



CENTRE FOR BIOINFORMATICS
UNIVERSITY OF KERALA

SOORYAKIRAN BIOINFORMATICS
UNIVERSITY OF KERALA

Molecular Visualization Softwares

◇ Rasmol ◇ Swiss PDB Viewer ◇

HANDOUT #2

Swiss PDB Viewer (now *Deep View*) – in a simple manner

Swiss-PDB Viewer is an application that provides a user friendly interface allowing to analyze several proteins at the same time. The proteins can be superimposed in order to deduce structural alignments and compare their active sites or any other relevant parts. Amino acid mutations, H-bonds, angles and distances between atoms are easy to obtain.

1: Double click the icon named **Spdbv** in the desktop.



Spdbv.lnk

Observation.....

2. Go to the **File** menu, click **Open PDB File**. Select the data file for the **H₂O** molecule

Observation.....

3: Now click on the icon show below. Then drag the mouse inside the dark window, keeping the left button pressed.



Observation.....

This is the **translation** tool.

IMPORTANT!!! Look at the following **message area** of the **spdbv** window, for timely messages.



4: Position the water molecule to the right end of the black window area (use the above icon). Now click the icon shown below.



Now position the water molecule at any place in the dark window area and click the icon shown above. Do it 2 or 3 times.

Observation.....

This is the **centralizing** tool.

5: Click on the icon show below. Then drag the mouse inside the dark window, keeping the left button pressed.



Observation.....

This is the **zooming** tool.

6: Click on the icon show below. Then drag the mouse inside the dark window, keeping the left button pressed.



Observation.....

This is the **rotation** tool.

7: Now click on the icon show below. Then click on the two Hydrogen atoms



Observation.....

8: Click on one of the Hydrogen atoms. Then click the oxygen atom

Observation.....

9: Go to the File menu and select the **Close** option.

Observation.....

10. Open the data file for **H₂O** molecule. Click the icon shown below. Then click on the oxygen atom, now on the two hydrogen atoms one after another.



Observation.....

11. Now click on the icon show below. Then click on all the atoms in the molecule one by one. Look at the message area after each click.



Observation.....

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12. Select the **File->Close...**Option.

Observation.....

IMPORTANT:- Always **Close** the previous molecular data file before opening the new molecular data file.

EXERCISE

13. Open the data file for H₂SO₄ molecule and find the following:-

Bond distance (S-O bond):-.....

Bond distance (O-H bond):-.....

Bond angle (all the bonds):-.....

.....

14. Close the H₂SO₄ molecule. Now open data file of ammonia (NH₃) and find out the following details:

Find out:-

Bond distance (all the three N-H bond):-.....

.....

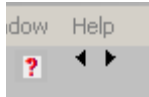
Bond angle (all the three H-N-H bond):-.....

.....

15. Open the data file for H₂SO₄ molecule. Click the following icon.



Now click on the Sulphur atom and any of the Hydrogen atoms. Look at the message area also. Then click on the arrow towards the right direction shown below.



Observation.....

16. Close the H₂SO₄ molecule. Now click the **Preferences** menu and select the **Colors...**Option. Now click on the button for any of the atom name displayed. The following small window color shows the color for the selected atom.



Now click on the **OK** button. Then check the default colors of all atoms, bonds, amino acid kind, structures, background etc... These colors will help us to identify different atoms present in a complex protein molecule. Last press the **OK** button...

Observation.....

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17. Open the data file for the **insulin** molecule. Write down the possible atoms present in the molecule by looking at the colors. Rotate insulin and look at the complexity of the protein.

Observation.....

18. Select the **window-> control panel...**option.

Observation.....

Points to note:- The control panel gives the information about insulin. On the top left, we have the protein name.

19. Click the square named **visible**.

Observation.....

20. Again click the square named **visible**.

Observation.....

Points to note:- The column named **group** gives the names of amino acids present in the displayed protein. The capital letters displayed on the left most part of the control panel shows the different parts of the protein. The letters present in between the capital letters and the group names gives information about α -helix (the letter **h**) and β -strands (the letter **s**).

21. Scroll the mouse till you reach the end of the control panel area. How many different parts you found for insulin?

Observation.....

22. Then write down the number of α -helix and β -strands present in each different part of the insulin.

Observation: -

Part A.....

Part B.....

Part C.....

Part D.....

23. Now write down the names of the amino acids present in each of the α -helix and β -strands present in insulin.

Observation:- Part A.....

.....

Part B.....

.....

Part C.....

.....

Part D.....

.....

24. Now click on any of the letter **A**. What is your observation in the control panel and in the dark display area?

Observation.....

25. Then write down the observations for the parts **B**, **C** and **D**.

Observation.....

Points to note:- The letter **v** present in the column names **show**, **side**, **labl** represents “**visible**” . If **v** is not present it means “**invisible**”.

26. Now select the part named **A**. Then click the column named **show**.

Observation.....

27. Then click the column named **labl**.

Observation.....

28. Now rotate the part of the molecule displayed. Click on the control panel menu.

Observation.....

29. Now click on any of the letter **v** present in the column named **labl**, keeping the SHIFT key pressed.

Observation.....

30. Now click on any of the letter **v** present in the column named **side**, keeping the SHIFT key pressed.

Observation.....

31. Now click on any of the letter **v** present in the column named **show**, keeping the SHIFT key pressed.

Observation.....

31. Now click on the space corresponding to the first amino acid (here GLY1) of part **A** under the column named **show**.

Observation.....

32. Now click on the spaces corresponding to all the amino acids of part **A**.

Observation.....

IMPORTANT:- Study how the amino acid residues connect each other by looking into the colors of the atoms.

33. Now click on the space corresponding to each amino acid under the column named **side**, one by one.

Observation.....

34. Now clear all the **v** under the column named **side**, following the similar steps done for the **show** column.

Observation.....

35. Now click on the space corresponding to each amino acid under the column named **labl**, one by one. Last clear all the **v** under the column named **labl**.

Observation.....

36. Now display part **A** (without **side** & **labl**). Slightly rotate. Now click the column named **ribn**.

Observation.....

37. Clear all the **v** under the column named **ribn**. Now click on the column named **v**.

Observation.....

38. Display **side** chains also. Identify the change in the area of van der Waal's effect. Clear all the **v** under the column named **v**.

Observation.....

IMPORTANT:- It displays the various **van der Waal's** radii existing in the displayed molecule.

Points to Note:- We can change the color of each amino acid by clicking on the small square shown corresponding to that amino acid under the column named **col**. We can change the color of all or part of a molecule with the option **select->all**. We can remove the selection with the option **select->none**.

39. **Close** the control panel & the display window of insulin. Now open the data file for **insulin**. Open the control panel also. Then go to the menu option **Select-> Group Kind-> Gly (G)**. Now click the column named **show** in the control panel.

Observation.....

40. Now display all the **Val (V)** residues present in the insulin molecule. Count the number, label each one, and display the side chains also.

Observation.....

41. Now go to the menu option **select-> group property-> select basic amino acids**. Now click the **show** column in the control panel.

Observation.....

42. Now write down the names of each amino acids displayed in the above step.

.....
.....
.....

43. Now check all the options in the **select->group property** menu (like acidic, polar etc). Each time click the **show** column in the control panel.

Observation.....

44. Now go to the menu option **select -> secondary structure -> strands** option. Now click the **show** column in the control panel. Rotate to get a clear view.

Observation.....

45. Now check the options of **helices** and **coils** present in **select -> secondary structure** menu option. Rotate to get a fine view. Last close the data file for insulin molecule.

Observation.....

EXERCISE:-

Open the data file for **Lysozyme**. Find out the following:-

Number of parts: -

Number of helices: -

Number of strands: -

Display only the helices: -

Display both helices and strands (you can select both helices and strands by clicking, while keeping CTRL key pressed): -

46. Open the data file for **insulin**. Go to the **Edit -> Find Sequence...** menu option. Now enter sequence **FVNQ** in the displayed text area & press the OK button. Then click the **show** column in the control panel. Also find out the names of matching amino acids. Last close the insulin molecule window.

Observation.....

47. Now open the data file for **insulin** molecule. Then go to the **Tools->Compute molecular surface...** option.

Observation.....

48. Now go to the **File -> Discard -> Discard Surface...**Option.

Observation.....

49. Take the **Tools-> Electrostatic potential...** option. Now you select the values of the different parameters shown in the dialog box. Last click OK button.

Observation.....

50. Now go to the **File -> Discard -> Discard Electrostatic potential...**Option. Last close the data file for insulin molecule.

Observation.....

51. Now open the data file for **insulin** molecule. Go to the **Select-> All** Option. Then go to the **Window->Ramachandran Plot** Option.

Observation.....

IMPORTANT:- The Ramachandran Plot contains one small dot (actually a small square for glycines and a small plus sign for all others) for each selected residue (here we selected all the residues). When you place mouse over any of the dots, the name of corresponding amino acid will be displayed at top left corner of the plot.

52. Now change the position of the dots present in the plot & look at the protein structure.

Observation.....

52. Now show only ALA (A). Then display its Ramachandran plot. Change the position of the dots present in the plot. Last close the data file for insulin.

Observation.....

EXERCISE

53. Open the data file for the **Lysozyme**. Show the Ramachandran plot for the whole molecule.

Observation.....

54. Now show the plot for only VAL (V).

Observation.....

55. Now go to **Window-> Alignment** option.

Observation.....

Points to Note:- It shows the amino acid sequence of the **insulin** according to the order shown in the control panel.

56. Now place the mouse over any of the letters in the alignment shown.

Observation.....

57. Then click on any of the letters shown. Last close the data file of insulin.

Observation.....

58. Now open the NOTEPAD and type the following in capital letters:-

> **MYSEQUENCE**

GHTESAARTNMKTGDDDCGEQQASD Save the file as **myseq.txt** in the directory "**c:\spdbv**". Close the notepad. Then go to **SwissModel-> Load Raw Sequence to Model...** option. Now select the file named **myseq.txt** and click Open. Rotate to get a nice view.

Observation.....

.....

IMPORTANT:- The swiss PDB Viewer gives a possible helix corresponding to our raw sequence. Using this facility we can model the structure of a known sequence.

59. Go to control panel and check whether the displayed structure is a helix or not. Now take the Alignment of the structure. Compare with our sequence.

Observation.....

60. Display the Ramachandran plot for the displayed structure.

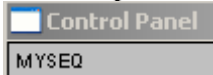
Observation.....

61. Close the Ramachandran plot. Now open the data file for **insulin**, without closing the raw sequence structure. Then take the **Window->Alignment** option.

Observation.....

IMPORTANT:- The vertical lines show exact match between the corresponding amino acid residues. The symbol ":" shows not exact match but in a similar group. "." Tells that they are in dissimilar group. You will get the **rms value** from the alignment window by, if you place the mouse over any letter of the raw sequence.

62. We can display each loaded molecule separately using the following area of the control panel.



Now click on the label **MYSEQ**.

Observation.....

63. Then click on the label **insulin**.

Observation.....

64. Now go to **File-> Close All Layers...**option. Open the data file for **insulin**. Now click on the icon shown below.



Then click on any of the amino acid residues present in the insulin.

Observation.....

65. Now select any of the residue displayed. Look at the message area also.

Observation.....

IMPORTANT:- The **rotamer** gives the possible staggered conformations of the selected side chain. The **score** value gives the score for the current conformation.

66. Press the “*” key, present at the top right of the keyboard (NUMlock should be on), repeatedly and look at the selected side chain. Look at the message area for the values of **rotamer** and **score**. Last go to **File->close...**option.

Observation.....

Points to Note:- The **green** colored dashed lines shows the potential **H-bonds**. The **pink** colored dashed lines show the possible **clashes**.

67. Open the data file for **myoglobin**. Now go to **Color** menu and study the options present there.

By CPK: -

By Selection: -

(Here you can combine this option with different **Select-> Group.....**options)

68. Close the **myoglobin** molecule. Load the raw sequence **myseq.txt** (we already done). Now load data file for **insulin**. Now go to **Fit-> Fit raw sequence...**option. Centralize the molecule using the left most icon in the Toolbar.

Observation.....

69. Now take the control panel. Click the column named **show** for both **insulin** and **myseq** (use label present at top left corner of control panel). Rotate the molecule for a better view.

Observation.....

70. Now display the **alignment** window and identify the fitting region. Use the scroll bar present in the alignment window. Last close the window for insulin.

Observation.....

71. Open the data file for **insulin**. Now click on the icon shown below. Look at the message area also. Now click any atom.



Observation.....

72. You can select various options shown including the radius of selection. The default is 6.00 Angstrom. Now click the OK button.

Observation.....

73. Now using the control panel display the whole insulin. Now click the icon shown below. Look at the message area also. Now click any atom.



Observation.....

74. Now display the control panel. One amino acid residue will be in red color. Now click on the **show** column.

Observation.....

IMPORTANT:- This shows the amino acid whose atom is selected by us.

75. Display the whole insulin molecule using control panel. Now click on the icon shown below. Look at the message area also. Now click on any of the atom.



Observation.....

IMPORTANT:- It displays the Φ , ψ and ω angles.