Getting to know RNA Polymerase:
A Tutorial For Exploring Proteins in VMD
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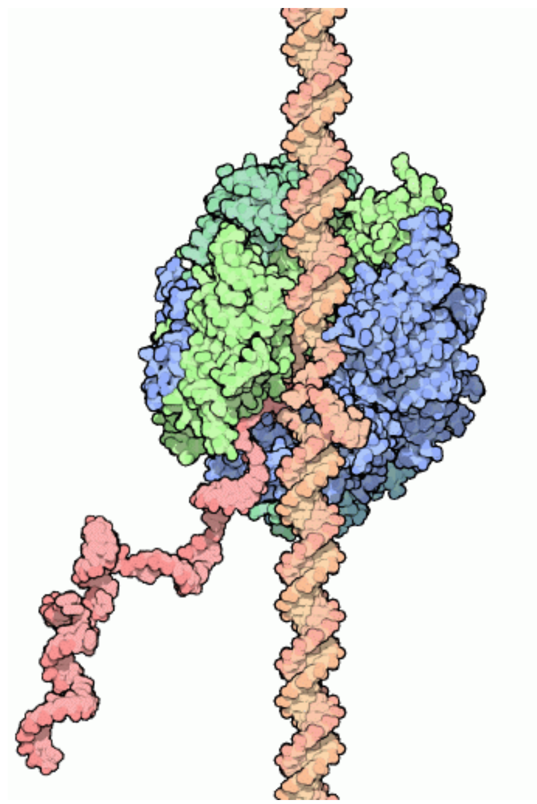
1. You will need to answer some questions and write down some observations during this activity, so please take out a pen or pencil and some paper.
2. Double click on the "VMD" icon in red green and blue (with black background) on your desktop. The window labeled "VMD Main" is the control panel and the window labeled "OpenGL" is where the molecule(s) will be displayed.
3. Select "file", then "new molecule". Type in the PDB ID "1msw" and click "load". Your molecule should be visible now in he OpenGL window (if it is not, see me).



4. In the VMD Main menu, select "Representations" under the Graphics menu. Click the "Create Rep" button in the upper left corner and then type "protein" in the selected atoms field. Now select the "Drawing Method" drop down menu in the bottom left hand corner and select "New Cartoon".
5. Now select "Create Rep" again and type "nucleic" into the drop down menu. Choose "VDW" as the drawing method and change the coloring method to "chain".
6. Highlight the first representation (the selection listed as "all") in the blue part of the Graphical Representations box and delete it by clicking the "Delete Rep" button in the upper right hand corner.

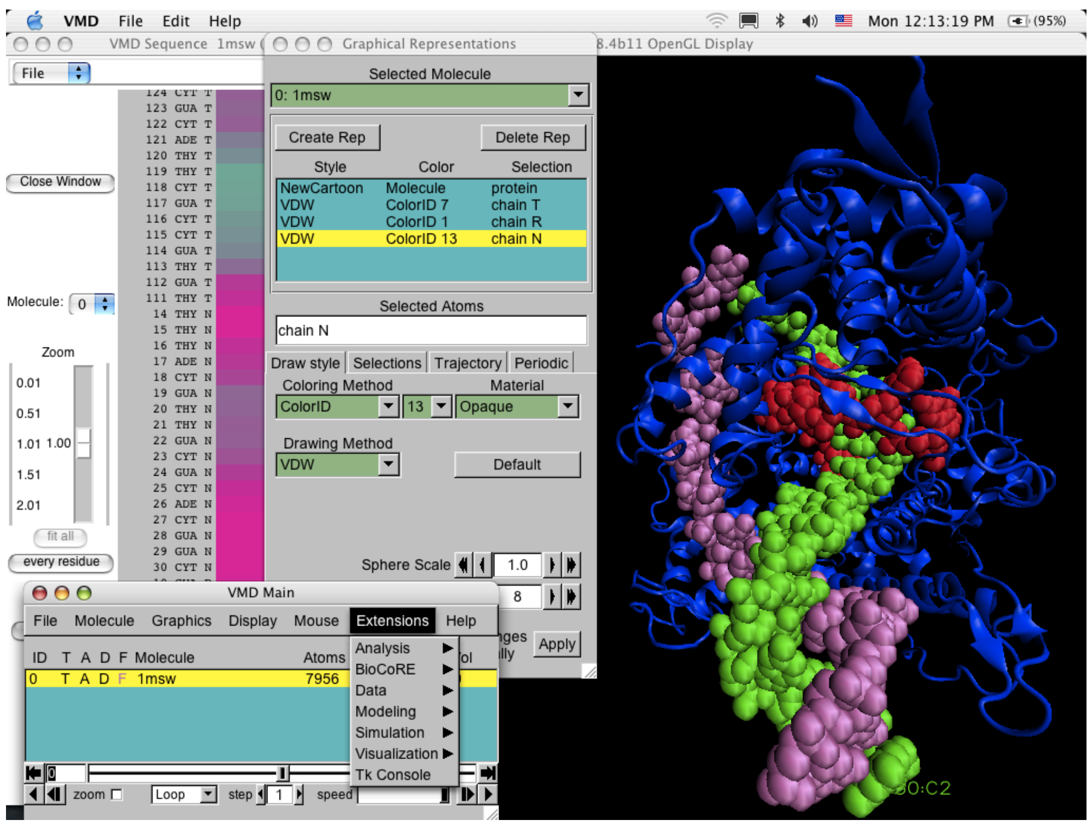
7. Now let's go back to the OpenGL screen to have a look at the molecule. You can scale (magnify or shrink) the molecule by pressing the letter "s" on your keyboard and then clicking and dragging the mouse from side to side (try this). You can rotate the molecule by selecting "r" on your keyboard and again clicking with the mouse and moving to one side or the other (try this, too). You can translate the molecule by pressing "t" on your keyboard, and you can choose the center point about which rotation takes place by pressing "c" on your keyboard.

List of VMD Keyboard Shortcuts (also accessible under the "mouse" menu):

Key pressed	Action Performed
t, T	Enter translate mode for moving entire molecule
R, R	Enter rotation mode, stop rotation of selected molecule
S, S	Enter scale mode for magnifying or shrinking the selected molecule
c	Choose center about which rotation will take place
x, X	Begin rotation about the x axis, rock back and forth about x axis
y, Y	Begin rotation about the y axis, rock back and forth about y axis
z, Z	Begin rotation about the z axis, rock back and forth about z axis
1	Label atoms selected with mouse left click
2	Enters "bond label" mode, which gives the distance between two atoms selected by successive mouse left clicks

8. The protein is shown in blue. It contains many ribbon-like structures which look like telephone cords – these are called alpha helices- and some others which look like arrows – these are beta strands. **Take some time to explore the protein structure and write down some of your observations here:**

9. You will also notice in the center of the protein, what look like a bunch of balls in red, pink and green. These are the nucleic acids. More specifically, the pink and green structures each represent two strands of a DNA double helix which has been unwound so that a piece of RNA could be made from this template. The RNA is shown in red. If you haven't already, take some time to read about how RNA Polymerase makes RNA from the PDB website (www.rcsb.org).



10. Go back to the Graphical Representations window and double click on the representation for protein. This will hide the protein so we can look more closely at the DNA & RNA. Now click on the "nucleic" representation. Change the coloring method to "ResName". This will color each of the DNA & RNA bases a different color. Here green corresponds to Cytosine, pink to Alanine, gray to Guanine, and White to Thymine. Can you figure out which of these

four bases is absent from the RNA molecule? To help you figure this out, press the number “1” on your keyboard and then click on any atom. You should see to a label appear. The label reveals the identity of the atom you clicked. For example, the label A1:O3 means you clicked an Alanine which is the 1st amino acid in the protein chain. The “O3” means the specific atom you clicked in the Alanine was Oxygen number 3. Press “r” on your keyboard to exit the label mode.

11. Change the drawing method for this “nucleic” representation back to lines, can you tell which bases are always paired together in the double helix? Spend some time exploring the nucleic acid structures by choosing different coloring and drawing methods and by rotating the molecule around. How far is it across the DNA double helix (how wide is a base pair)? To figure this out, press the number “2” on your keyboard and then click on one side of the helix, then on the other side. You should see a white dotted line appear with a number. That number is the distance in Angstroms – that’s 10 **billion** times smaller than the equivalent distance in meters!! **Write your answer here:**

12. Now you need to save this image. Select “Render” under the File heading in the VMD main menu. Select “Postscript” from the “Render Using” drop down menu. Now select Browse and select the directory where you want to save, then click “Start Rendering”.
13. Now go back to the Graphical Representation menu and the nucleic representation to make it disappear. Now double click on the protein representation. This should cause the protein to reappear in the OpenGL menu – check to make sure this happens. Change the coloring method to “structure”. What happened? What color are the alpha helices and what color are the beta sheets? **Write your answers here:**

14. Save this image as you did for the nucleic acids. Save it as "yourlastnamePolymeraseCartoon" in your period's folder.
15. Now go back to the Graphical Representations page and change the coloring method to "ResType". This will color all positively charged amino acids blue, negatively charged amino acids red, polar amino acids green, and hydrophobic ones white. Now change the drawing method to "Surf", this will calculate the surface of the protein. It will take some time, so be patient. When you have your protein surface, rotate it around. Does the exterior of the protein appear to be mostly white, or mostly red, green, & blue? **Why do you think that is? Write your answer here:**