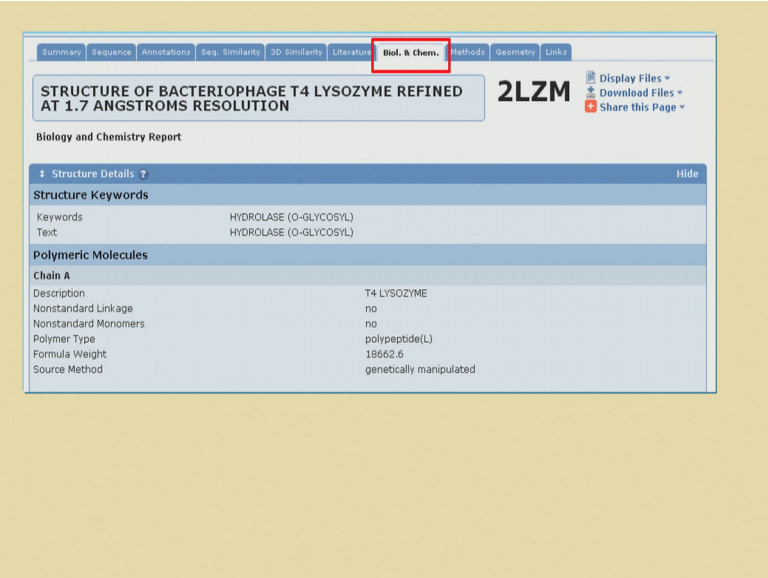

So, you get the biology and chemistry.

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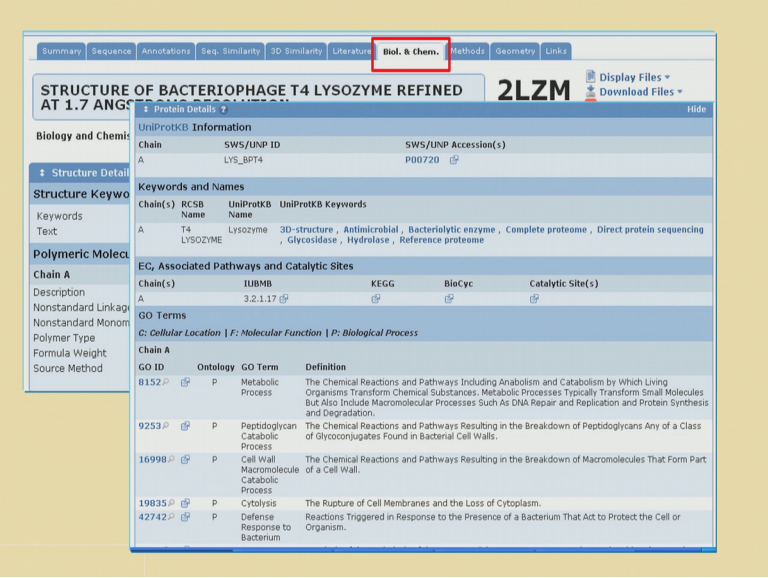

So, you can give the structural keywords right as well as the description of the proteins the weight and the source method and so on right.

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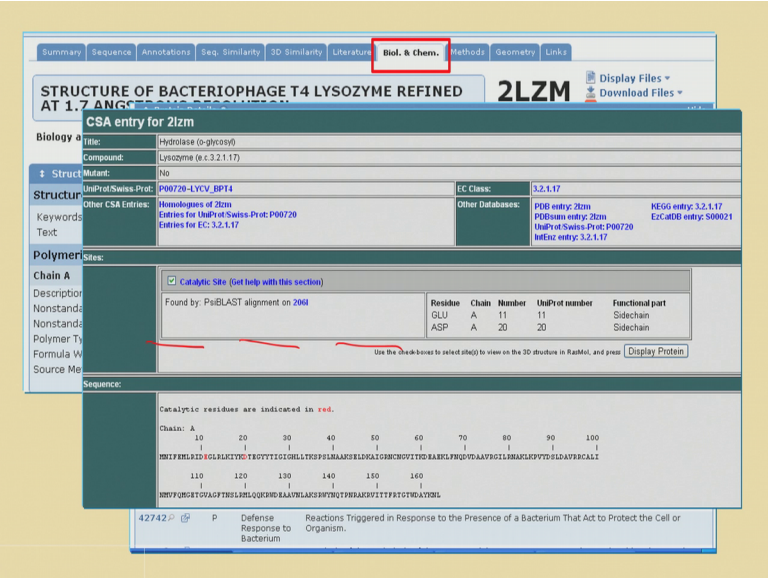

And we can get the information regarding the go terms like the cellular location, molecular function or biological process; and you can if it is enzymes and we can get the catalytic site residues right. So, what is catalytic site residues?

Student: Residue which perform catalysis.

Catalysis right this is shorter, to small sequence right. So, we can see for example, which is the database you get the catalytic site residues?

Student: Catalytic Site Atlas

Catalytic Site Atlas right you can see a CSA right we will get this information you can see, these are the residues right which are important and acting as a catalytic site residues.

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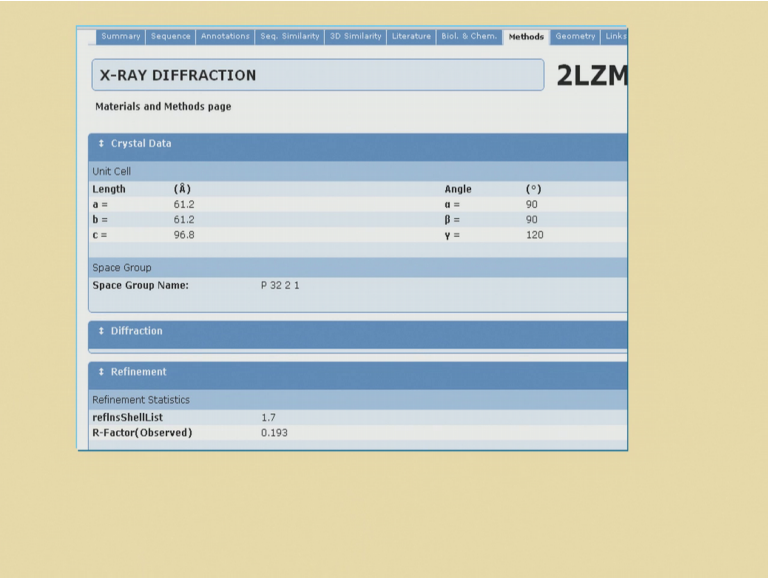

So, the X-ray diffraction they will give the crystal data for example, if we have the any crystals, they have the length abc and the space groups right and they give all this information.

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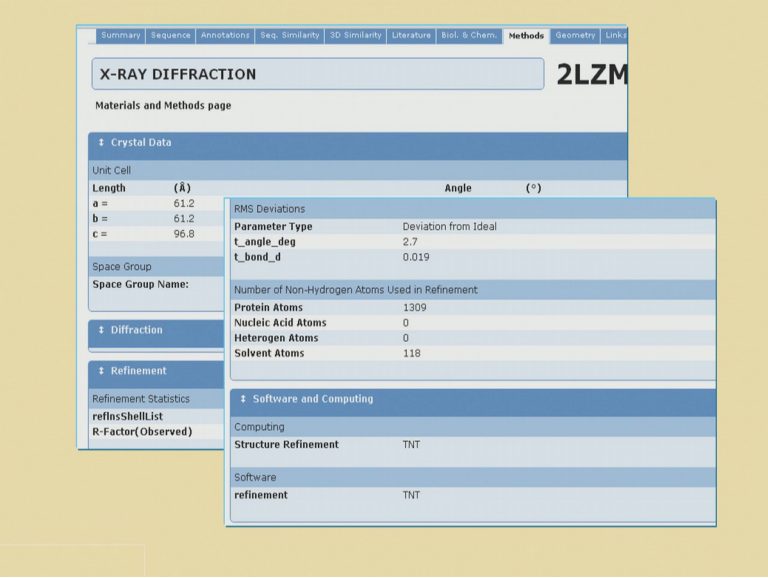

As well as the number of hetero atoms, solvent atoms, and a refinement.

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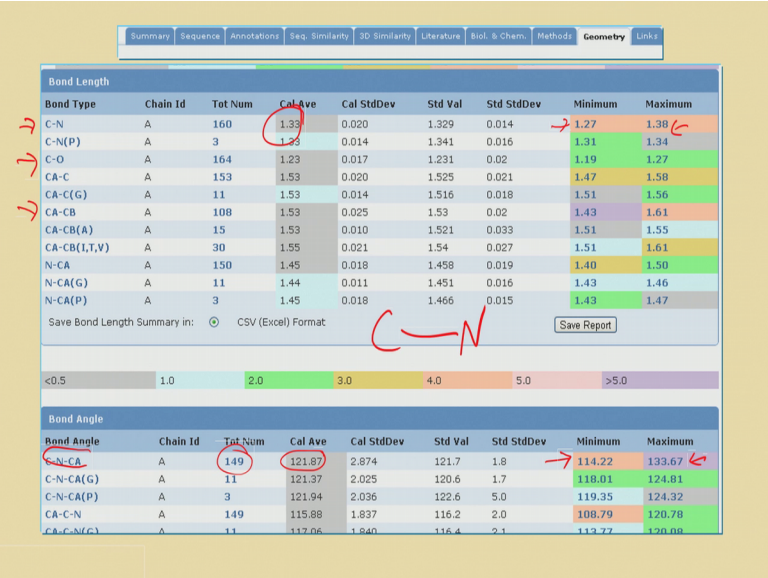

And then here you can give the bond length right. There are various types of atoms like between C and N and C and O, Cα and Cβ right.

So, different types of this bond length, they give the average and the standard deviation. For example, if you have a C and N what is the bond length for the C and N where is 1.33 right because C and N right. So, you can see this is 1.33 and the standard deviation we give. These are minimum 1.27 this is 1.38 right this is the minimum and this is a maximum fine then in case of bond angle, how many atoms are required to look at the bond angle.

Student: 3.

Three right. So, you can put the C and Cα right if it is C and N and Cα right. So, you can see this is the average where 149 angles 129.87 is the average. So, the deviation is also not much right 114 to 133. So, this is the minimum value, this is a maximum value and you can see the average as well as the deviation then take a torsion angle.

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So, we discussed earlier about torsion angle. So, you can see the four different atoms right. So, the phi and psi angles right you can give the average values the minimum and the maximum is over here and you can see the average value for the different dihedral angles.

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Then we go with this the methods the and the and the geometry right as well as the given links; the structural summary, structural features, ligand features and so on this you can get all the information right. So, then you go to the PDB right https://www.rcsb.org/

right, then you can get all the information regarding a protein. So, just you try with any of the PDB IDs right and you can read the details, which are available in Protein Data Bank right.

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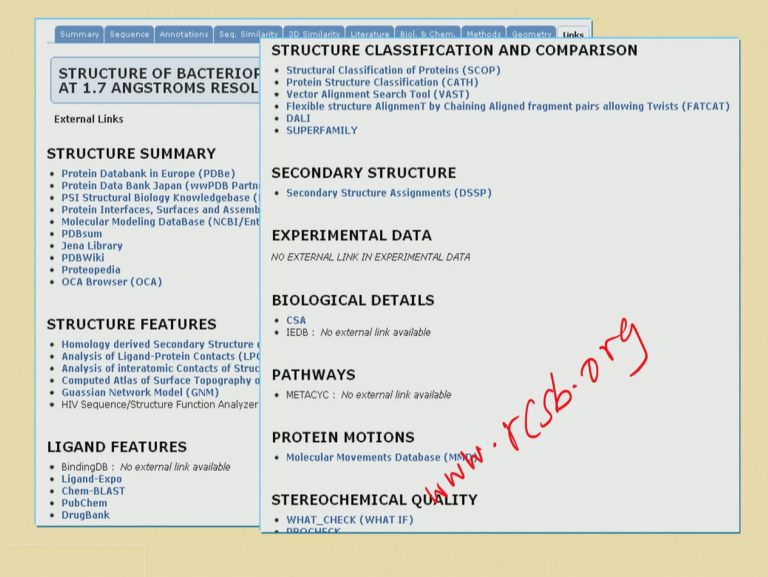

So, the classifications and then biological details and other information regarding the pathways and motions and so on. So, the PDB has several options to search and to get the data; first you can use the simple search, in this case you can search with the UniProt or any PDB ID or you can the names right any keywords. So, you can use any of this information in the simple search and you will get the information.

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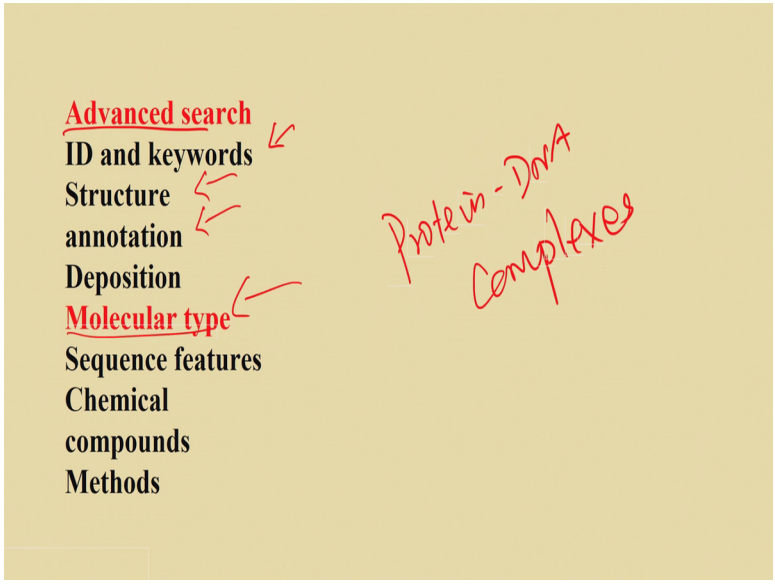

And they have the advanced search; in this case you can search with the various other options. You can check with the ID and keywords or the structure or any type of annotation or the molecular type, sequence features, chemical compounds and methods.

For example if you want to get the data for all protein-DNA complexes right if you are interested in the protein-DNA complexes right. So, in this case which keywords you have to search which option you have to search for to get the protein DNA complexes.

Student: Molecule type

These are molecular type because there are several molecular types and I show at the beginning, there are many proteins and several nucleic acids and as well as some protein nucleic acid complexes. If you want to have the protein-protein complex, you can select the proteins and see where we need the monomer or the dimer or the trimer and so on right. If you are interested in protein-DNA complexes right you go to the molecule type there you can get the, ok next box will open.

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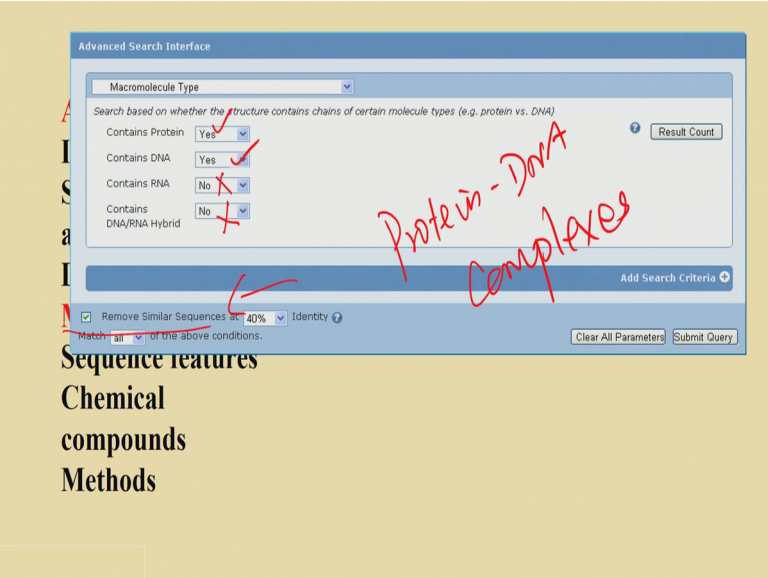

So, you have you have the questions. So, first the question is whether it containing protein right yes or no? yes because we need protein DNA complexes.

So, this is yes and it contains DNA you need? yes right. So, you put yes then it contains RNA no right because here we do not need this RNA, because we are interested in protein DNA complexes. Then we need to contain protein DNA and the RNA hybrid, there also no need because we are mainly interested in protein DNA complexes. So, if you want to have the protein DNA complexes, we search for the proteins and DNA.

So, if you do this right we can get the data; in this case you also have another option whether do you need to remove the sequences with some redundancy, if you want to remove you can also remove the redundancy you can cut say some cutoff identity. If you do not want just you do not have to remove; if you want to remove you have to put this and then give; there are several options you can click which redundancy do you want. So, you have a 40 percent identity. So, then now we get the data.

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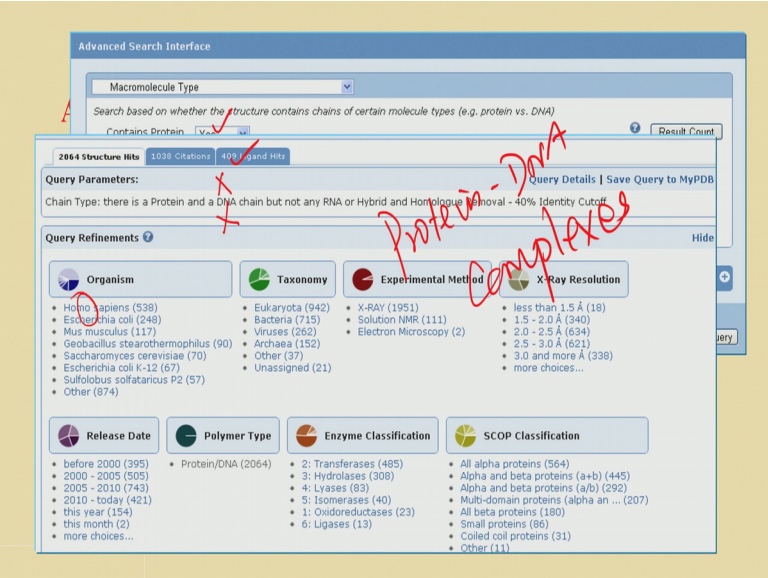

So, here also they classify different groups, you can see the organisms you will get the homo sapiens 538, and equal to 48. So, you can make the classifications and you can analyze separately if you are interested. Then you have the taxonomy different methods and resolution. If you want a higher resolution structures, you take these right you will get the good number of structures, then you are interested in latest data. So, you can have the data which are very latest. So, in this case we get this month, they have 2 structures deposited in the database for the protein nucleic acid DNA complex.

But polymer type is protein DNA then we have a different enzyme classification. So, these are the different classifications and different types of proteins right this I will discuss later about the SCOP classification. So, if you want to have a group of proteins, you can get the group with different aspects. We can give the different organism, different taxonomy, different methods and different enzyme classification and so on. If you want to have a data on protein-protein complexes you know what to do.

Student: Check on protein-protein.

You can get the proteins, but you need to have the complex means, at least you require 2. So, in this case you can select the number of chains right minimum 2. If you want to have the different proteins not the homodimer or a homopolymer, if only heterodimers or heteropolymers then if you have to mention the chain length should be different then you

can get the heterodimers or heteropolymers right. So, likewise you can get the information and collect the data from the Protein Data Bank.

So, now if you have these complexes and we can get lot of information on the proteins right and you can also use these structures to obtain various parameters, right and you can also visualize the protein and the protein structures I show one static structure, right, this is a right this is a kind of static structure.

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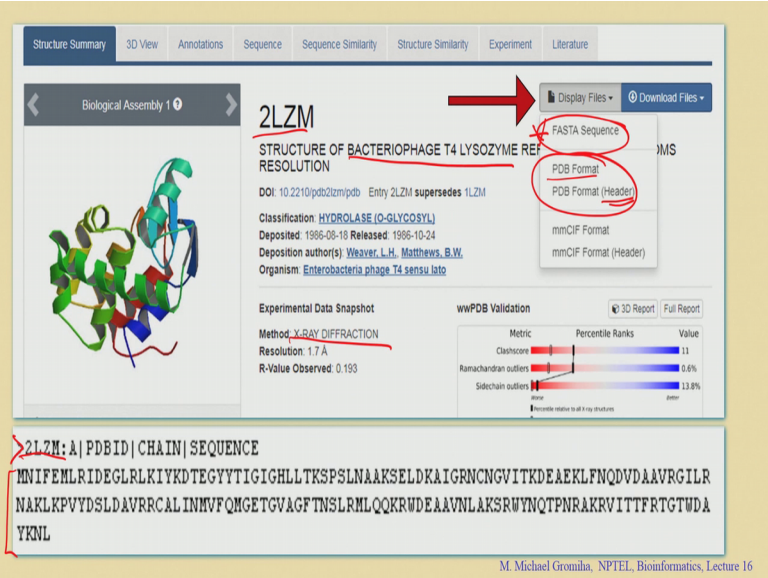

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So, you can see only one motion right this is only one view. So, you can view this protein and you can view in different directions and also you can observe various information from these particular proteins right.

So, there are several software available, to visualize the proteins and to get the information from these protein structures.

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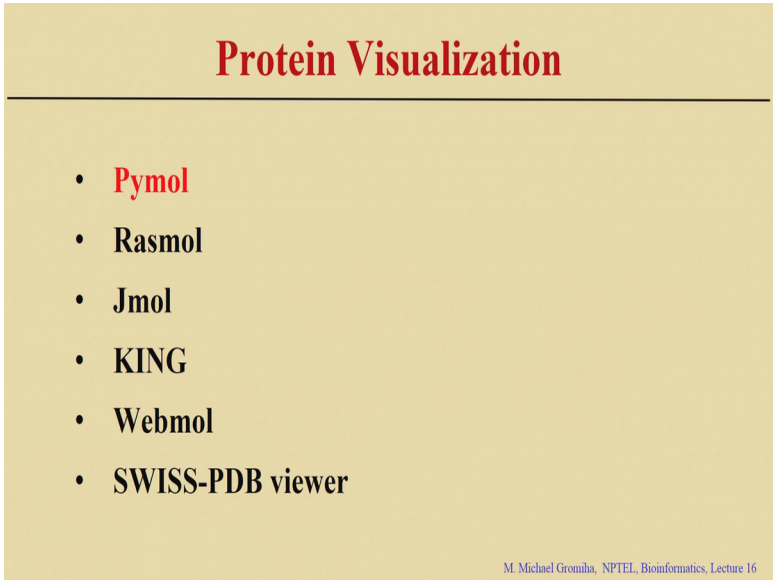

The commonly available software for visualizing protein is the Pymol and Rasmol Jmol KING and Webmol they are developed earlier days and Swiss-PDB viewer. So, Rasmol is one of the oldest ones right we just to view this a protein structure to and to understand how they make the contacts and what are the interactions and all these things right currently Jmol, Swiss-PDB viewer, and Pymol are widely used software to visualize protein structures.

And among all these things Pymol is getting famous, because you can get the publication quality figures. And also there are several options available in Pymol, right I can you can be fruitfully utilize the Pymol for rotating several information for a protein structure. I will show you short demonstration right about the utility is available in the Pymol, in earlier days when they started the Pymol, it was free for everyone right then after sometime when it is getting famous because many users is started to use its Pymol software then the Schrodinger bought this Pymol and they incorporated inside this Schrodinger software. So, they became commercial right; however, they are kind enough to give this for free for educational purposes with the most of the utilities.

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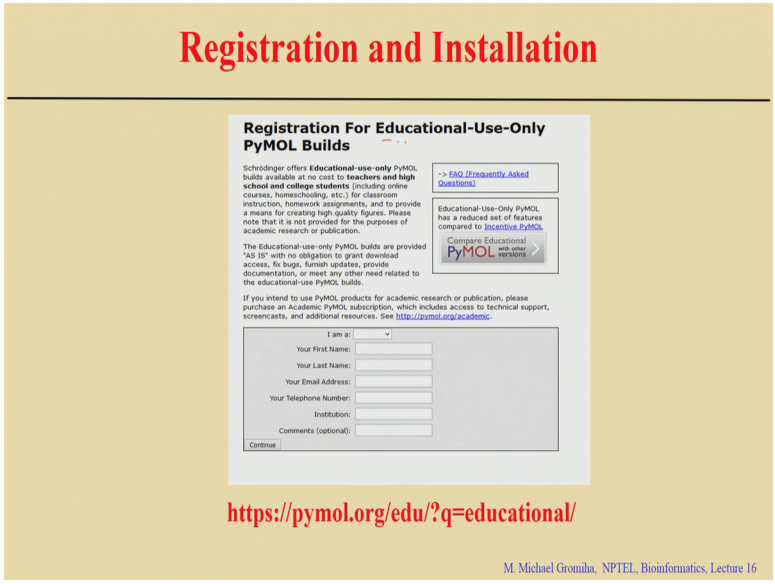

So, if you want to get this Pymol for the educational use, first we need to register and you have to get the software right by giving the necessary information right to the developers. So, you give a necessary information, then they will give the key right and then you can register right and you can install the software right in your desktop. So, here this is the web website where you can get the Pymol login, fine. So, once you get this Pymol, right and then you start to use it. So, when you install and even you launch Pymol, we can get 2 windows, right.

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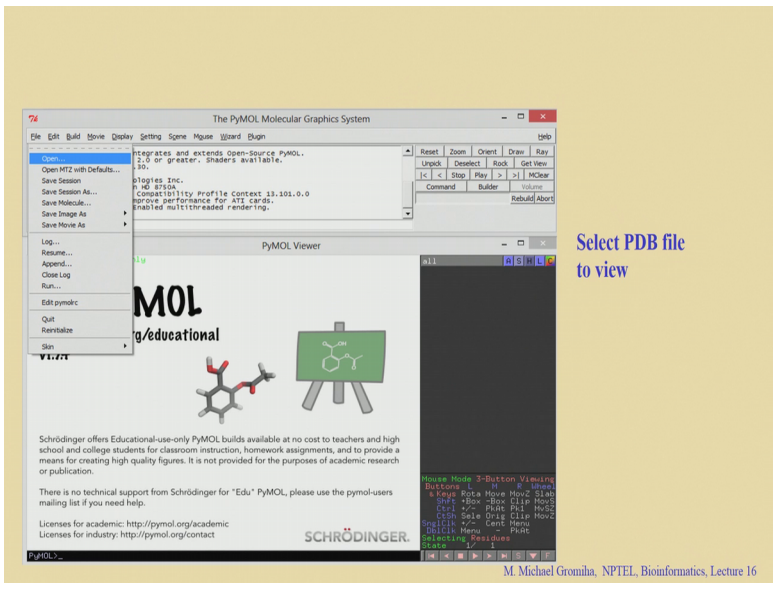

So, you can see this is one window and this is with a command prompt, we can use any command right in this space and execute the program. Then you can see the next one the down. So, here this is the viewer window. So, here you can see the; your molecule and you can do some manipulations in this a protein molecule right. So, first we need a structure. So, it accepts the PDB and also several other formats for the PDB just if you go to the file and then we take the option open, it will ask you the file which you want to open.

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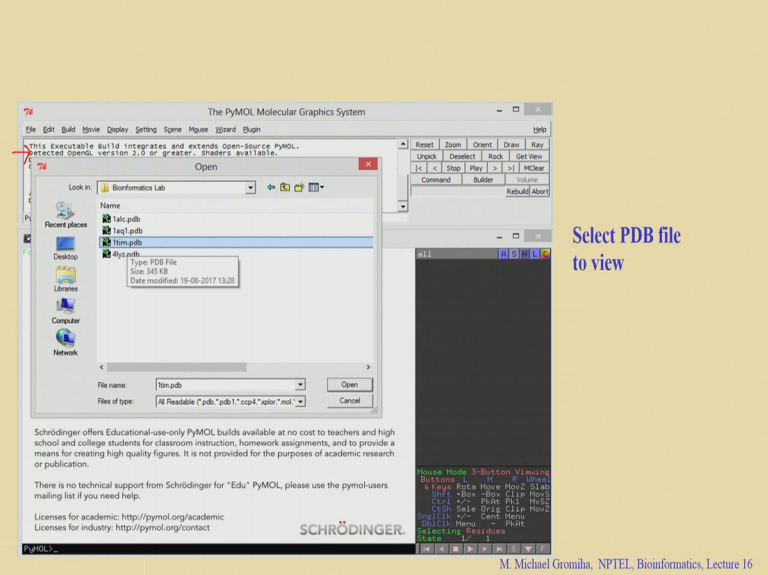

So, then we go to your directory. So, 1tim.pdb this is the one if you choose right when you open it right then you can see these structure here right.

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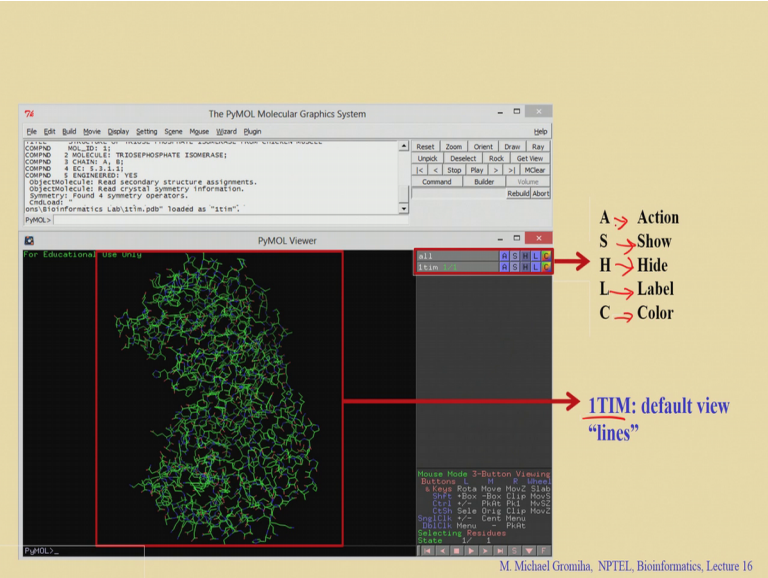

You can easily see the structures. So, default is lines. So, we can see several lines here, here we represents the PDB ID 1TIM right this is the PDB ID which you can see in this picture right. So, when you see the right side then you can see these 5 letters ASHL and C; A is for the action this will tell you what you want to do and S is for to show right whether you want to show the atoms or show the structures or not and H is to hide.

Now, if you do not want to see then you can hide and L is to label and C is to color right and A is for the action right. I will tell you a few examples through how we use these.

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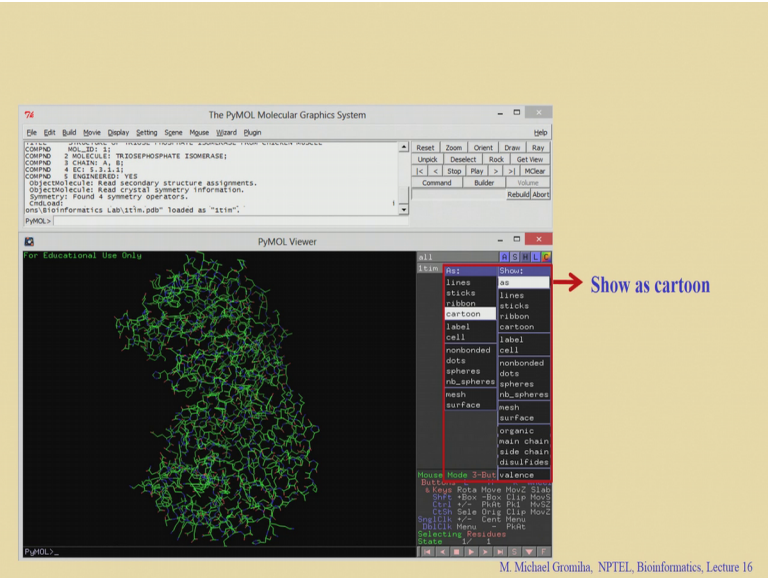

So, first you want to show this as a cartoon. So, we use this s right we can see this is the S here. So, you want to show this as I got currently it is lines if you want to show in cartoon right then you go to S and show as cartoon if you do like this, then you can get the picture figure like this; it is a kind of cartoon. If you see this one, it is very difficult to see where are the helix and strand can we see this where you can see the helix and strand? We cannot see that right it is very difficult.

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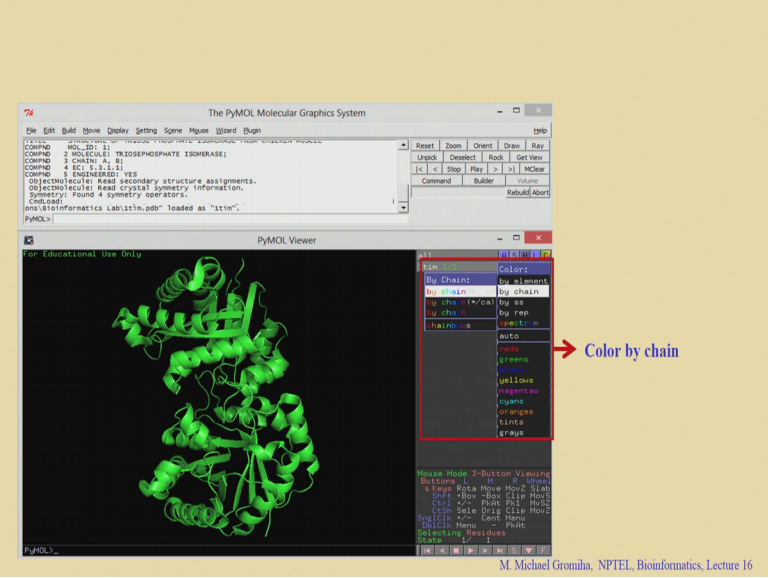

If you see here then here you can see where the helix are located, and where the strands are located now you can see the spirals here they represent the helix and you can see the arrows that we can see these are strands then also you can color by chains. If you see this one how many chains in this structure we do not know right may be 1 maybe 2 right if you color by chain right automatically it will color right.

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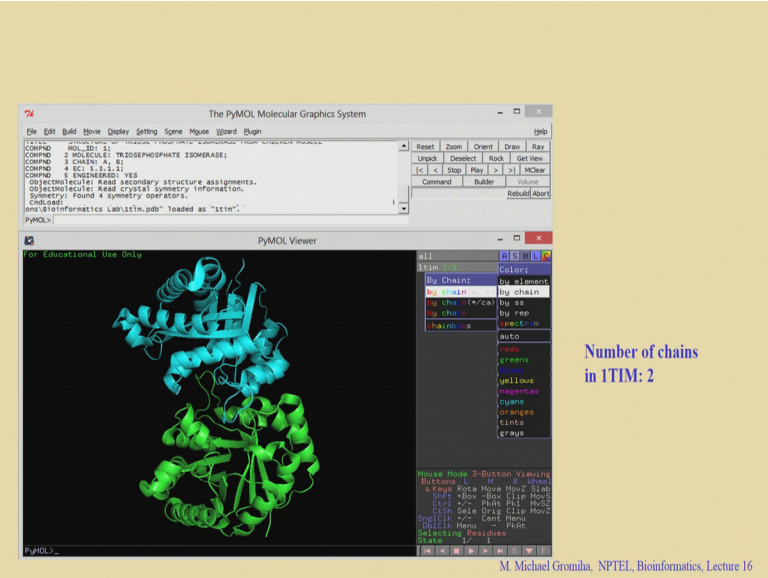

Now, we can see how many chains 2 easily you can see right. So, you can use this information current information, we can see now there are 2 chain this is one and this is two right in this chain.

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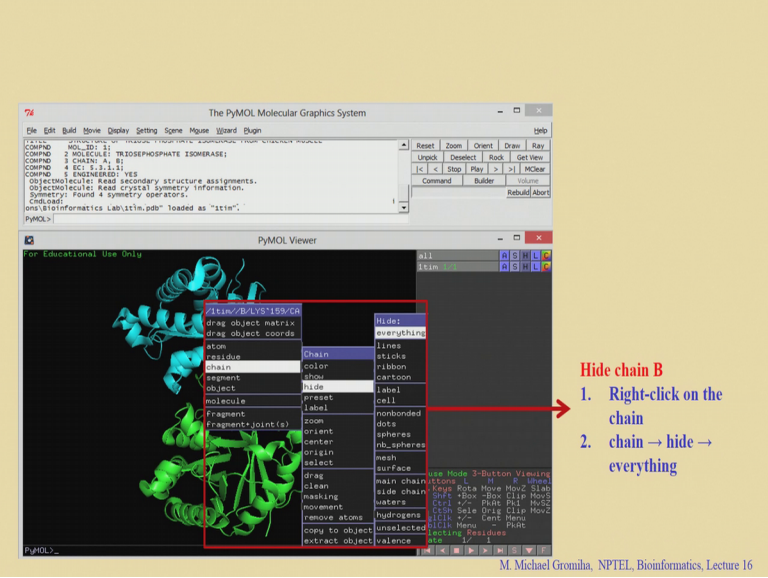

So, now we can also hide for the 2 chains here if you want to hide one chain. So, you right click on the chain right and you can get this information like for example, chain information and if you go to this hide right the chain and hide. So, on click on everything right and you can see one chain is hide here 2 chains. So, we select one chain this chain

we selected and if you hide that chain. So, now, that chain is hide then we can see one chain. It is also possible to zoom in and zoom out and also you can change the orientations also change the locations, we can move this mouse and you can change it to the different orientations right and you can have different views as well as you can zoom in or the zoom out this particular structure.

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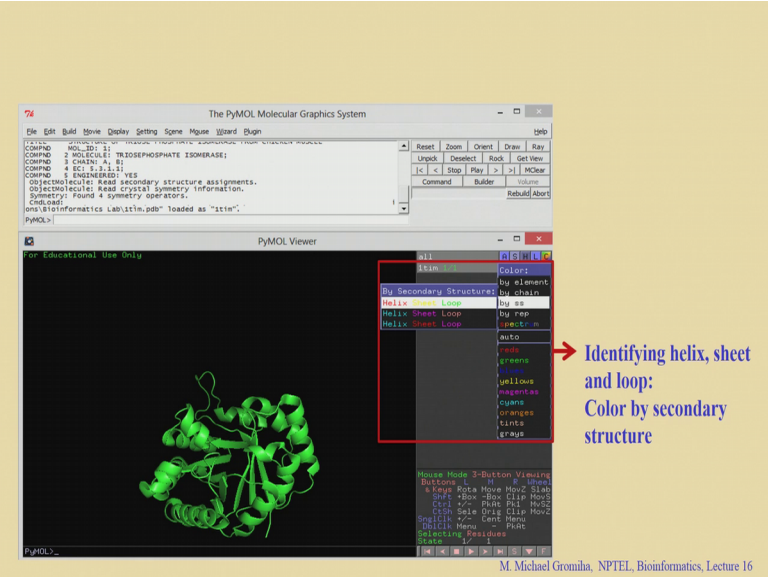

So, now if you want to see the different secondary structures in different colors; for example, if you want to see the helix strand and the loop. So, the different color options, here we use red as helix, and yellow as the strand and the green as loop right in this case you can see this is the case red is helix right. You can say helix here and you can see the strand in this yellow one and the loop right in this green one you can clearly see the difference between all these secondary structures.

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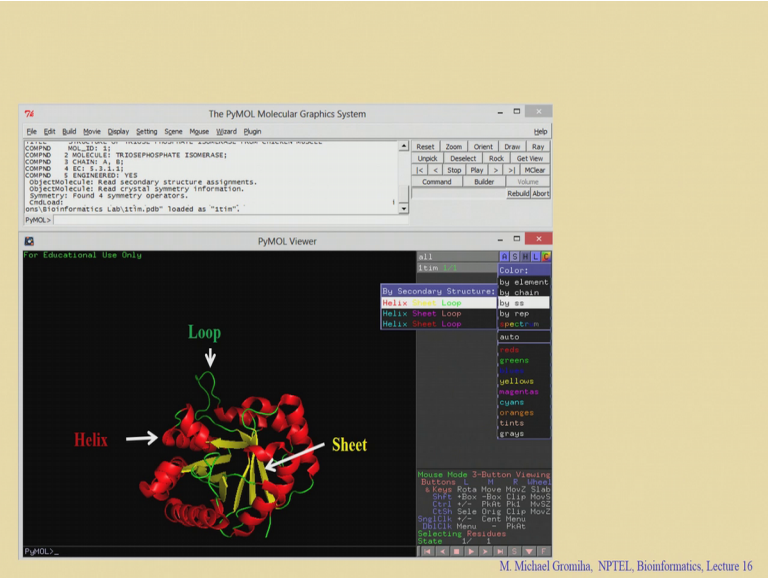

So, now if you want to display a sequence now we would dealing with the sequence in the structure.

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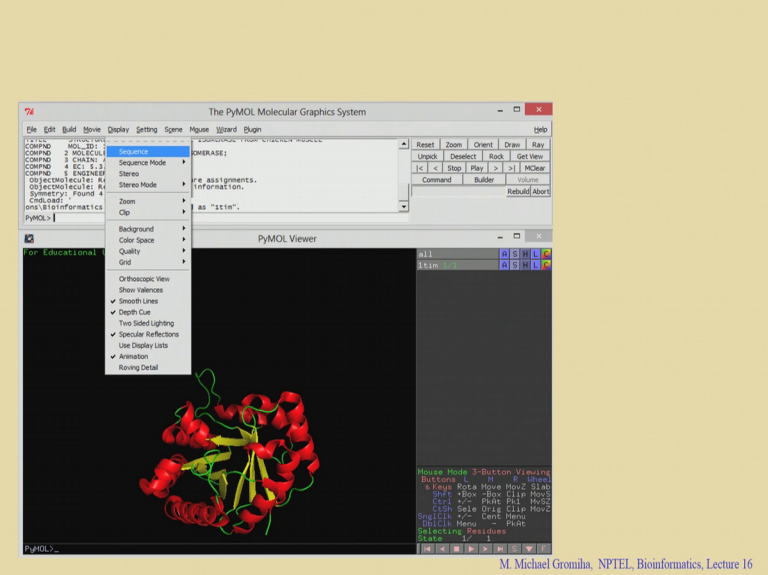

If you want to show the sequence and see; where are the helix is. In this case you go to the display option right you have the display option here, and you get this option you called the sequence right if you show the sequence then you can see a sequence.

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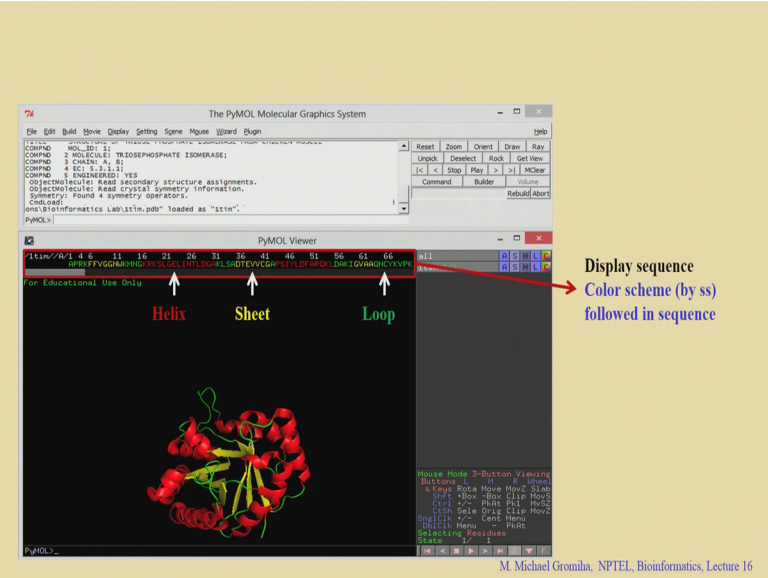

Also if you see this region corresponds to helix here, and this region corresponds the strand and this region corresponds the loop right.

You can see the same color we applied to a sequence and the structure. So, you can map and see where you are the helical segments strands as well as the loops, in the sequence as well as in the structure.

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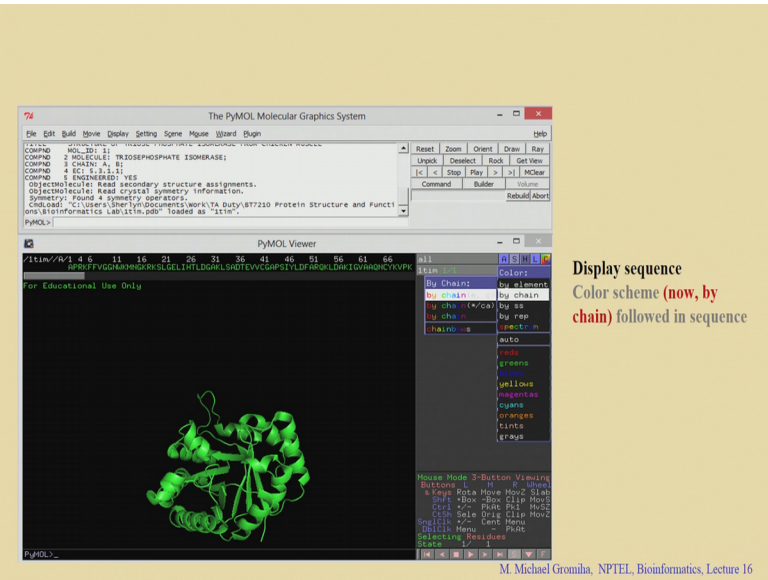

So, you can also change the color in terms of the chains right if we were to this very long if you drag through, then you can see one sequence in one color right and the another sequence in another color.

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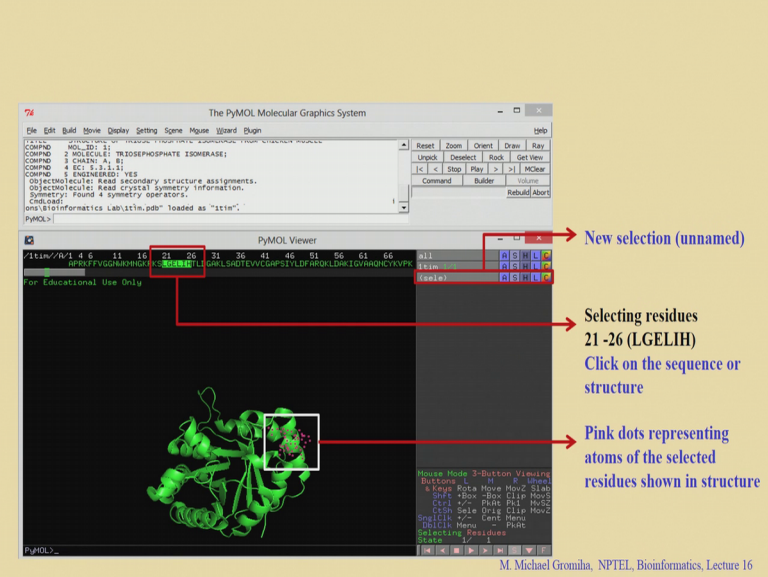

So, now if you want to see a few segments any segments or if you want to measure any bond length or bond angle or torsion angle. So, you have selected the segment 21 to 26 right it is very simple just you click on this sequence, then that is represented in the structure.

You can see the same in the structure the pink dots these are the residues which represent the same in the sequence for example, LGELIH.

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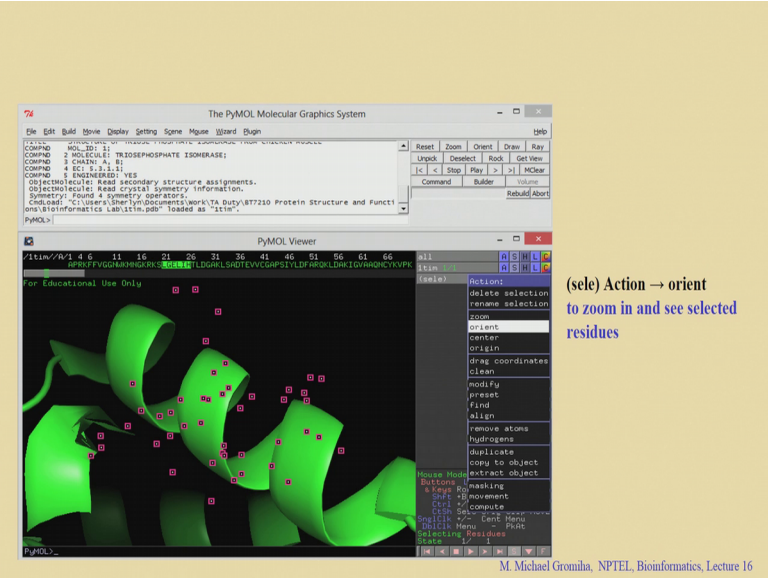

So, now you can see and you can zoom in to select the residues, you can see the pink ones these are the selected residues and you can hide all others.

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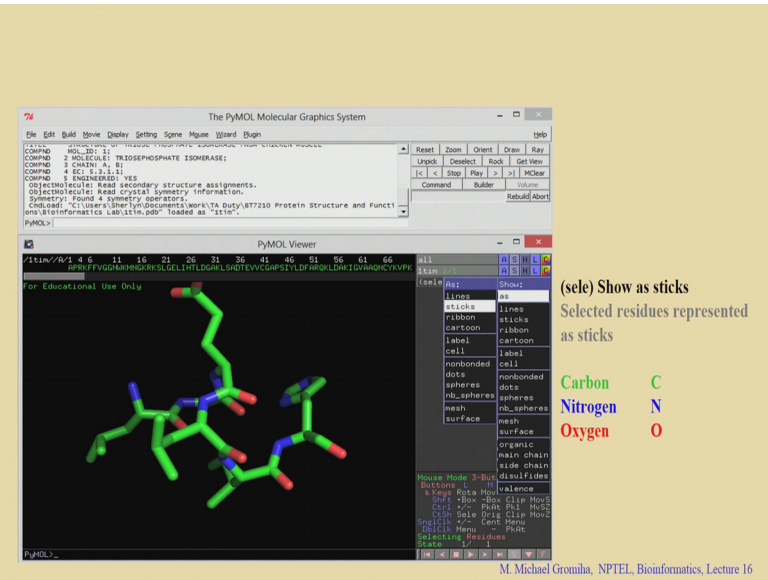

So, if you see these specific residues in the ball and sticks, right what is ball and stick model?

Student: A bond.

Yeah sticks represent the bonds and the balls represent the atoms. So, if you see here there are different colors right they follow a specific color for any specific atoms for example, the green as carbon and N for this nitrogen is a blue right and the oxygen is in red right this is oxygen right this is the nitrogen and you can see this is the carbon now you can see this.

Now, you can label the residues right. So, here this is the; we have the residues GLU-23 is here 23, leucine 24 and isoleucine is in 25. So, this is the one we selected. So, these residues are given here. So, we take glutamic acid 23 it is marked here.

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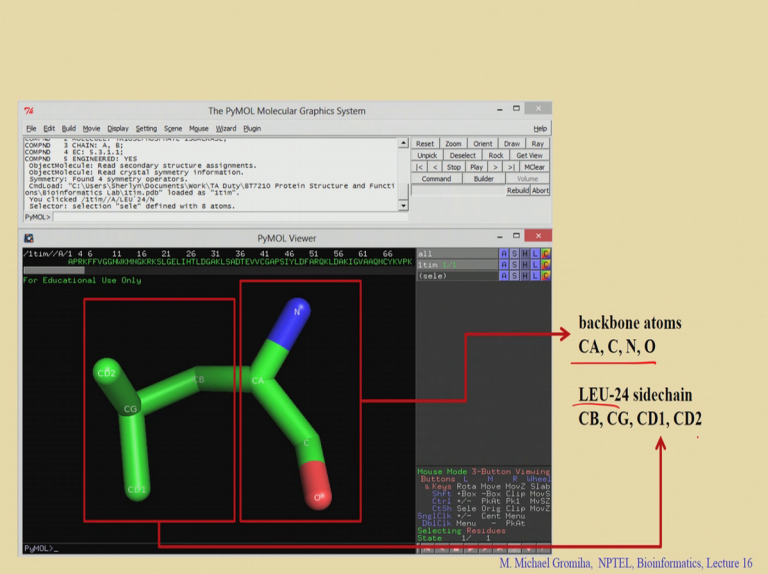

So, you can also know the selected using 24 and you can also mark with this atom name here you labeled this is Cα and we have Cβ Cγ this is the main chain right and here the side chain ok.

So, marked here these are the main chain atoms then what are main chain atoms.

Student: (Refer Time: 24:15).

N, CA, CO, right, this is a main chain atoms you and this one right the backbone atoms and here these are the side chain atoms right this is leucine.

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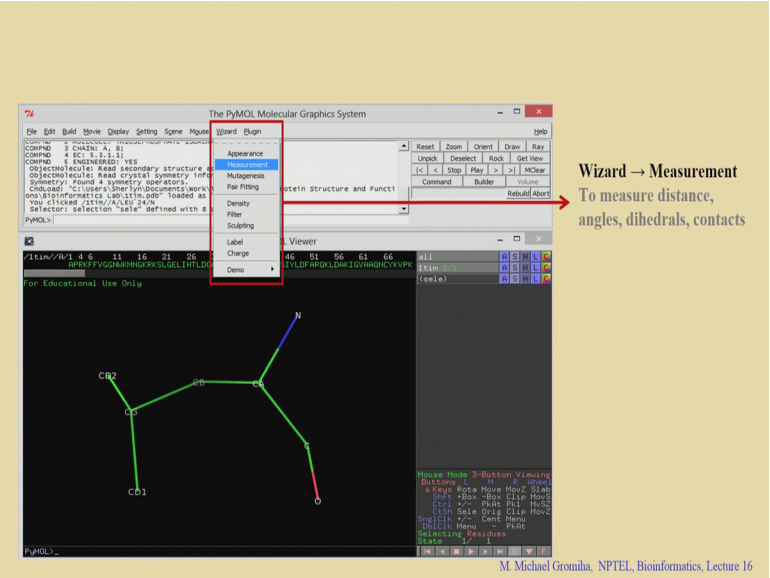

So, they have a side chain Cβ, Cγ, Cδ1, Cδ2 right this is a shown here, then you can also see in this a line a line options and so on. It is also possible to measure the bond length bond angle and torsion angle. So, in this case go to wizard right and then go to the measurement right it will ask for the atoms to measure the distance, angles, dihedrals as well as the contacts how many attempts are required to get the distance?

Student: 2.

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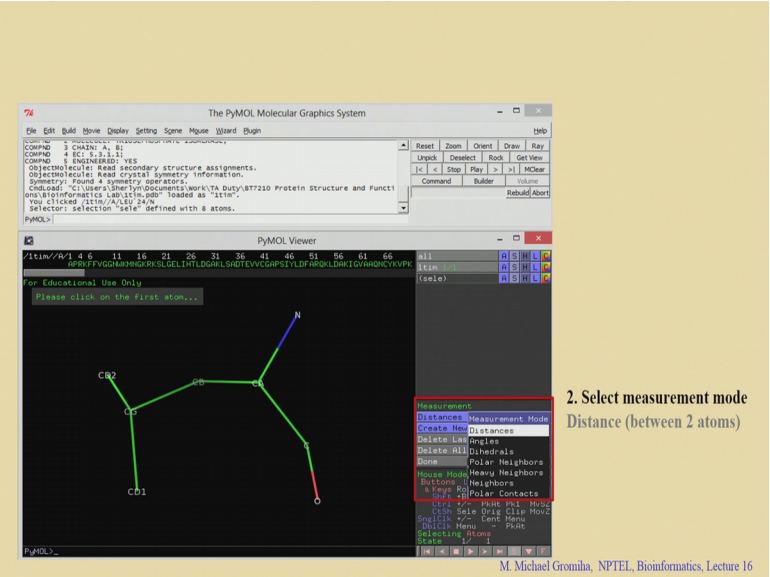

Two right. So, if you want to get the distance, it will ask the atoms select the first atom right to click on the first atom.

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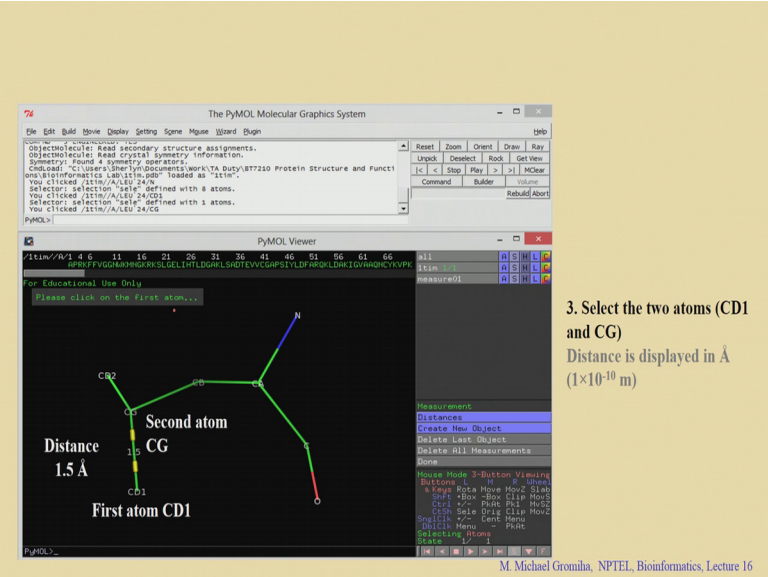

So, we click on the first atom right say this one right and last 2 are the second atom. So, they click on second atom. So, now, it is CD1 and the CG right. So, what is the distance is 1.5 Å. So, Å the Å it is equal to one into 10^{-10} meter right 10^{-8} centimeter right.

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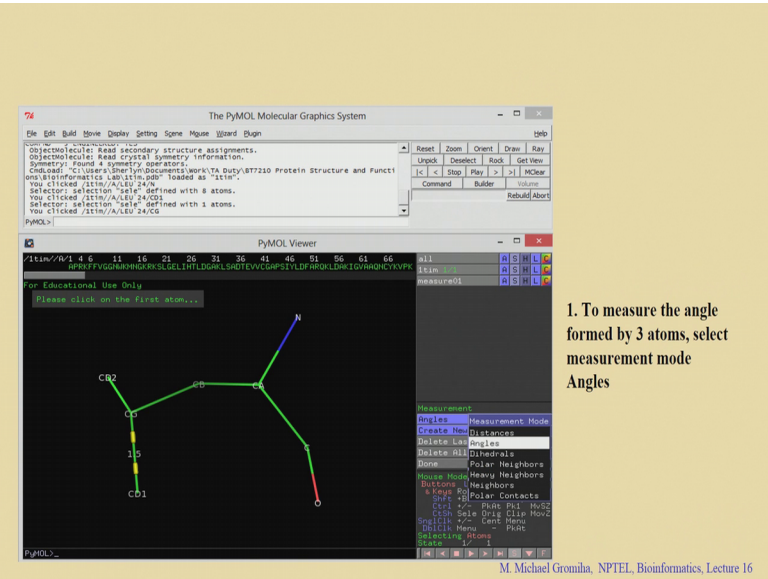

So, we can see this is the angle this distance 1.5 Å between cG and the CD1 like we have this angle how many atoms you require 3 right. So, we have to select 3 atoms to get the angle.

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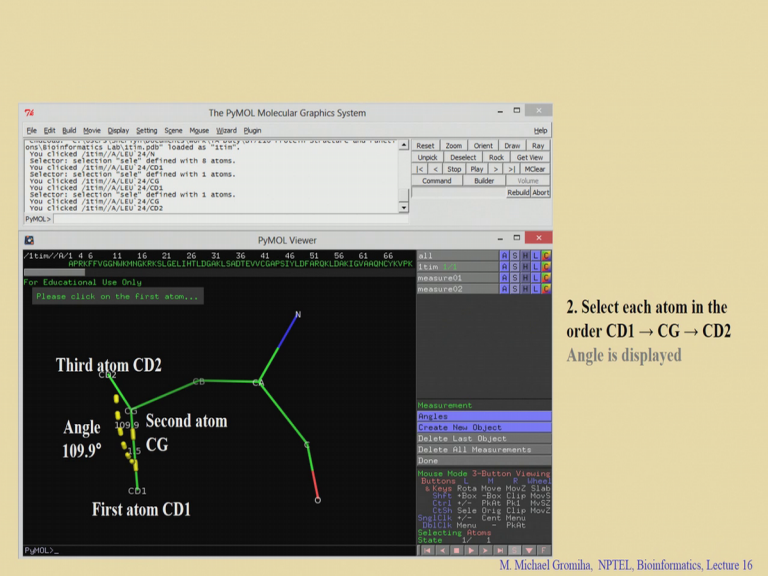

So, you can see that CD1 right 1 2 3 right if you CD1, CG and CD2, if we give click 3 atoms then this will give you the angle. So, the angle is 109.9 degrees likewise we can use this Pymol for various aspects you can see the mutations, you can see the molecular surface and you can see the interactions, you can see the contacts right for example, hydrophobic interaction this electrostatic interactions.

So, we can play around a lot with this Pymol. I will show one more example for example, to visualize B-factors.

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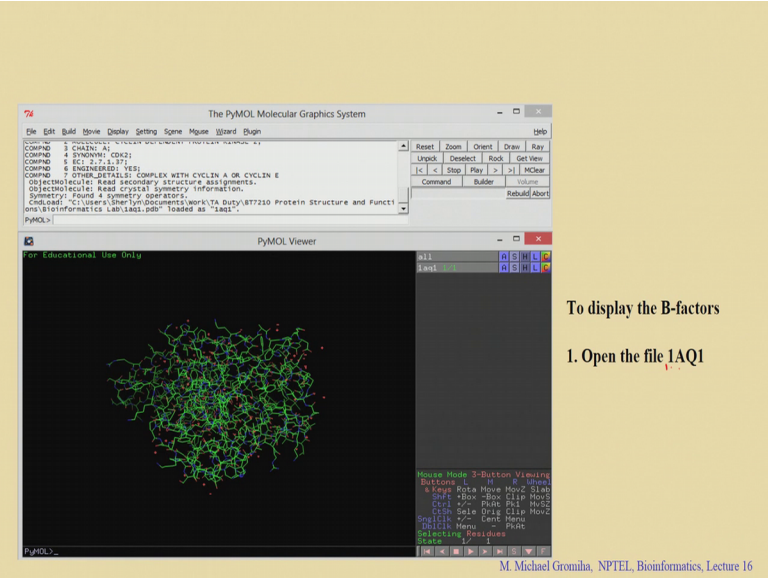

Now, we discussed B-factor what is the B-factor? Its temperature factor this will give you the fluctuations of each residues right for example, how much they fluctuated and how far they are rigid. So, if you see this one if I take this file. So, I take 181 right they open this file in this line lines right.

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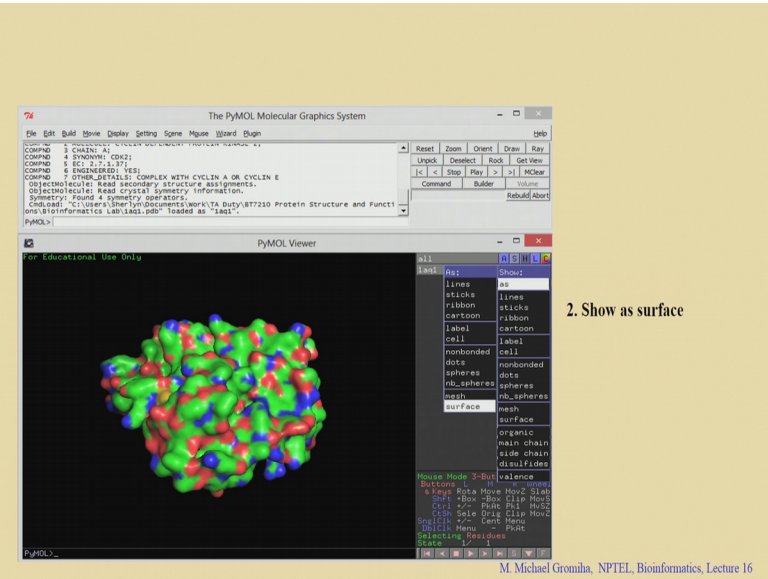

So, this is you can see on a surface right this is the line one and you can see the surface and from this you can see the B-factors the different colors.

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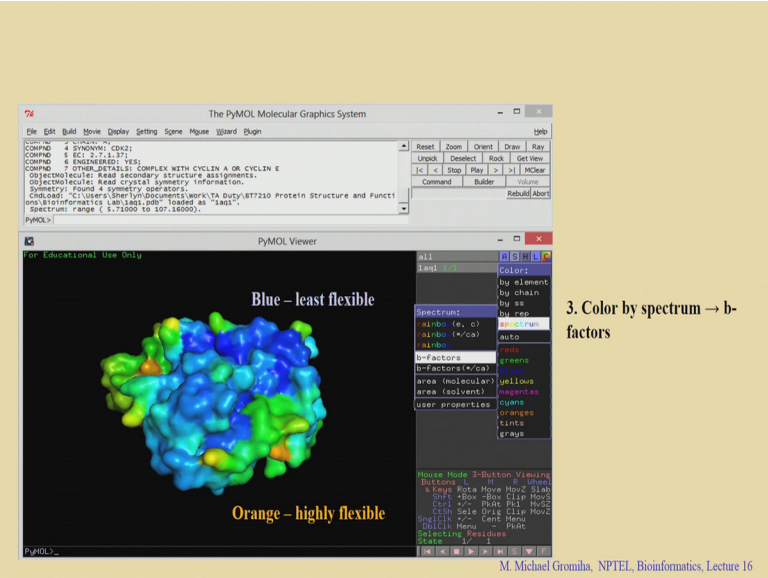

You can see the blue colors this is rigid right, there is less flexible and you can see the orange ones here and there right here. So, you can they are highly flexible. So, we see very residues are rigid because they could accommodate the residues within the electron density map. So, in this case several residues are rigid and some cases they are fluctuating these residues are highly flexible right they have a more B-factors.

So, then if you have the Pymol, it has several applications for example, you can see the combined 2 structures, whether they are similar or not. You can mutate any specific residue and see what is the changes because of these substitutions and you can get the halogen structures and also you can get measure the bond angle, bond length and the torsion angles you can under analyze various types of interactions, that you can manipulate or you can play around this Pymol to get various information; you can also get very high resolution figures right this is acceptable in publications right.

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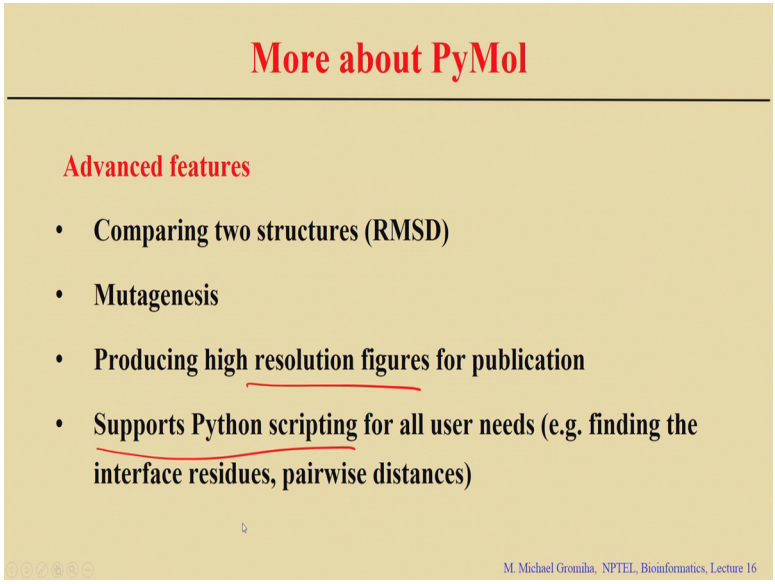

And another important fact is it supports python script for the use the necessity of this user's right, you can find the interface residues pairwise distance and so on. For more information you can look into the tutorials right you can see the websites right.

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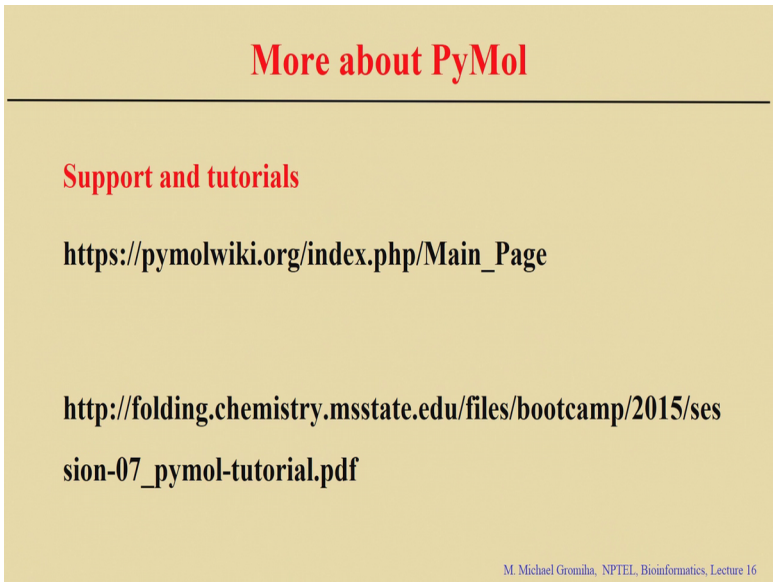

And we can get more information right and you can use this Pymol right as an effective resource right in your project or in your reports or your papers or anything or any applications. So, to summarize today's talk. So, what did we mainly focused on?

Student: Protein 3D structures

Protein 3D structures 3D structures provides which information.

Student: Atomic 3D coordinates

Atomic information XYZ coordinates right. So, what are the various experimental techniques used to determine 3 D structures.

Student: XRD and NMR

X-ray crystallography and NMR spectroscopy these are the widely used methods right electron microscopy also now used for determine the structures right. So, what is the resource, what is the database which contains protein 3D structures?

Student: PDB.

PDB right Protein Data Bank right. So, this is organized by the different institutions right different places now we have the worldwide PDB right fine. So, which information what are the other informational which can get the PDB, for actually we take the coordinate file. The coordinate file gives the information on the atom number, atom name residue number, residue name and the chain information and the coordinates, occupancy and temperature factor; what is occupancy?

Student: in unit cell how many orientations

That the orientations which the atom can take how many different orientation if only one orientation this will be 1 different orientations the total sum will be one then temperature factor right. So, then we discussed about the visaulization tools right and we gave the demo on one tool which one we discussed Pymol. What are the applications of Pymol? We can get the structures, you can view the structures, we can see the various orientations, and you can map sequence and structures and the mutations, and get different types of interactions and you can measure the bond length, bond angle right and you get a lot of applications right for by using Pymol.

So, we discuss more about 3D structures and the coordinates, now the question is we have a lot of data; like the PDB contains 133,000 structures right. So, what can we do with these structures for the various information you can get? In the subsequent classes, I will discuss about the parameters or the properties right which we can derive right from

their own 3 D structures, and how these parameters can be utilized for understanding the structure or understand the function of these proteins as well as their complexes and so on.

Thank you for your attention.