(Note: These tutorials are meant to provide illustrative examples of how to use the AMBER software suite to carry out simulations that can be run on a simple workstation in a reasonable period of time. They do not necessarily provide the optimal choice of parameters or methods for the particular application area.)


# TUTORIAL B2

## Using VMD with AMBER

**By Ross Walker**


This tutorial is designed to give you an introduction to using VMD with AMBER. How to load AMBER trajectory files, inpcrd files and then how to manipulate the data. It is not designed to exhaustively cover all of the many features that are present in VMD.

## *Introduction*

Visual Molecular Dynamics (VMD http://www.ks.uiuc.edu/Research/vmd/) is a very powerful and feature rich molecular visualisation package for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. Its development is funded by the National Institute of Health under the guidance of Klaus Schulten. It is available free of charge to academic researchers and can be downloaded from the above link after registering.

VMD is an ideal tool for visualising results produced by the Sander module of the AMBER software suite. However, its use is not necessarily intuitive. This tutorial is designed therefore to give a brief introduction to visualising and manipulating trajectories produced from AMBER simulations.

This tutorial is based on VMD v1.8.3 (with the updated plugins v1) which at the time of writing (3rd June 2005) was the most up to date version. If you use a different version of VMD you may find that some features are not available or the interface is slightly different. However, it should still be possible to complete the vast majority of this tutorial.

This tutorial also assumes that you are using Linux. If your operating system is different some of the layout and/or procedures may be slightly different.

This tutorial consists of nine sections:

1. section1.htm : Loading VMD and Customising the Initial Window Layout
2. section2.htm : Loading a PDB File
3. section3.htm : Changing Representations
4. section4.htm : Loading AMBER inpcrd and restrt files
5. section5.htm : Aligning Molecules and Measuring RMSD's
6. section6.htm : Visualising AMBER Trajectories
7. section7.htm : Saving a Single Set of Coordinates
8. section8.htm : Following System Parameters Over the Course of a Trajectory
9. section9.htm : Creating a Movie

CLICK HERE TO GO TO SECTION 1

(Note: These tutorials are meant to provide illustrative examples of how to use the AMBER software suite to carry out simulations that can be run on a simple workstation in a reasonable period of time. They do not necessarily provide the optimal choice of parameters or methods for the particular application area.)

# TUTORIAL B2 - SECTION 1

## Using VMD with AMBER

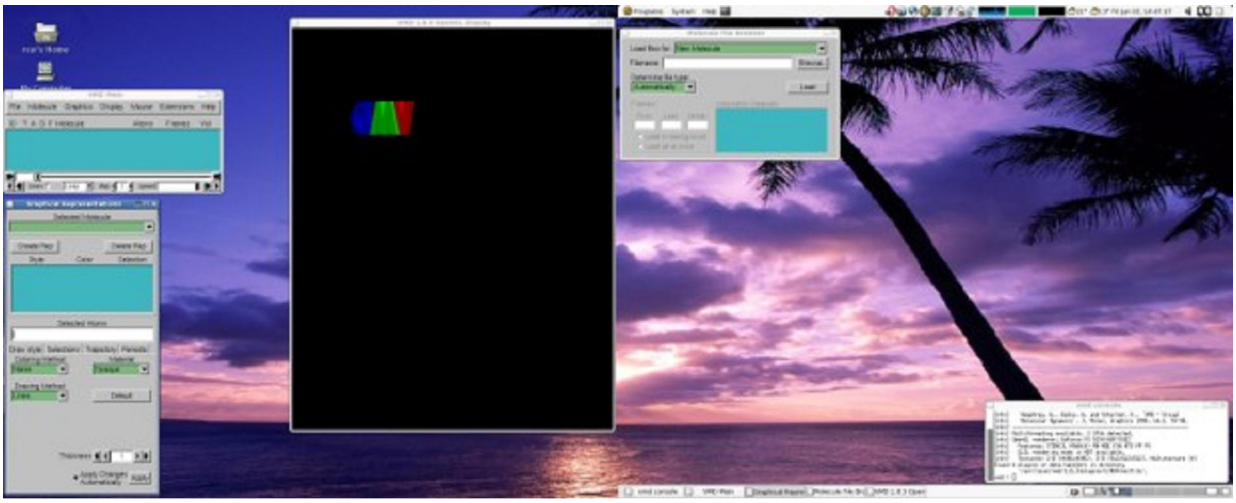
**By Ross Walker**

## *1) Loading VMD and Customising the Initial Window Layout*

Before we start looking at some AMBER trajectories you should ensure that VMD is correctly installed on your machine and working correctly. When you issue the command 'VMD' it should load without error messages. If you can't get VMD to work please refer to the VMD website for further info.

Lets start by customising the way VMD starts up so that we have a similar display layout. (If you are confident navigating your way around VMD you can skip this step.)

I tend to use a dual screen system so I configure my VMD to load with the windows distributed across the two displays as shown below:



However, since most people will be using single display machines to run this tutorial we will step through creating a startup script for a single display.

VMD's initial layout is controlled by a file called **.vmdrc**. Here is a .vmdrc file you can use to obtain what I consider to be a *good* initial layout.

vmdrc

```
# turn on lights 0 and 1
light 0 on
light 1 on
light 2 off
light 3 off

# position the stage and axes
axes location off
stage location off

# position and turn on menus
menu main on
```

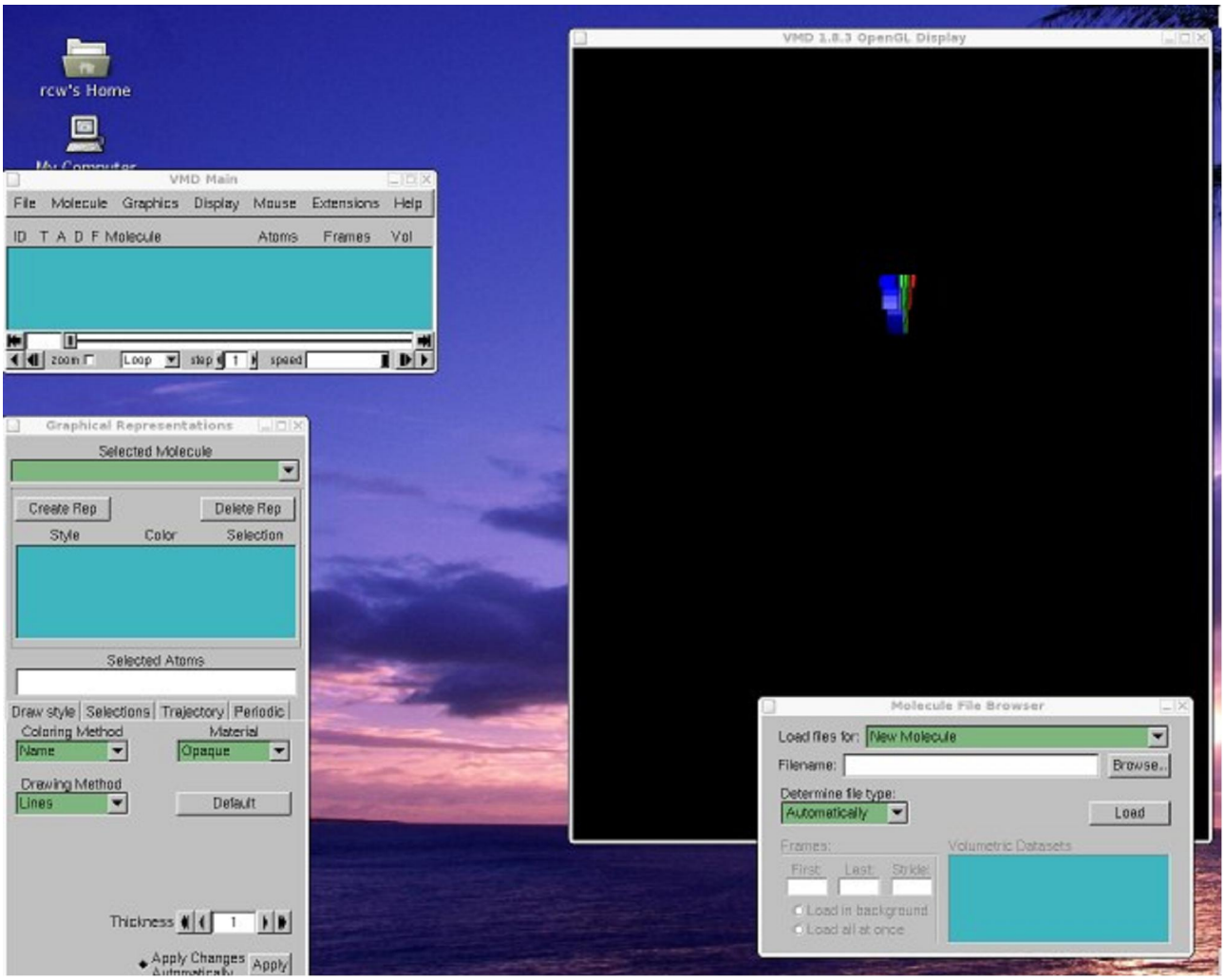
```
menu graphics on
menu files on

menu main move 5 196
menu graphics move 5 455
menu files move 800 750

display projection orthographic
```

If you have a file called .vmdrc in your home directory (check with cd ~, ls -la) either delete it or rename it. Then save the file above as "**.vmdrc**" in your home directory. (Note the dot before the vmdrc).

This file is sourced automatically by VMD on load and does several things. First of all it switches on lights 0 and 1. It then turns off the Axis. This I feel creates a cleaner OpenGL window. It also sets the display projection mode to orthographic which in my opinion gives much better depth perception and less distortion when rotating on a screen that does not have an exact 4 by 3 ratio. E.g. my screen which has a resolution of 1280x1024. Finally it turns on the main menu, the graphics menu and the file menu. It then moves these to suitable locations on the screen. Note: this is designed for a screen resolution of 1280x1024. If your resolution is different you may need to play around with the numbers on the 3 move lines to get a layout that is reasonable.

Now run VMD and it should come up with a layout similar to that below:

>vmd



We are now ready to try loading some molecules.

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CLICK HERE TO GO TO SECTION 2

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(Note: These tutorials are meant to provide illustrative examples of how to use the AMBER software suite to carry out simulations that can be run on a simple workstation in a reasonable period of time. They do not necessarily provide the optimal choice of parameters or methods for the particular application area.)

# TUTORIAL B2 - SECTION 2

## Using VMD with AMBER

**By Ross Walker**

## *2) Loading a PDB File*

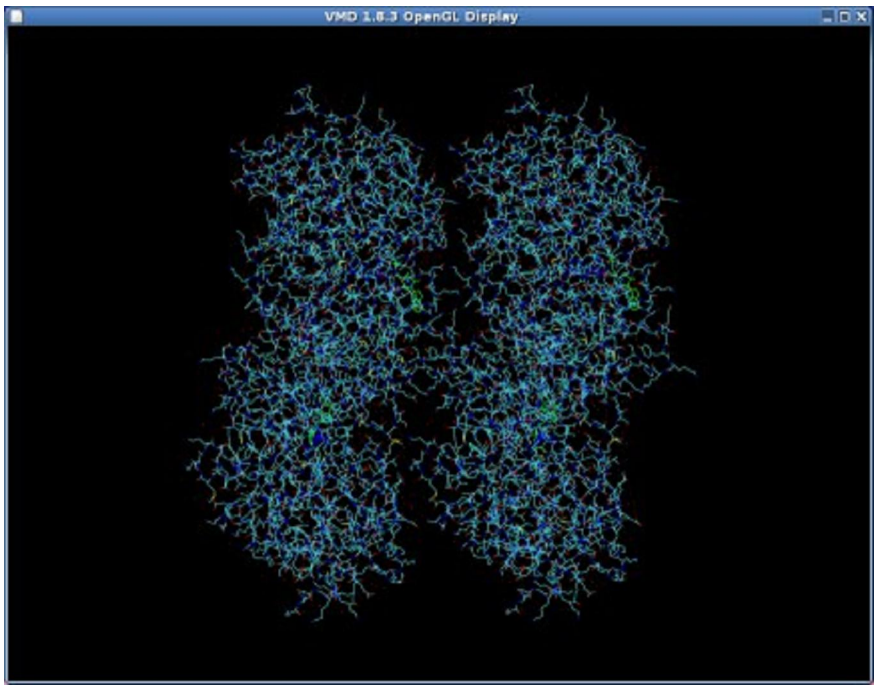
PDB files, as can be obtained from the Brookhaven protein databank can be loaded into VMD in one of two ways. You can either specify them on the command line, e.g.:

vmd my_structure.pdb

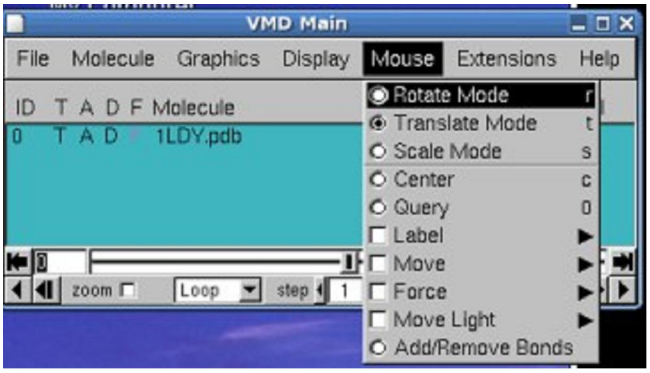
or you can load them via the "molecule file browser". Lets try loading Liver Alcohol Dehydrogenase (LADH) using the latter case. Here is a pdb of LADH (1LDY.pdb) Note: You may need to right click this link and select save as.

If it is not already up open the "**Molecule File Browser**" window by clicking File->New Molecule.

Then select **browse** and look for the 1LDY.pdb file you just saved. Next check the "**Determine file type**" box to ensure it says **pdb**. Never trust VMD to get this correct, especially when it comes to loading AMBER trajectories. Then hit **load** and up should pop the tetramer LADH:




By default the mouse will be in rotate mode. Holding down the **left** mouse button while the mouse pointer is inside the "Open GL" display will allow you to rotate the molecule. There are two other modes for the mouse. Translate which moves the molecule in the plane of the window and Scale which allows you to zoom in and out of the molecule. You can access these modes in 2 ways. The first is via the **Mouse Menu**:




The second, and arguably more convenient, method is to use the keyboard short cuts as displayed on the right of the Mouse Menu:

(r) = Rotate Mode
(t) = Translate Mode
(s) = Scale Mode

While your mouse is over the "OpenGL" window press "**s**" and then move your mouse from side to side while holding down the **left** button. Press "**r**" to return to rotate mode. If at any point you mess up click **Display->Reset View** to get back to the default view.

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CLICK HERE TO GO TO SECTION 3

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# TUTORIAL B2 - SECTION 3

## Using VMD with AMBER

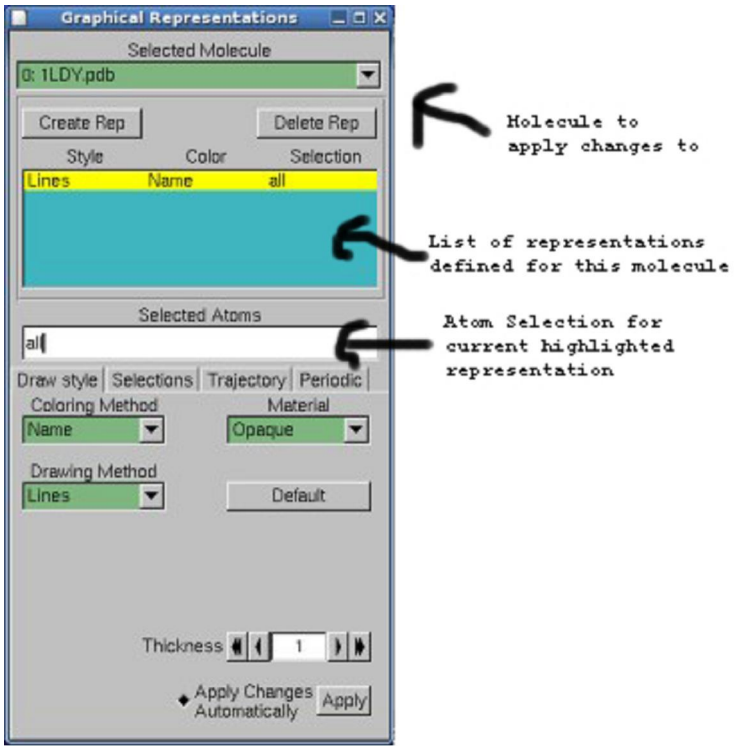
**By Ross Walker**

## *3) Changing Representations*

Now we have mastered the basics of manipulating a molecule's view the next thing to look at is how we can change the representation. This is done via the "**Graphical Representations**" window. If it is not already open click on **Graphics->Representations** to open it.

By default the Selected Molecule will be the last one you opened. In this case molecule **0: 1LDY.pdb** (BEWARE: VMD numbers from zero. This applies to residues as well. E.g. Residue 0 is actually residue 1!!!). By clicking the **down arrow** beside the selected molecule you can change which one we are applying changes to. In this case we only have one molecule loaded so it is the default.

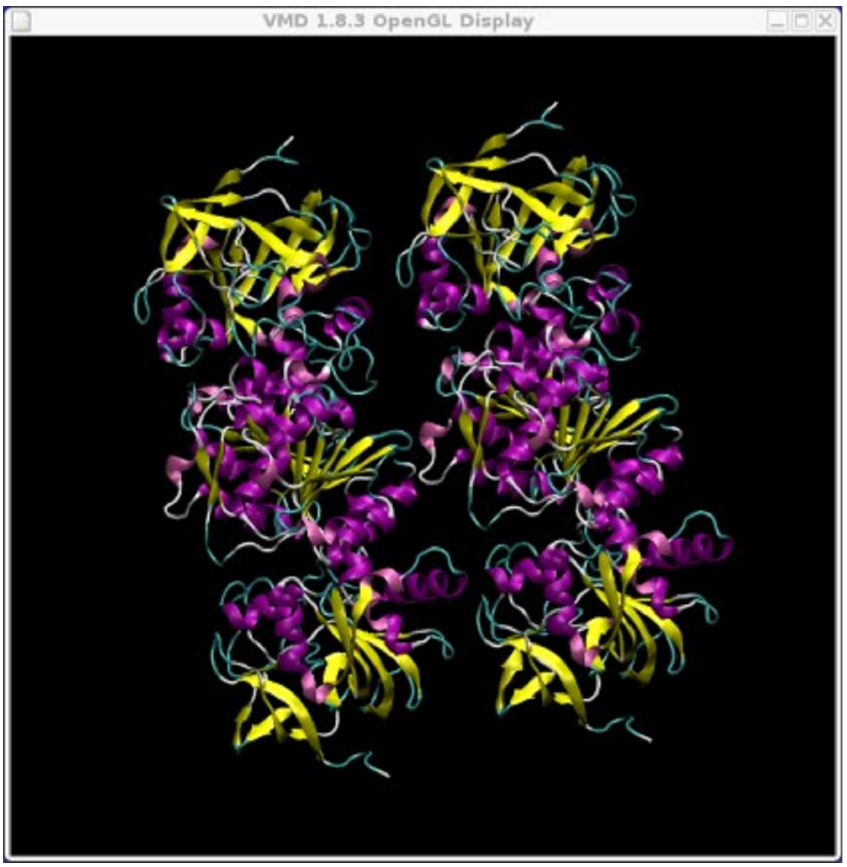
Lets start by removing the waters from the display. If you look at the display at the moment you will see all these little red dots. These are the oxygen atoms of crystallographic waters that were in the pdb file. We can remove them from the current representation by changing the **Selected Atoms** box:



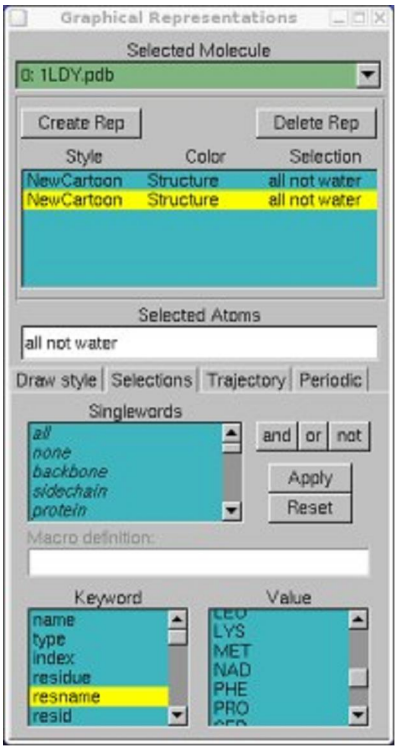

Replace the word "**all**" in the selected atoms box with the words "**all not water**" and hit **apply**. The red dots should disappear. While this example might not seem a stunning use of such a selection it is very useful when looking at explicit solvent calculations since often the water molecules will obscure your protein or system of interest. Next we will change the view to a cartoon view so we can see the structure more clearly.

In Coloring Method select "**Structure**". This will change the colouring to one where different residues are coloured differently depending on the secondary structure they are part of. Next

click select "**Cartoon**" from the **Drawing Method** box. (You can also try "**NewCartoon**" if you are using v1.8.3 or later). Your display should now look something like this:

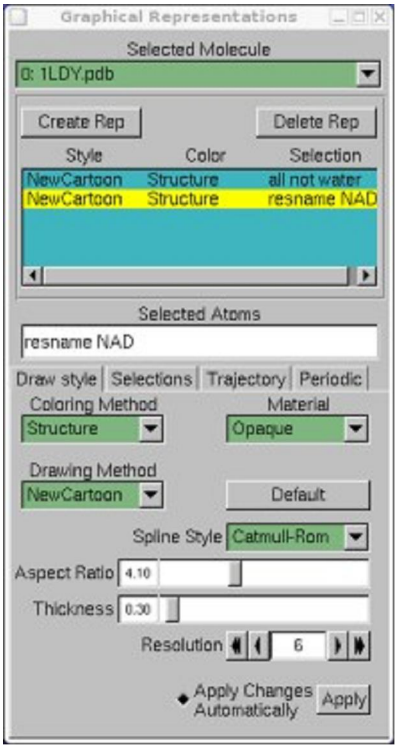



Next we will highlight the NADH coenzyme molecules in this protein so that we can see them. We will do this by creating a second representation for this molecule and selecting only those residues with the name NAD. So, in the "**Graphical Representations**" window click on "**Create Rep**", you should get a second representation created with the same representation as the original. Next click on the **Selections** Tab:



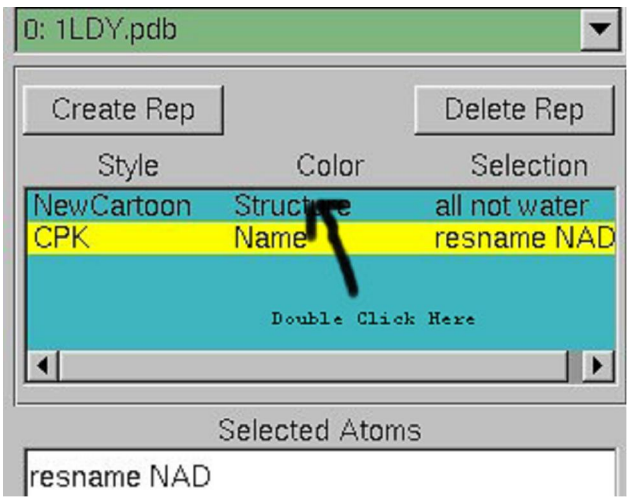

Here we can pick the selection we want in the "**Selected Atoms**" box. Note, we can also simply

type in this box, as we did to remove the water, if we know what we want. So, lets select only residues that have the name "**NAD**". First things first **delete the text** in the "**Selected Atoms box**". Then double click on **resname** (This should add **resname** to the **Selected Atoms** text box.) Then scroll down the list of values and **double click** on **NAD**. Then hit **apply**. Now we can go back to the **Draw Style** Tab:

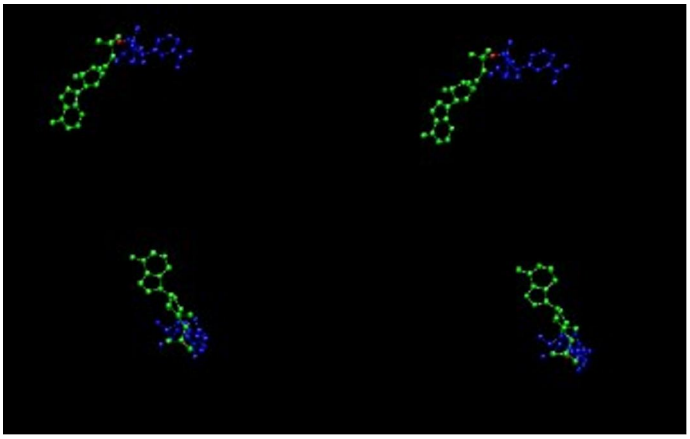



As it stands not much has happened to our molecule's representation. This is because the draw style is still set to NewCartoon. Lets change it to CPK so we can see the NADH residues. Step 1 make sure the second of the two representations is highlighted as above - we don't want to change the entire protein to CPK as this will really hurt out eyes (if you don't believe me, try it)...

Next change the **Coloring Method** to **Name** and the **Drawing Method** to **CPK**. Then hit **Apply**. You should now be able to see the 4 NADH residues. So, we have a tetramer. Well actually we have two dimers in close proximity. If you rotate the protein around you will be able to see that there is clearly a solvent filled void between the two dimers. You can temporarily turn off either of the representations by **double clicking** on it's name in the representation list:

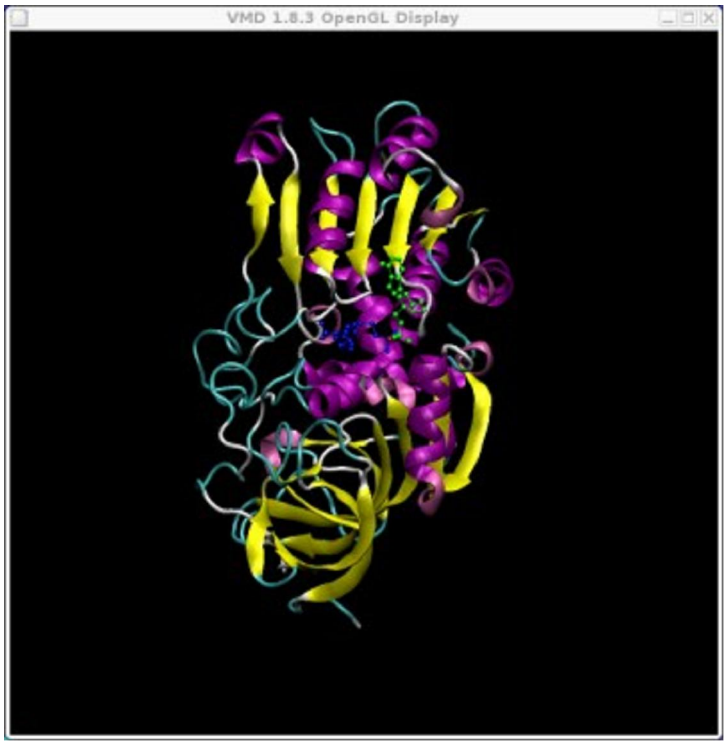



Try it, **double click** on the one that has "**all not water**" as its selection. You should be left with just the NADH residues.



**Double click** on it again and you'll get the protein back.

Now: See if you can work out how to display just chain A of the protein with it's single NADH residue:




*Hint: you will need to modify both representations selected atoms. You will also need the 'and' keyword.*

Click here for the answer.

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CLICK HERE TO GO TO SECTION 4

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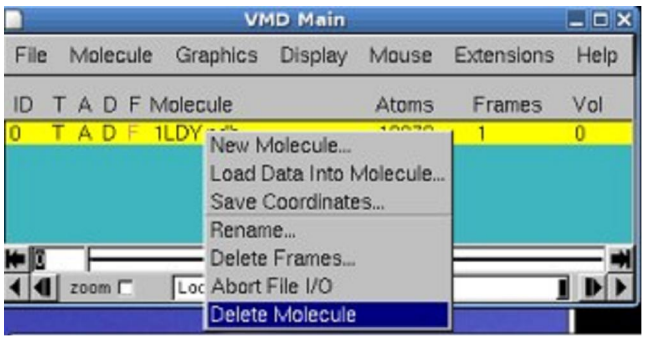
# TUTORIAL B2 - SECTION 4

## Using VMD with AMBER

By Ross Walker

## *4) Loading AMBER inpcrd and restrt files*

Lets remove the current molecule and try looking at an AMBER inpcrd or restrt file as created by xleap or sander. Start by removing the LADH molecule. **Right click** on the 1LDY.pdb file name in the "**VMD Main**" window and select "**Delete Molecule**". You may have to left click first to select it.

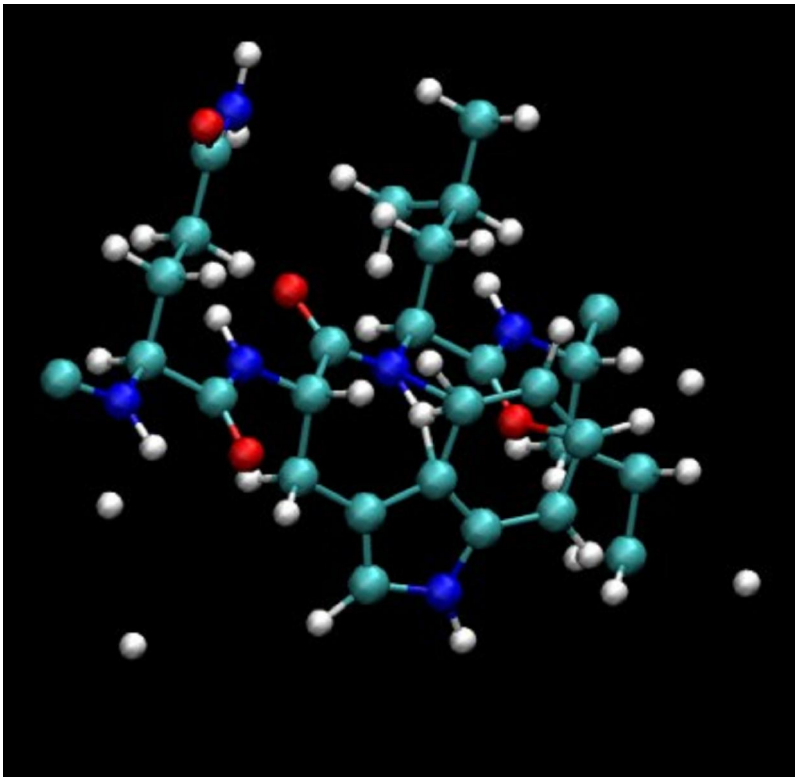



Next we will open a prmtop and inpcrd file I created with XLeap. Don't worry about how we create these files were created. That will be covered in a later tutorial. Here are the two files you will need: TRPcage.prmtop, TRPcage.inpcrd.

Loading AMBER structures is slightly different to how you load a pdb file since there are actually two files. The first file is the **prmtop** or **topology** file. This says nothing about the locations of the atoms in a molecule it simply defines what each atom is, what it is bonded to the parameters for each atom type. The **inpcrd** file on the other hand simply lists a set of coordinates, it says nothing about the atoms. Thus we need both these files to load the structure. Lets start by looking at one of the limitations of the pdb view. Here is a pdb of this TRPcage structure I created using ambpdb. (TRPcage.pdb).

This structure I created by hand using XLeap's sequence command. As such it has some very poorly placed protons and residue side chains. **Load** the pdb into vmd and see what you get. It should look pretty good. However, try zooming in on the central Tryptophan residue. What do you see?

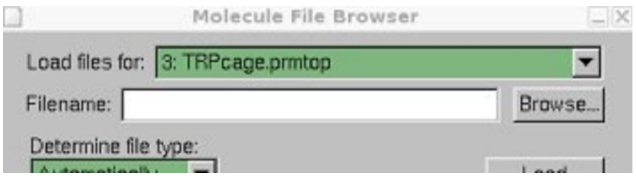
It might be easier to see what is going on if you remove the other residues. In "**Graphical Representations**" "**Selected Atoms**" enter "**all within 5 of resname TRP**". This will only show atoms that are within 5 angstroms of residues called TRP. Also **select CPK** as the **Drawing method** while you are there. Next **click** on the **Mouse menu** in the "**VMD Main**" window and click "**center**". This allows us to change the centre of rotation. Now **click** on the **backbone nitrogen** of the **tryptophan**. Now when you rotate it should rotate about this atom. (Press **r** to return to rotate mode).



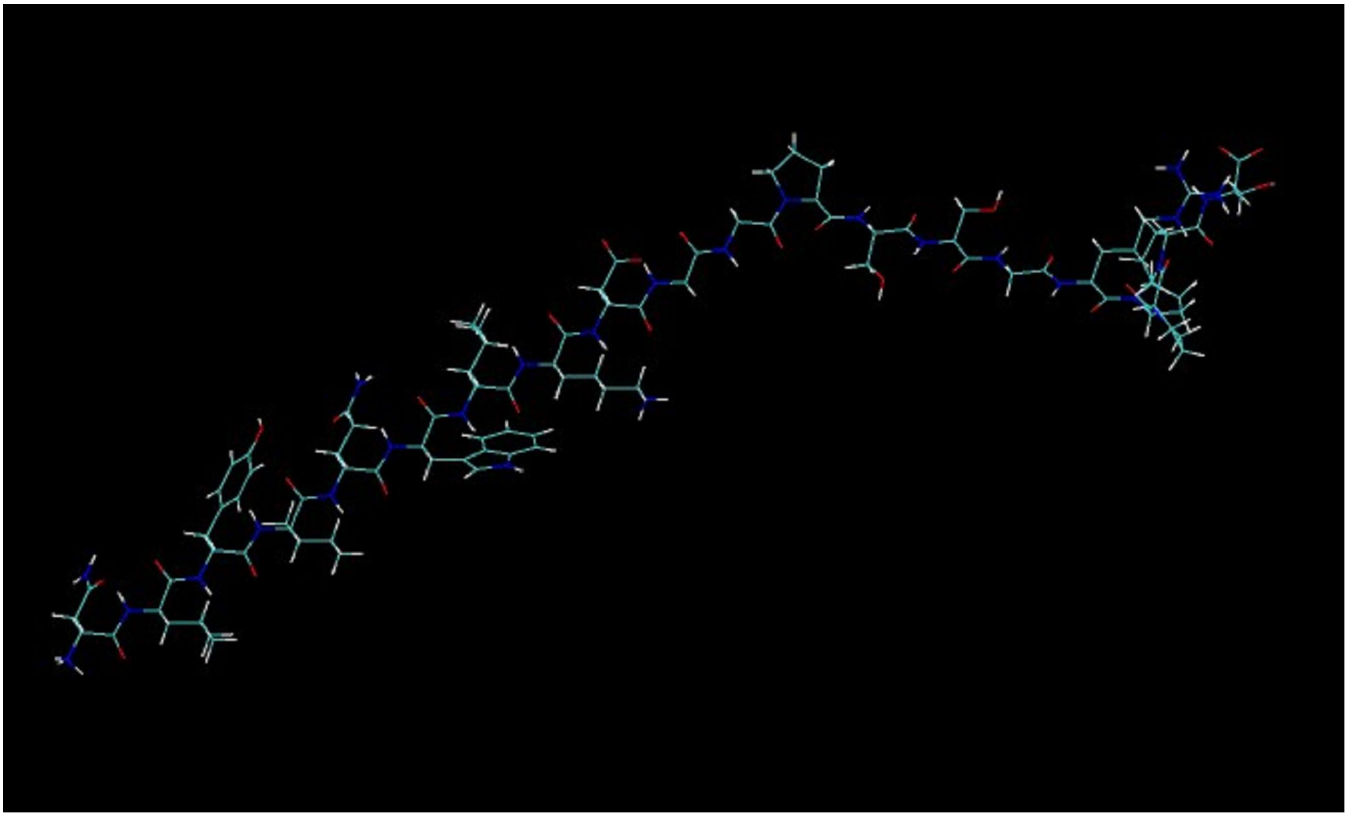
What are those strange bonds? We have a proton with 3 bonds to it. Surely the simulation was not setup in this way. Indeed, it wasn't. But the pdb I created has no bond information in it. As such VMD added bonds based on the distance between atoms. Since this is a "very" bad starting structure there are a number of atoms very close together and so vmd bonded them all. Hence looking a pdb files does not tell you where the bonds that AMBER will use are. In order to see how AMBER will treat the bonding of this molecule we have to use the prmtop file.

So, delete this molecule so that we can load a prmtop instead. When loading AMBER prmtop files it is important to know whether you have a new format prmtop file or an old one. PRMTOP's created with AMBER 6 or earlier are OLD format while those created with AMBER7 or later will be NEW format. The prmtop I gave you above is a NEW format one. So, go to the Molecule File Browser and browse for the prmtop file. Now, under "**Determine file type**" select "**parm7**"[vmd1.8.3] or **"Amber 7 Parm**"[vmd1.8.4]**.** This means NEW format prmtop file. (**parm** refers to the old format). Hit **load**.

Not much happened right? That is because the prmtop file contains no coordinates. However it should have created a new structure container called "**TRPcage.prmtop**". We can now load any number of structures into this molecule by making sure it is selected in "**Load files for:**" in the Molecule File Browser.



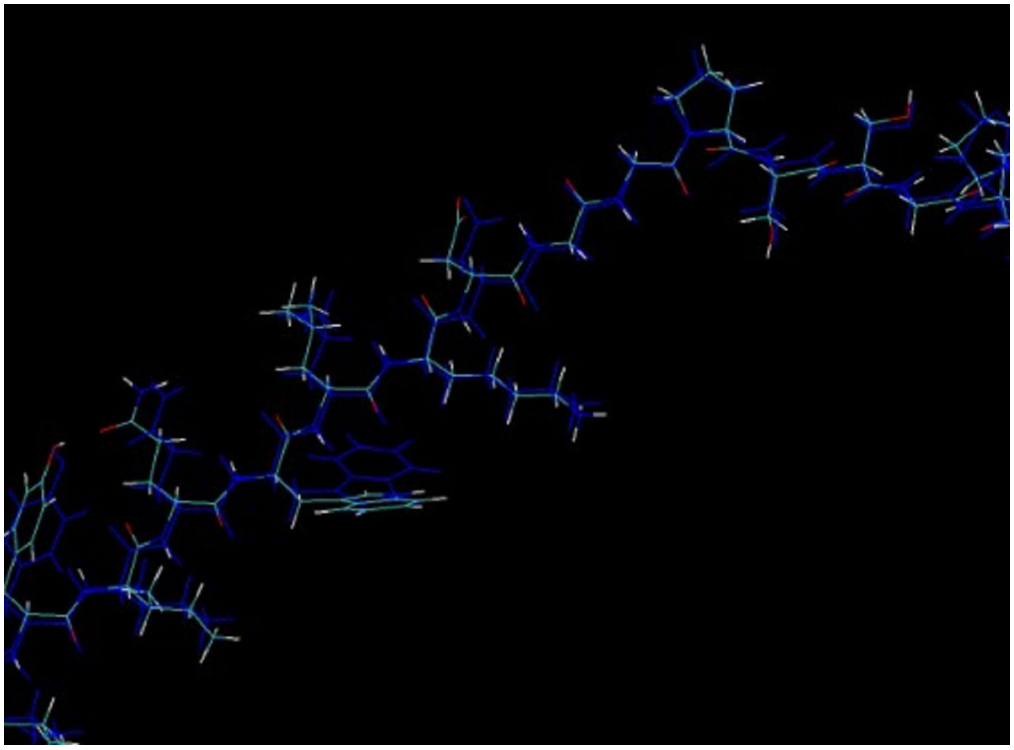

Now we can load more or less any molecule format into this molecule. If we load our pdb file into this molecule we will get the same as before but this time the bonding will be that defined in the prmtop file. Try it. We can also load an inpcrd file (as created by LEaP) or a restrt file (as created by sander) into this molecule. To do this we browse for the file (TRPcage.inpcrd) and select "**rst7**"[vmd1.8.3] or "**Amber7 Restart**"[vmd1.8.4] as the file type. Make sure **TRPcage.prmtop** is selected in the "**Load files for:**" box and then hit **load**.



The bonding should look much better now. This is still too strained a structure, however, to be able to run MD so I have minimised it for you using sander. Here is the restrt file from the end of the minimisation. (TRPcage.rst).

We can load this as either a new molecule (by loading the prmtop file again) or as a new frame in the current molecule. I want to see the two molecules side by side so I will load it as a NEW molecule. So go to the "**Molecule File Browser**" window again and in the "**Load files for:**" box select "**New Molecule**". Now hit the browse button and browse for the **TRPcage.prmtop** file. Select "**parm7**" as the type and hit **load**. Now hit **browse** again and find the **TRPcage.rst** file. Select "**rst7**" as the type and hit **load**. You should now have two molecules displayed in the "**OpenGL**" window. They will be very similar. In order to see the difference between them lets colour one of them in blue.

Go to the "**Graphical Representation**" window and under "**Selected Molecule**" select the first **TRPcage.prmtop** of the two in the list. This should be our initial (unminimised) structure. Then under Coloring Method choose "**ColorID**" and pick 0 in the box that appear to the right of it. You should see one of the molecules in the "**OpenGL**" window turn blue. You can now zoom in on this and look at the difference between the two structures.



As you might have guessed the minimisation has twisted the Tryptophan away from the backbone to avoid that really bad hydrogen contact we had. Can we calculate an RMSD for the minimisation change? We could do this using AMBER's ptraj command but we can also do it within VMD itself using the RMSD extension.

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CLICK HERE TO GO TO SECTION 5

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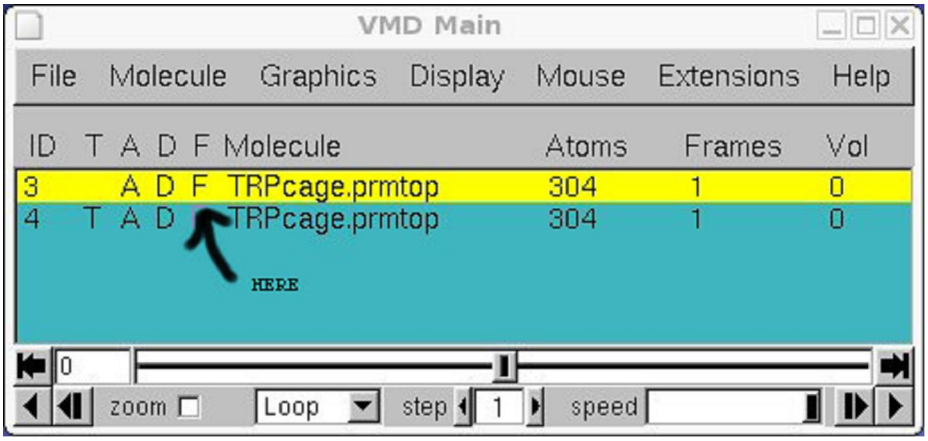
**TUTORIAL B2 - SECTION 5**

**Using VMD with AMBER**

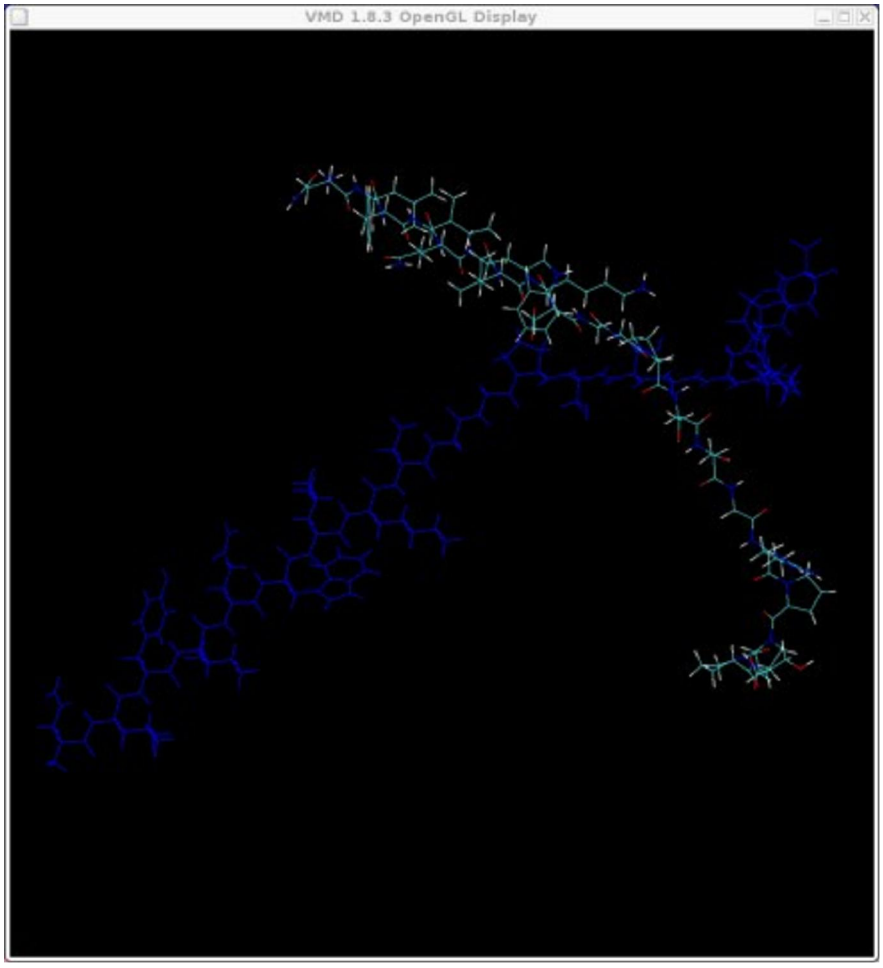
**By Ross Walker**

## *5) Aligning Molecules and Measuring RMSD's*

We do an RMSD fit in two stages. First of all we align the two molecules and then we measure the RMSD between the aligned structures. The alignment actually involves an RMSD fit but the actual value is not printed to the screen. To illustrate how the alignment works lets first rotate one of our molecules on its own. To do this we can remove the "Fixed" flag from the first molecule. We do this by **double clicking** on the letter **F** that is beside the molecule in the "**VMD Main**" window. It should change to black when you double click on it:




Then when you go back to the "**OpenGL**" window you should find that only the second structure (our minimised one) rotates. Now, rotate the molecule so that it no longer aligns with the first one, you can translate it a bit as well if you want:

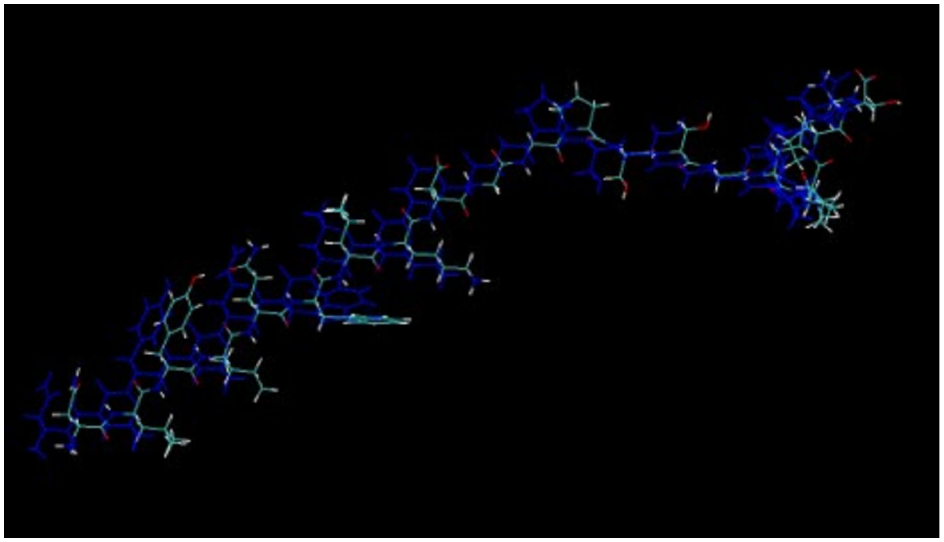



Now **double click** the **F** flag on the first molecule again so that it is no longer fixed. You will now find that the two molecules rotate together and it is difficult to see the structural differences between them. This is often what you will get if for example you load an AMBER trajectory and a crystal structure. They will almost never have the same origin or axis definition and so you cannot visually compare the two molecules. I will now show you a quick way to align the two molecules. Unfortunately we need to load a new file that has the coordinates shifted in order to do the alignment. (if we don't do this and just try to do the alignment as we currently have it VMD won't actually re-align the two molecules).

Here is a structure I have shifted by 2 angstroms in the x direction (TRPcage_shifted.rst).

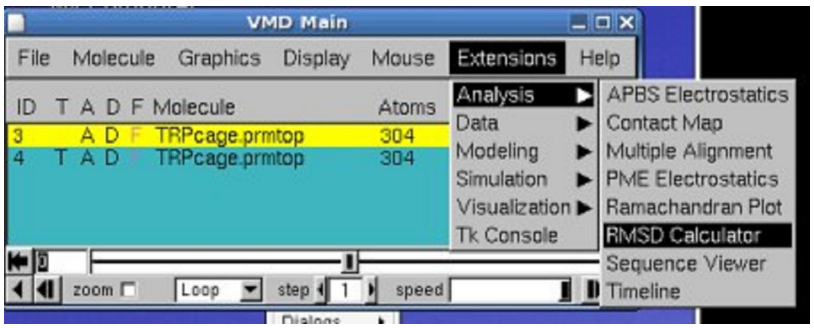
Now, to make sure we are at the same place quit VMD and then reload it.

**Load** the **TRPcage.inpcrd** structure. Remember to load the prmtop first, select **parm7** as the type. Then select **Load files for: New Molecule** and load the prmtop and **TRPcage_shifted.rst** structure. Then go to "**Graphical Representations**" and change the colouring of the first molecule (**0: TRPcage.prmtop**) to **ColorID 0**. Your display should now look like this:

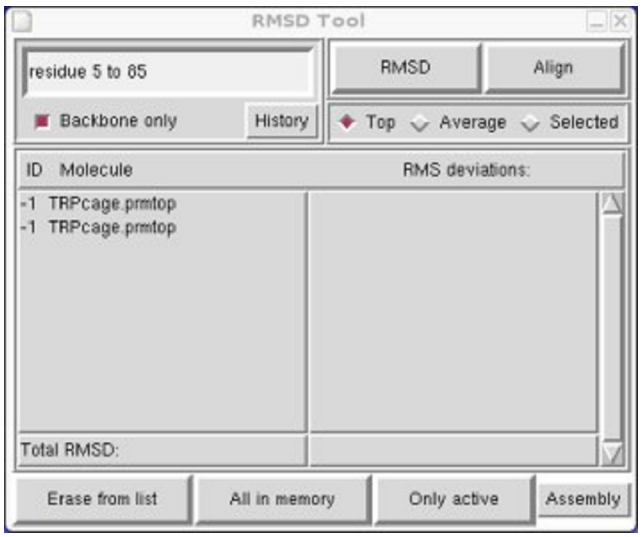


As you can see the two structures are no longer aligned and it is difficult to compare them.

In the early days of VMD you had to use AMBER's ptraj to manually align the two molecules before opening them in VMD. Indeed you can still do this and there are some situations, like when you have a really complex fit to do, or want RMSD as a function of time, that you will need to use ptraj. However, often you just want to do a quick comparison and for this you can use VMD's RMSD Calculator. To access this click on **Extensions->Analysis->RMSD Calculator**. Note this is a section that has changed quite a bit between versions so your options may look slightly different to mine:

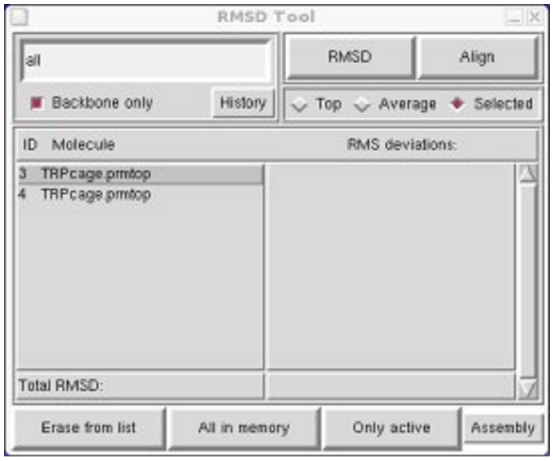



This should bring up the following window:




The first thing we need to do is enter what residues we want to fit in the text box. The alignment will be done on the whole molecule but the actual calculation will be done on what we specify. In this case we want to fit all residues so in the **text box** at the top of the window enter "**all**".

Next we only want to do the RMS fit against backbone atoms (C, CA and N) so make sure "**Backbone only**" is selected. Next we need to make sure the correct molecules are selected. I would start by hitting the "**Erase from list**" button until all of the molecules are removed from the list. Next hit "**All in memory**". This will add the two molecules that we currently have loaded. Next we need to select what we want to fit to what. Since we only have two structures here this is really a no-brainer but even so lets fit the second structure, the minimised one, to the first structure. Hit the **Selected tab**, this should unselect **Top**. Next click on the first molecule in the molecule list to select it:




Now, if we just hit RMSD at this point we will get the RMSD between our two structures which at the moment are very different as we rotated and translated one of them. Try it, hit the **RMSD button**. You should get around 2.2 angstroms. This is because one is offset from the other by 2 angstroms. Now click the **Align button**. You should see the two molecules become aligned in the "**OpenGL**" window. If you click RMSD now you will get the correct RMSD between the backbone atoms of the two molecules. In this case around 0.55 angstroms. This value is typical for a minimisation.

The final stage of this tutorial is how we load AMBER trajectory files so we can watch a "movie" of a structure changing over time.

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CLICK HERE TO GO TO SECTION 6

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# TUTORIAL B2 - SECTION 6

## Using VMD with AMBER

By Ross Walker

## *6) Visualising AMBER trajectories*

Note: Unfortunately VMD cannot yet load compressed (gzipped) trajectory files so when you download the mdcrd.gz files I provide here you will have to unzip then using *gunzip* before loading them into VMD.

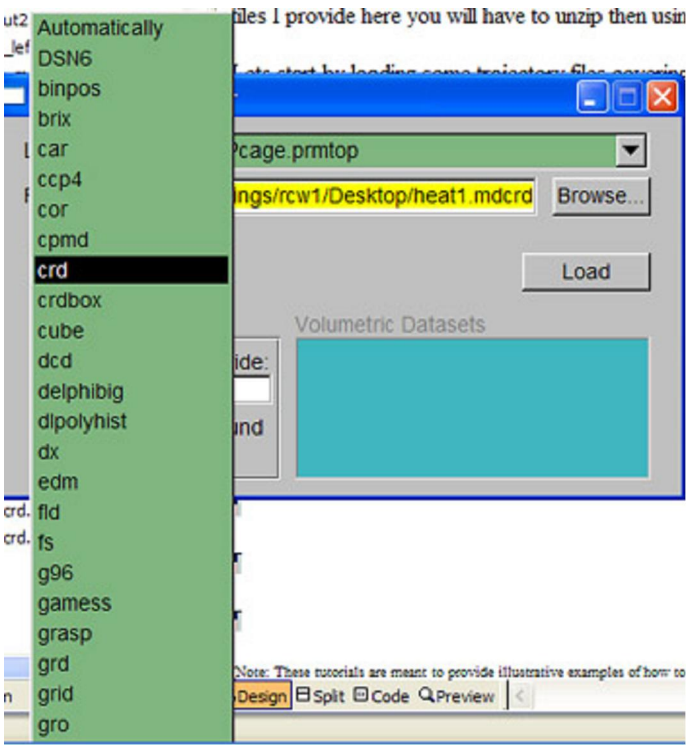
Lets start by loading some trajectory files covering the first 10ps of a Molecular Dynamics simulation of the TRPCage extended structure shown above. These simulations were run using Sander v8.0.

Here are the files you will need: TRPcage.prmtop (128 kb), heat1.mdcrd.gz (510 kb), heat2.mdcrd.gz (515 kb)

Start by decompressing the two trajectory files:

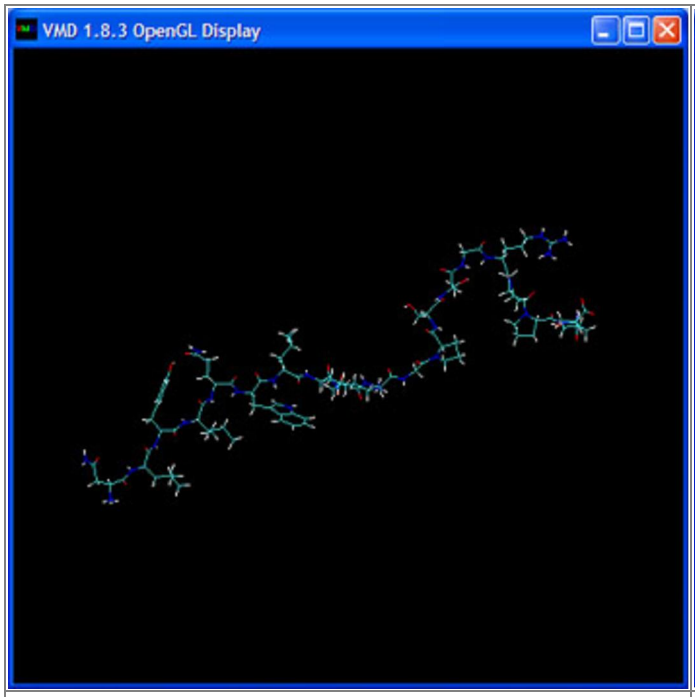
```
>gunzip heat*.mdcrd.gz
```

If VMD is running quit it. This way we should be starting from the same point. Load vmd and browse for the **TRPcage.prmtop** file. Select **parm7** and hit **Load**. Into this structure we will load the two trajectory files on after the other. So, load the first one, browse for **heat1.mdcrd** and then choose "**crd**" as the type and hit **load**.

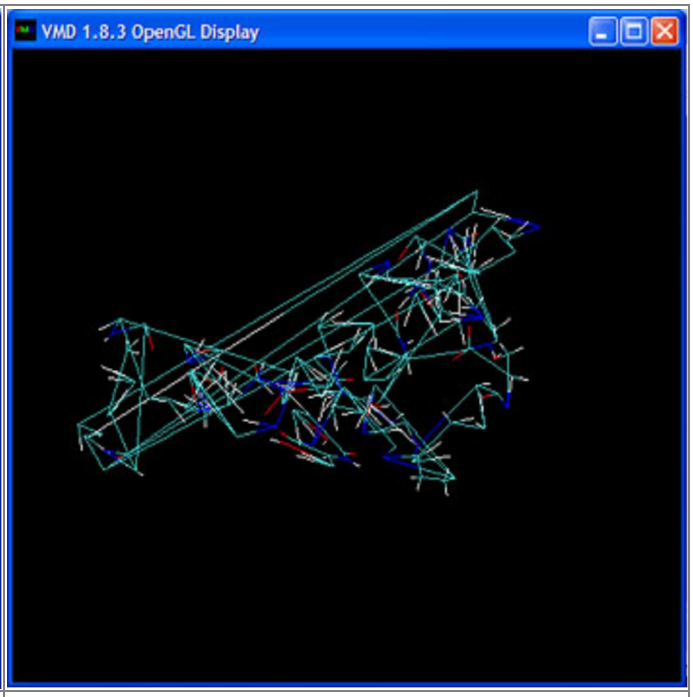



Note: there are two types related to amber trajectory (mdcrd) files. These are "**crd**" and "**crdbox**". The difference between the two concerns whether the trajectory file is from a gas phase/implicit solvent/solvent cap simulation (**crd**) or from a periodic simulation (**crdbox**). When Sander writes an mdcrd file from a simulation run with periodic boundaries it writes an extra 3 floating point

numbers to the end of each frame, these are the box size. VMD is not smart enough to work out what type of trajectory file it is so we need to tell it. In this case we have an implicit solvent calculation so select "**crd**". You can often tell if you have selected the wrong format because things will look very weird, feel free to try it. If you do load a simulation that looks strange try deleting the molecule and reloading it selecting the other format:

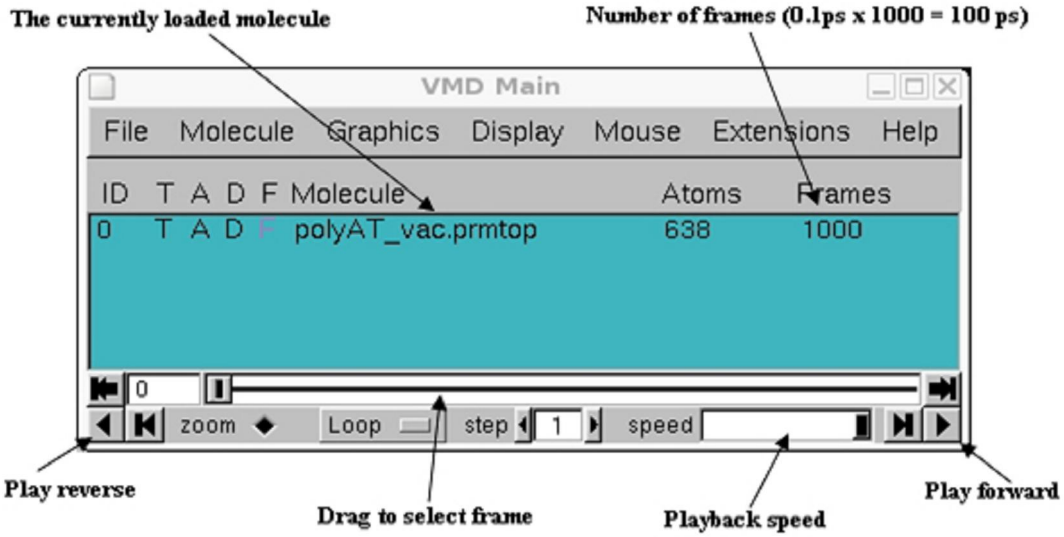



Last frame of heat1.mdcrd loaded with "crd"




Last frame of heat1.mdcrd loaded with "crdbox"

If it loads correctly you should see the TRPcage structure appear in the OpenGL window and start to move. Next click **browse** again and find **heat2.mdcrd**. Load this in the same way, you don't need to reload the prmtop file. Make sure **TRPcage.prmtop** is selected in the "**Load files for:**" box. This will append the frames in heat2 to the frames we have already loaded. In this way you can load a number of different trajectory sets into a single animation so that you can watch the full trajectory without interruption. You should now have 400 frames of TRPcage loaded. This covers 10ps of heating from 0K to 100K. Try replaying the trajectory. You can use the **movie controls** in the "**VMD Main**" window for this:

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CLICK HERE TO GO TO SECTION 7

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(Note: These tutorials are meant to provide illustrative examples of how to use the AMBER software suite to carry out simulations that can be run on a simple

workstation in a reasonable period of time. They do not necessarily provide the optimal choice of parameters or methods for the particular application area.)

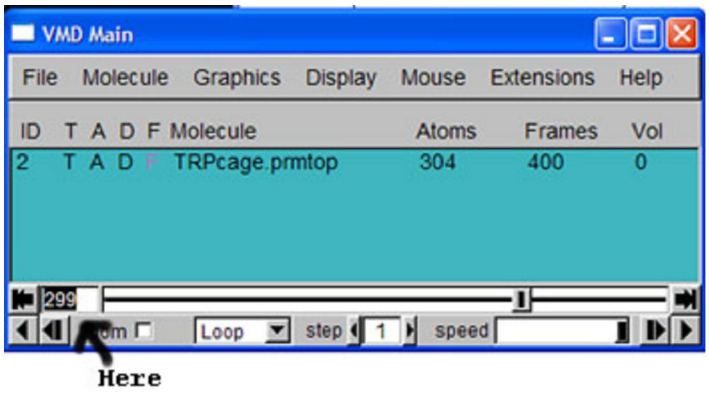
# TUTORIAL B2 - SECTION 7

## Using VMD with AMBER

**By Ross Walker**

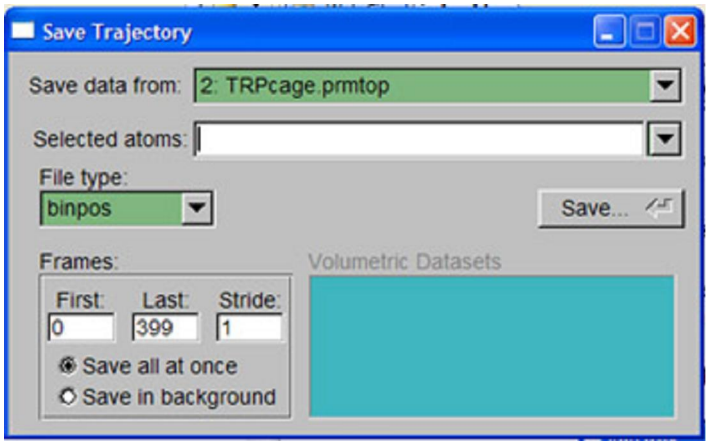
## *7) Saving a single set of coordinates*

Now we have our trajectory loaded lets save frame 300 as pdb file. First of all we have to make sure we have frame 300 displayed in the window. VMD numbers everything from zero so this is actually frame 299 in "VMD speak". We can easily jump to a specific frame by typing the frame number in the text box next to the drag bar in the VMD Main window. Try it now. Enter **299** as shown below and hit enter.




This is the structure we are going to save.

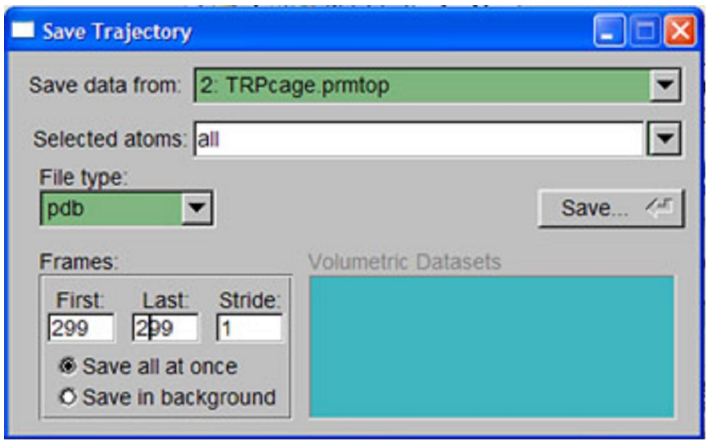
Next click on the "**molecule name**" - The text line that has the T A D and F flags. This should highlight the line in yellow. Then click **File->Save Coordinates...** The following window should appear:




This tool will actually allow us to save the entire trajectory as a different type. E.g. binpos. Or even pdb, VMD will save each frame of our trajectory as a new molecule in a single pdb file. Quite how to interpret such a pdb file, however, would appear to be ambiguous. Some programs, such as rasmol, will load all the molecules together and overlay them all while others, such as VMD, will load each molecule as a frame in a trajectory.

For our purposes we just want to save a single frame as a pdb file. So, start by typing **all** in the **selected atoms** box, this will save all of the atoms in our structure. Next under **file type** select

**pdb**. Finally in the **Frames box** select the **first** frame as **299** and the last **frame** as **299**:




Finally hit **save** and save the file with a filename of your choosing. Here is the pdb file you should get: (frame_300.pdb) Feel free to load it back into VMD if you want.

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CLICK HERE TO GO TO SECTION 8

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(Note: These tutorials are meant to provide illustrative examples of how to use the AMBER software suite to carry out simulations that can be run on a simple workstation in a reasonable period of time. They do not necessarily provide the optimal choice of parameters or methods for the particular application area.)

# TUTORIAL B2 - SECTION 8

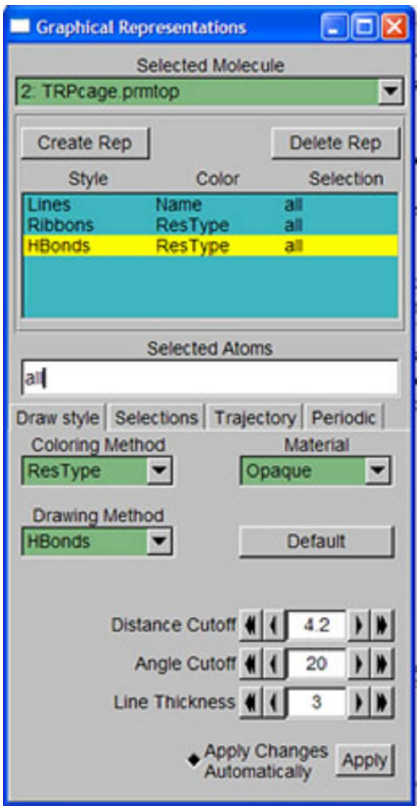
## Using VMD with AMBER

**By Ross Walker**

## *8) Following system parameters over the course of a trajectory.*

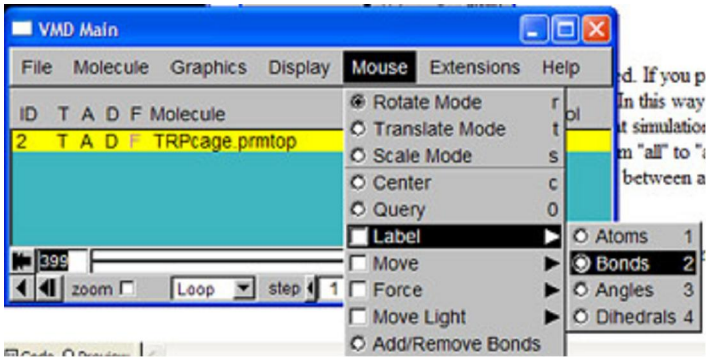
We have two more useful things we should look at in this tutorial. The first is to use VMD's label tools to watch how the distance between two atoms changes during our trajectory.

Lets start by making our currently loaded trajectory a little prettier. Click **Graphics->Representations** to bring up the "**Graphical Representations**" menu if it is not already up. Next click "**Create Rep**" and change the **drawing method** to "**Ribbons**" and the **Coloring method** to "**ResType**". Then hit "**Create Rep**" again and change the **drawing method** to "**H bonds**" and then change the "**Line thickness to 3**" so things are easier to see. Also change the "**Distance Cutoff**" to **4.2** angstroms. This is a little long for what would be considered a regular hydrogen bond but it is just for demonstration purposes since this trajectory is not long enough for any real hydrogen bonds to form. Your window should now look something like this:

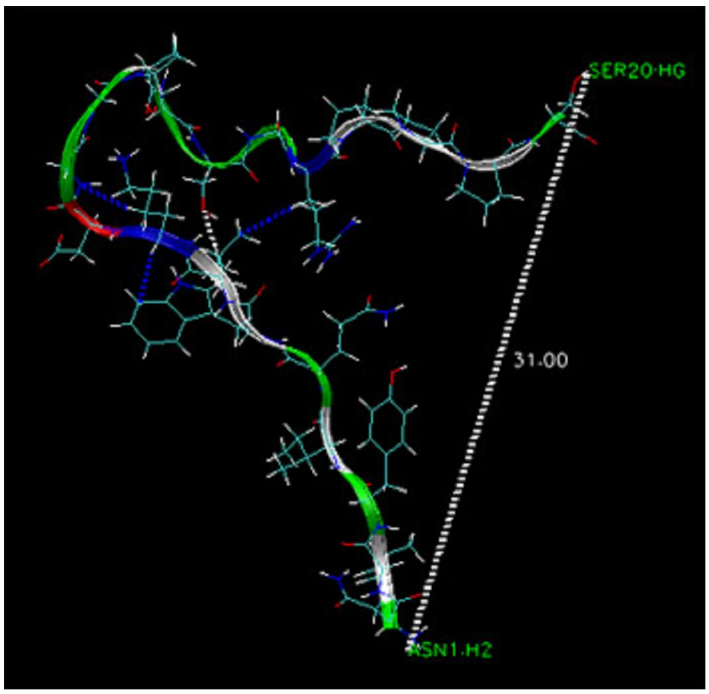



Detected hydrogen bonds will now appear as dashed lines between the two atoms involved. If you play through the trajectory you will see that they are formed in places and then broken and then reformed. In this way you can visually track the presence of hydrogen bonds over a trajectory. Note if this was an explicit solvent simulation you would probably want to change the selected atoms for each of the 3 representations we have from "**all**" to "**all not water**". This is especially true with the HBonds case. Otherwise you will be swamped with dotted lines between all of the hydrogen bonded water molecules.

Finally we will add a bond label between the two ends of out peptide chain. This will allow us to monitor the distance between the chain ends as we run through our simulation. Go to the "**VMD Main**" window and select **Mouse->Label->Bonds**. This will change the mouse left click action to bond selection.




Then go to the "**OpenGL**" window and click on one atom on each end of the peptide chain. You should see a dashed line with the distance between them displayed. If you get things wrong you can use the **Graphics->Labels** tool to delete labels so that you can create them again. Note: The bond, angle and dihedral label options don't actually refer to bonds, angles and dihedrals. The labels you add don't actually have to be between bonded atoms. Bond means distance between any two atoms (in angstroms), angle means angle between any 3 atoms (in degrees) and dihedral means dihedral angle between any 4 atoms (in degrees).




Now play through the trajectory and you should see the value change and the TRPcage peptide starts to fold up. We don't really learn a lot about the system here but this is only designed to show you some of the things VMD can do. Over a much longer production simulation we could learn a lot more and measure more relevant parameters.

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CLICK HERE TO GO TO SECTION 9

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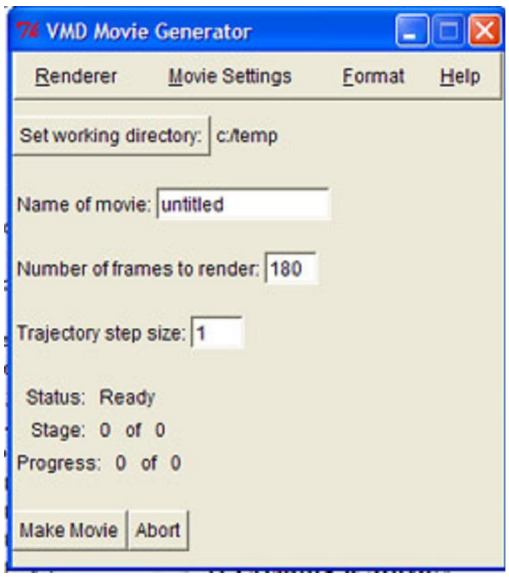
# TUTORIAL B2 - SECTION 9

## Using VMD with AMBER

**By Ross Walker**

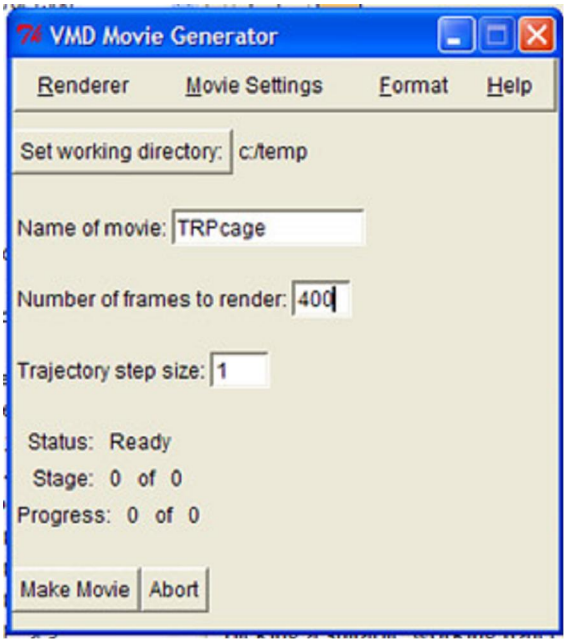
## *9) Creating a Movie*

Finally lets learn how to create a movie of our trajectory so that we can use it in a talk. Note, this may not work on all systems due to compatibility of various compression codecs. However, give it a try on your system and see how you get on. Start by Clicking **Extensions->Visualization->Movie Maker**.




There are a large number of different options available here. I won't try and cover all the options, see the VMD website for more information. In this example I shall just just step through creating a simple movie of the trajectory. Start by picking a suitable working trajectory. The screen shots here are from the Windows version of VMD. It may look slightly different in Unix.

Next enter a name for the movie, e.g. **TRPcage**. We next need to pick the number of frames we want. We have a total of 400 frames in our trajectory so any setting below 400 will loose frame and any setting over 400 will have some frames showing the same thing. We should bare in mine however that the movie will be playing at 24 frames per second. (See **Format->Change Compression Settings** for the frame rate). Hence 400 frames will give us about 16 seconds for our movie. This is reasonable, if we wanted it to last around 8 seconds we could cut the number of frames to 200 and we would get every other frame rendered. Alternatively we could set it to 800 and get a 32 second long movie. The movie length is something you should always consider since it needs to be compatible with your talk. So, enter **400** in the "**Number of frames to render:**" box. We want every frame of the trajectory so leave the step size at 1.




Next we want just a single run through of our trajectory so select **Movie Settings->Trajectory**. Then under Format select **MPEG-1**. This will create an MPEG-1 format video file. By all means play about with the AVI format if you want.

Then hit on "**Make Movie**". Hopefully after about 3 minutes or so you should find a movie file in your working directory.

Here it is TRPcage.mpg (2.9 mb)

This ends the tutorial. This hopefully has given you the knowledge you need view and analyse AMBER files and trajectories using VMD. Bare in mind, however, that we have not even scratched the surface in terms of what VMD can do. If you go to the VMD website you will find much more information covering the more advanced features in VMD.



Return to Index



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