DEEP VIEW Tutorial - Introduction to Program

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Lesson Date: 09/20/06 - W

A Bit about DEEP VIEW

The following program (DEEP VIEW version 3.7, formally called SWISS-PDB VIEWER) is used to translate a PDB file containing detailed molecular structure information into a picture. The PDB files from published structures (from both nuclear magnetic resonance spectroscopy and x-ray crystallography) are available at the Brookhaven Protein Data Bank http://www.rcsb.org/pdb/index.html.

This shareware free software is a more robust visualization program than RASMOL and is commonly used by many structural biologists. Although the rendering is not as nice as in RASMOL, it provides a number of powerful tools for displaying and manipulating macromolecular structure that RASMOL can not. The user can display multiple structures, display electron density or electrostatic maps, display crystal symmetry (useful for displaying an entire molecule), create 'mutants', perform sequence alignments, superimpose related molecules, perform energy minimization's, and so on. If you are interested in structural biology research, you should learn how to use this program thoroughly. For more information on what DEEP VIEW can do, please see the introduction to Gale Rhodes tutorial as well as the ExPASy (**Ex**pert **P**rotein **A**nalysis **Sy**stem) Molecular Biology Server. Both web addresses can be found below.

DEEP VIEW as an Analytical Tool.

- Build models from scratch
- Find H-bonds within proteins and between proteins and ligands
- Examine e-density maps from crystallographic structure determination
- Judge quality of maps and models
- View several proteins simultaneously
- Superimpose structures to compare structure and sequence
- Carry out energy minimization
- Creates homology models with SWISS-MODEL

Computing Platforms for running DEEP VIEW. DEEP VIEW runs best on a Macintosh PowerPC, a UNIX computer (e.g. an SGI), or a Pentium based computer running Windows or NT. Other computers can be used but tend to be slow. In addition to

the computers available for this course, suitable computers can be found in the CCIT computing labs and the Biology Learning Center.

- CCIT http://www.ccit.arizona.edu
- Biology Learning Center (BLC) http://www.blc.arizona.edu

Downloading DEEP VIEW and PDB files. To run DEEP VIEW, you must obtain the program DEEP VIEW 3.7 (already downloaded on the Biochemistry Lab computers), and a Protein Data Bank (PDB) file (which contains the coordinates for the structure to be viewed).

- DEEP VIEW Umbrella Page (ExPASy) http://www.expasy.ch/spdbv/mainpage.html
- Download DEEP VIEW version 3.7 http://us.expasy.org/spdbv/text/disclaim.htm
- Download PDB files (PDB site) http://www.rcsb.org/pdb/

DEEP VIEW User Guide and Help

- User Guide http://us.expasy.org/spdbv/text/main.htm
- Help directions http://www.usm.maine.edu/%7Erhodes/0Help/GetSPdbV.html)

Additional DEEP VIEW Tutorials

- Gale Rhodes (U. Southern Maine) http://www.usm.maine.edu/~rhodes/SPVTut/index.html (MOST RECOMMENDED!)
- From DEEP VIEW Homepage (Expasy) http://us.expasy.org/spdbv/text/tutorial.htm
- U. Arizona - formally used in Graduate course 585: Biological Structure http://www.biochem.arizona.edu/classes/bioc585/protnuc/example/example.htm

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Tutorial Exercise

This exercise is designed to teach you the basics of molecular graphics display using the program DEEP VIEW. If you have any questions, please ask! We will be using the enzyme lysozyme in complex with the trisaccharide inhibitor tri-(N-acetylglucosamine) or tri-NAG. Atomic coordinates contained in the Protein Data Bank have a pdb code of **1HEW.pdb**.

Tutorial Exercise Objectives:

- Start and download structures into DEEP VIEW
- Understand the Windows of DEEP VIEW
- Become familiar with the Control Panel

- Become familiar with the Tool Bar
- Practice keyboard modifiers

Part I. Getting Started and Knowing the Various Windows of DEEP VIEW

- Creating a DEEP VIEW folder
- Obtaining the PDB file 1HEW.pdb
- Starting DEEP VIEW
- Opening a PDB structure
- Opening Various Windows (Control Panel, Alignment, Layers Infos, Ramachandran Plot)

- **Create a DEEP VIEW folder in your directory**.
  Unlike RASMOL, you do not need to save everything dealing with DEEP VIEW in this folder to have the program work properly. However, for organizational purposes, I highly suggest that you keep everything dealing with DEEP VIEW in this folder.

- **Obtain the PDB file 1HEW.pdb.** (This can be done 1 of 2 ways:)
  1. On the **course website** under Computer Section/Shared PDB's and RASMOL Scripts.
  2. Go to the **PDB and retrieve** the coordinate file for lysozyme in complex with tri-NAG that has the name **1HEW**.

- **Start DEEP VIEW**. Double click on the DEEP VIEW icon on your desktop. A window that has credits will pop up Close this window. You will now see a window with menu pull downs as well as picture icons. This is called the Tool Bar and will be referred to as such from this point on.

- **Opening a PDB structure.** Go to the 'File' pulldown menu at the top of the Tool Bar window. Scroll to 'Open PDB File...'. Scroll to your Deep View folder and open 1HEW.pdb. The protein should appear as a wireframe model in a black window, which is labeled with the name of the PDB file. This is called the in the Display window and will be referred to as such from this point on. *Note: Unlike RASMOL, DEEP VIEW displays only in wireframe.* In addition a window called inputlog.txt opens...don't worry about this, thus close it.

- **'Window' pulldown Menu**
  Go to the 'Window' pulldown menu at the top of the Tool Bar window. Scroll to the following to see its location and what each entails:
  - **Control Panel.** Opens to the right of the Display window. The Control Panel is very important. It lists the amino-acids residues and other contents of the PDB file. From here you select residues, label residues, color residues, ect. We will go into more depth in Part III of this tutorial, thus do not close this window.

- **Alignment**. Opens below the Display window. This window shows the amino acid sequence of the protein in one-letter abbreviations. This window comes in handy when comparing sequences of two or more proteins. For now, close this window.
- **Layers Infos**. Opens to the right above the Control Panel. This table allows control of multiple protein models when needed. You can choose which model is visible, which model can move, and which model has certain features displayed. For now, close this window.
- **Ramachandran Plot**. Opens to the left of the Control Panel. As learned in lecture, a Ramachandran plot allows you to judge the quality of a model and find residues whose conformational angles lie outside allowed ranges. For now, close this window.

PART II. Moving your Model.

To make your model active, click on the Display window. The following Tool Bar buttons will manipulate your model. Take time to play with these tools. More to come on the Tool Bar in PART IV.

Tool Bar Buttons (First 4 buttons starting from left to right):

- **Zoom/Center** (arrows pointing in toward a residue): This automatically zooms to fill the screen with whatever is currently on display. Use this function when ever a view becomes awkward

- **Translate** (hand): This translates your model when you click and move your mouse over your model.

- **Zoom** (boxes): This zooms your model.

- **Rotate** (circular arrow): This rotates your model.

- *Tip: Pressing **'TAB'**: Cycles through the translate, zoom and rotate functions from **left to right**.*
    - *Pressing **'SHIFT + TAB'**: Cycles through the translate, zoom and rotate functions from **right to left**.*

PART III. The Control Panel.

The control Panel is very important. It lists all the groups in your model and lets you select, display or hide parts of the model. It may seem overwhelming at first, but as with RASMOL, the more you play, the easier it will all come.

Raw (i.e. Column) Headings (From Left to Right):

- **Far most left** (which is blank in this case): When a protein contains more than one **chain**, the letter designation (Usually A & B) for each chain appears here.

- **'s' & 'h'** (to the left of the 'group' column): **secondary structure** (sheet and helix respectively)

- **'Group'**: lists the **residue and hetero** group names and numbers.

- **'Show'**: displays the **backbone** of an individual or selected residues

- **'Side'**: displays the **sidechains** of an individual or selected residues.

- **'Labl'**: **Labels** individual or selected residues

- **Dots**: displays a dotted van der Waals or accessible surface of an individual or selected residues depending on which is activated.

- **'Ribn'**: Stands for Ribbon; draws a smooth-stranded cartoon of the selected backbone

- **'Col'**: Shows the **color** of each residue when colored.

- **Far most right**: Chooses what you want to color (ex. backbone + sidechains, backbone only, label, ect.)

Tips and keyboard modifiers:

When click on a **group name**:

- **SHIFT**: acts (meaning selects/deselects) on all groups.

- **CTRL**: acts only on selection without affecting other groups.

- **SHIFT + CTRL**: deselects

- **Right Click**: centers a group or select groups belonging to the same secondary structure

- In general, to **select a group of residues** in a row:

  - **Click and drag** on those residues in the '**group**' column OR

  - **Click** on the **first** residue and **'SHIFT + Click'** on the **last** residue of interest.

When click on a **checkmark raw**:

- In general, clicking **in the checkmark raws** next to a group acts on **individual** residues/groups.
- In general, clicking **on a heading** at the top of the raw acts on **all selected** (i.e. red) residues.
- **SHIFT**: acts (meaning checks/unchecked) on the **whole raw**
- **SHIFT + CTRL**: acts on the **whole raw of each layer**

Additional:

- **'Enter': adds selected** groups and **removes unselected** groups.
- **'+'** on the numeric key pad: **Toggles on and off the selected groups** without affecting the other (unselected) groups. Make sure you NUMBER LOCK IS ON!!!

Exercise: Now Let's play with these a bit:

- First, **scroll** down to the bottom to see how many amino acids and the names of the hetero group(s) the protein contains. Hetero group(s) are always listed last.
- **Select LEU 25- SER 36**: Click and drag on the word LEU 25 through SER 36. These residues are now selected and should turn red.
- **Press 'Enter'**. Notice only those residues **selected (residues 25-36) remain** in the display window and have a check next to them in the 'show' and 'side' raws. Move the display using the manipulation tools learned previously. What type of secondary structure is this?

  *Note: When using the Control Panel, a sidechain is only shown if the residue is displayed. You can display only the sidechains without the backbone by using the 'Show Sidechains even when Backbone is Hidden' under the 'Display' pulldown in the Tool Bar.

- **Click the checkmark in the 'show' raw next to CYS 30.** Notice that CYS 30 disappears. Click in the same space to make it reappear. Try the same in the

'side', 'label', and 'surface' raws and see what happens. Now **remove** the checks from the **'label' and 'surface'** raws simply by clicking on the checkmark.

- **Click on the raw heading word 'label'**. Notice all selected residues are now labeled.
- **Click on the raw heading picture of 'dots'.** This shows a dotted van der walls or accessible surface on all selected residues depending on which is activated.
- **Click on the raw heading word 'ribn'.** This draws a smooth-stranded cartoon of the selected backbone.
- **Remove all labels, surface and ribbon.** Try both of these ways:
    - '**SHIFT + Click'** simultaneously **on a checkmark** in the respective raw OR
    - **'CTRL + SHIFT + Click** on the raw **heading**

*Note: To add all labels, surface and ribbon again simply use the above in an empty space in the respective raw.

- **Add, but not select, residues 16-24 to your model.** Click from residue 16-24 in the 'show' raw . Notice checks appear, however **they do not turn red**. This means that residues 25-36 are selected and shown, while residues 16-24 are shown, but NOT selected.

- **Press '+' on the numeric key pad.** This **toggles on and off the selected groups** without affecting the other groups. End with residues 16-36 displayed.

- **Press Enter.** Notice that residues 16-24 disappear because they were not selected .

- **Select and display residues 13 and 19 in addition to what is already selected.**
    - **'CTRL + Click'** on residues 13 and 19 in the **'group' raw**. They should turn red.
    - Press **'Enter' to add** them to the display.
    - Click on the raw **heading 'side'** to turn on their **sidechains** .

- **Click anywhere in the far most left, blank raw.** Notice the entire chain (in this case, the entire model) has been selected and thus turns red. Press **'Enter'** to display the chain.

- **Click on any 'h' in the second column.** This selects all residues in that **helix**. Press **'Enter'** to display the helix.

- **Click on another 'h' or 's'**. This changes your selection. Press **'Enter'** to display.

PART IV. The Tool Bar.

The Tool Bar allows you to perform a variety of actions. We will not be able to go through all the icons or pulldown menus today so I suggest playing on your own. Instead we will have a brief overview of the icons not mentioned in PART II and of some of the more basic and/or useful operations in the pulldown menus.

Buttons (From Left to Right): To use, simply click on the button and follow the directions which appear below it in red.

- **Zoom/Center** (arrows pointing in toward a residue): This automatically zooms to fill the screen with whatever is currently on display. Use this function when ever a view becomes awkward

Manipulative:

- **Translate** (hand): This translates your model when you click and move your mouse over your model.
- **Zoom** (boxes): This zooms your model.
- **Rotate** (circular arrow): This rotates your model.

Most Commonly Used Tools:

- **Distance** between two atoms
- **Angle** between three atoms
- **Dihedral angles** (By default, gives a measure of omega, phi and psi angles of the picked amino-acid)
- Atom **Identification**
- Display/Undisplay selected groups in a certain **radius**
- **Center** the molecule on one atom
- **Fit** a molecule onto an other (More advanced fitting features available in the 'Tools' pulldown)
- **Mutation** tool
- **Torsion** tool (Allows to rotate sidechains atoms)

Menu Pull-downs

- **File** - Commands as most programs.
- **Edit** - Commands as most programs.
- **Select** - Provides commands for selection in addition to those in the Control Panel
  - **all**: selects all
  - **inverse**: selects opposite of what is selected
  - **visible**: selects those residues that are currently visible
  - **pick on screen**: selects those which you click on in the display
  - **group kind**: selects by amino acid, nucleic acid, heteroatom, solvent or disulfide bonds
  - **group property**: selects based on acidity or polarity
  - **secondary structure**: selects alpha helices, beta sheets or coiled
  - **accessible aa**: selects amino acids over a certain accessible cut off (determined by user)
- **Build** - Useful when rebuilding a model during a process called refinement. For now, don't worry about this menu.
- **Tools** - Provides various advanced tools, some of which we will discuss in later lessons.
- **Fit** - Allows various operations such as superimposition of molecules. This pulldown will only be active when more than one molecule is present.
- **Display** - Allows options on different ways to display molecule. The most important are:
  - **Show CA trace only**
  - **Show sidechains even when backbone hidden** (command noted in PART III)
- **Color** - Provides many different ways to color a model. Color is not trivial. It can reveal structural, chemical and comparative features. It is to note that the same operations in this menu can also be done through the Control Panel (i.e. the last two raws to far right)
  - 1st: Choose an 'act on...' (BB & SC, BB only, ect.)
    - Backbone + Sidechains
    - Backbone
    - Sidechains
    - Ribbon
    - Label
    - Surface
  - 2nd: Choose a 'by...'
    - CPK: carbon = gray, nitrogen = blue, oxygen = red
    - Type: basic (+) = blue, acidic (-) = red, nonpolar = gray, yellow = polar, uncharged

*Note: aromatics are included into one of the above categories. (Ex. Tyr is yellow, thus polar and uncharged)

- Secondary Structure: alpha-helices = red, beta-sheets = blue, coil = gray

- Accessibility: The darker the color, the less accessible to solvent

- **Preferences** - Sets how you want to the program to perform. In other words, you can customize tools to your liking. I suggest not changing anything for this class and use the programs default preferences.
- **Swiss-Model** - Creates homology models. This is beyond the scope of this class, thus ignore this menu.
- **Window** - Please see PART I for details.
- **Help** - Provides help files for the Tool Bar, Control Panel, Layer Info, Alignment, and Ramachandran Plot Windows. (Note: These help files can also be found by clicking the red '?' in each window.) Also provided here is a web or local-based copy of the user manual.

Exercise: Now Let's play with these a bit. Since many of the menus and buttons are relatively intuitive, there will be less guidance on getting the end result and more questions asked. Please put answers on a separate piece of paper: you will be asked to hand these in the Wednesday after the exam.

We will concentrate on the **Select, Display and Color pulldown menus** first.

1. Select and display the whole molecule and color it CPK: Go to the 'Select' pulldown menu, then to 'all'. To display residues, press 'Enter'.
   - Again, what were the steps you used to accomplish this?
2. Select and display accessible residues with a cut off of 30: Go to the 'Select' pulldown menu, then to 'accessible aa...'. Enter a cut off of 30 and then press 'OK'. To display only these residues, press 'Enter'.
   - Where are most of these residues located? (Hint: color by accessibility)
   - What type of residues are they? (Hint: color by type)
   - Name two of these residues.
3. Select and display all residues involved in beta-strands. Notice the characteristic pattern of hydrogen bonds in the strands. (Note: To turn on H-bonds, go to the 'Tools' menu pulldown and then choose 'Compute H-bonds'. To turn off H-bonds, go to the 'Display' menu pulldown and then uncheck 'Show H-bonds'.)
   - How many strands are shown?
   - Are they close in the primary amino acid sequence?

4. Select and display only the residues whose sidechains carry positive charge (i.e.. basic residues).
   - Where are these residues located?
   - What color are they?
   - Name two of these residues.
5. Select and display only the histidine residues and their side chains.
   - How many histidines are present in lysozyme?
   - When colored by type, what color are histidines?
6. How many disulfide bonds are present in this model? What are the residue names and numbers involved in these disulfide bonds?
7. What is the approximate length of a disulfide bond?
8. What is the approximate length of a hydrogen bond? (Hint: you first have to 'Compute H-bonds' from the 'Tools' menu pulldown then measure the distance).
9. Name two residues within 6A of the heteroatom NAG.

Extra Problem:

10. Make a model in which lysozyme is shown only as a ribbon, colored by secondary structure, and tri-NAG is shown in normal (CPK) colors with a dotted van der Waals surface.

- What are the steps you used to accomplish this view?