The Model Panel and Ensembles Tutorial

This tutorial focuses on using the **Model Panel** and handling ensembles of structures (such as those determined by NMR).

We will view solution structures of a toxin that binds to sodium channels. Separate ensembles were determined for *cis*- and *trans*-proline conformations of this toxin:

> L. Volpon, H. Lamthanh, J. Barbier, N. Gilles, J. Molgo, A. Menez, and J.M. Lancelin, "NMR solution structures of δ-conotoxin EVIA from *Conus ermineus* that selectively acts on vertebrate neuronal Na+ channels" *J Biol Chem* **279**:21356 (2004).

On **Windows**/**Mac**, click the **chimera** icon; on **UNIX**, start Chimera from the system prompt:

```
unix: chimera
```

A basic Chimera window should appear after a few seconds; resize it as desired. Open the **Command Line** (choosing **Tools... General Controls... Command Line** is one way).

If you have internet connectivity, structures can be obtained directly from the Protein Data Bank:

> *Command*: **open** **1g1p**
> *Command*: **open** **1g1z**

If you do not have internet connectivity, you can download the files 1g1p.pdb.gz and 1g1z.pdb.gz into your working directory and then open them in that order as local files (with **File... Open**). It is not necessary to uncompress the files.

Simplify the view to α-carbon traces and thicken the lines:

> *Command*: **chain** **@ca**
> *Command*: **line** **2**

An α-carbon trace connects the α-carbons of amino acid residues that are directly bonded to each other, either sequentially in the peptide chain or by sidechain crosslinks such as disulfide bonds.

Rotate, translate, and scale the structures as desired throughout the tutorial. Optionally, use the **Side View** to scale the view and move the front and back clipping planes. There are several ways to start tools, including from the menu (in this case, **Tools... Viewing Controls... Side View**) or with a command:

> *Command*: **start** **Side View**

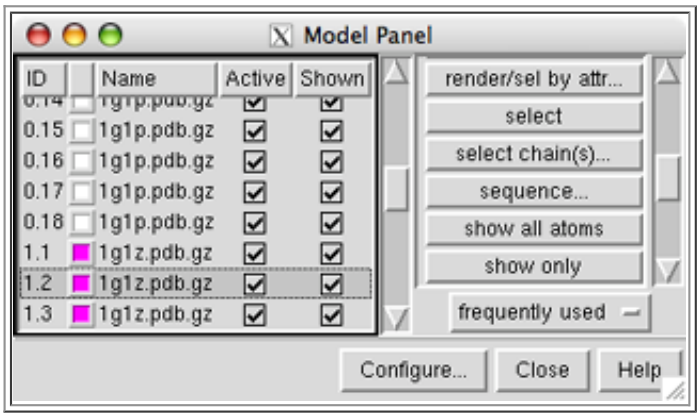
Open the **Model Panel**:

> *Command*: **start** **Model Panel**

Each file of coordinates opened in Chimera becomes a ***model*** with an associated ID number and

model color. Some PDB files are further subdivided into multiple structures designated with MODEL and ENDMDL records; these are assigned ***submodel*** numbers. Each structure can be specified independently by number (**model.submodel**) and handled just as if it were a separate model. Thus, the term "model" often indicates anything with its own line in the **Model Panel**, whether it is a submodel or a model not subdivided into submodels.

Each of these files contains an ensemble of 18 structures. **1g1p** (*trans*-proline conformations, white) has been opened as models 0.1-0.18 and **1g1z** (*cis*-proline conformations, magenta) as models 1.1-1.18.



At first, most of the functions on the right side of the **Model Panel** are grayed out because none of the models are chosen. Choose model **1.2** by clicking its ID or name on the left side of the **Model Panel**, then try various functions:

> **show only** - hide the other models
> **show all atoms** - display all atoms
> **select** - select the entire model for further operations

in the menu: **Actions... Color... by heteroatom**
in the menu: **Select... Chemistry... element... H**
(this changes the selection to hydrogens in *all* models)
in the menu: **Actions... Atoms/Bonds... delete**
(in general, use **hide** instead of **delete** when the atoms might be needed later)

Sulfur atoms are shown in yellow; the structure contains three disulfide bonds.

Back to the **Model Panel**:

> **sequence...** opens a sequence window for the model. In that window, choose **Structure... Secondary Structure... show actual**. Two very short β-strands (positions 24-25 and 29-30) are highlighted in green. Placing the cursor over a residue in the sequence reports the corresponding structure residue number near the bottom of the window. The β-strand locations were read from the input file along with the coordinates. Highlight a string of residues in the sequence with the mouse and see how they become selected in the structure. **Quit** from the sequence window, then act on the selection with the menu: **Actions... Color... cyan**

Clear the selection, display ribbons, and hide atoms:

in the menu: **Select... Clear Selection**
in the menu: **Actions... Ribbon... show**
in the menu: **Actions... Ribbon... rounded**
in the menu: **Actions... Atoms/Bonds... hide**

The ribbon shows the β-strands as arrows. Although the input file specifies the strand locations as 24-25 and 29-30, the paper describes three β-strands, comprised of residues 8-10, 23-26, and 28-31. Such differences are common because secondary structure assignments are method- and parameter-dependent. Rather than trying to reproduce these assignments by recomputing secondary structure, change the assignments directly:

> *Command*: **setattr r isStrand true :8-10,23-26,28-31**

This sets the residue attribute named **isStrand** to **true** for the specified residues in all models. Although not necessary in this case, the previous assignments could have been cleared first, for example with:

> *Command*: **setattr r isHelix false**
> *Command*: **setattr r isStrand false**

Secondary structure assignments can also be changed by selecting amino acid residues, opening the **Selection Inspector**, and changing **Residue** settings.

Back to the **Model Panel**:

> **color by SS...** (to see this button, it may be necessary to change from the **frequently used** list of **Model Panel** functions to the **infrequently used**) opens **Color Secondary Structure**. The model chosen in the **Model Panel** (1.2) is automatically already chosen in this dialog. Click **OK** to use the default colors.
>
> uncheck the **Shown** checkbox for model 1.2
>
> check the **Shown** checkbox for model 1.2

The **Shown** checkboxes toggle model display without changing the display settings of individual atoms, bonds, and ribbon segments. Using the **Shown** checkbox is equivalent to using the command **modeldisplay**. Show all of the models:

> *Command*: **modeldisplay**

The **Active** checkboxes in the **Model Panel** control what can be moved:

> uncheck the **Active** checkbox for model 1.2 and try moving the structures with the mouse; now only the other models can be rotated and translated
>
> check the **Active** checkbox for model 1.2 and try moving the structures again

Restore the position of model 1.2 relative to the others:

> *Command*: **matrixcopy #1.1 #1.2**

The first number could have been the number of any other model, since only model 1.2 was moved separately.

We will use **Ensemble Cluster** to cluster each ensemble and identify representative structures, then compare the representatives with **Ensemble Match**.

Start **Ensemble Cluster** (under **Tools... MD/Ensemble Analysis**) and choose **1g1p** as the ensemble to cluster. Leave the **Parts to Match** blank to use all atoms and click **OK**. Results are shown in a cluster list dialog; three clusters were found. In that dialog,

click the black arrowhead to reveal the **Treatment of Chosen Clusters**

choose all three cluster lines in the dialog with the mouse; this recolors all the **1g1p** structures, using three different colors for the three clusters, and chooses their lines in the **Model Panel**

change the third **Treatment** option to choose only the **representatives** in the **Model Panel**

Click **show only** on the right side of the **Model Panel** (to see this button, it may be necessary to switch back to the **frequently used** list of **Model Panel** functions). Delete the rest of the **1g1p** ensemble in model 0:

Command: **delete #0/!display**

This deletes models with ID number 0 and model display turned off (**!display** is the opposite of **display**). **Quit** from the cluster list dialog.

Start **Ensemble Cluster** again and cluster **1g1z** using all atoms. This time, four clusters are found. In the cluster dialog, make sure the treatment is to choose only **representatives** in the **Model Panel**. Choose just the two clusters with more than one structure and then, as before, click **show only** in the **Model Panel**. **Quit** from the cluster dialog and delete the rest of the **1g1z** ensemble:

Command: **delete #1/!display**

In the left side of the **Model Panel**, drag with the mouse to choose all five remaining models. On the right side,

click **show only** to show all five models

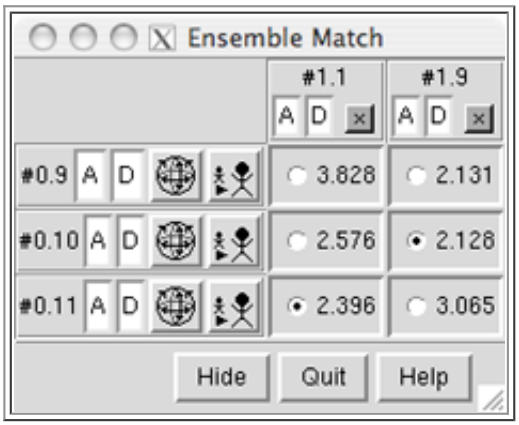
click **rainbow...** and in the resulting dialog, click **OK** to give each **model** a different color in the rainbow range

click **tile...** (it may be in the **infrequently used** list) and in the resulting dialog, decrease **Border scale** to –0.2 and click **OK** to spread the models out in a plane

Finally, compare the structures with **Ensemble Match** (under **Tools... MD/Ensemble Analysis**). Choose one ensemble as the reference and the other as the alternative. For **Parts to Match** just specify the backbone atoms:

@n@ca@c@o

Click **OK** to calculate the matches. Results are shown as a 3 x 2 (or 2 x 3) table with entries for all pairwise comparisons between the ensembles. The **A** and **D** buttons control model activation for motion and model display, respectively. The numbers in the table are pairwise RMSDs using the atoms that were specified as **Parts to Match**.



The structures are not yet superimposed. Clicking a button next to an RMSD value performs the corresponding match and reports in the status line the number of atom pairs used. Superimpose each *cis*-proline conformation in model 1 on the most similar (lowest-RMSD) *trans*-proline conformation in model 0.

In this case, *cis* and *trans* refer to the peptide bond between leucine-12 and proline-13. Display these residues as ball-and-stick:

> *Command*: **disp :12-13**
> *Command*: **repr bs**

When finished viewing the structures, choose **File... Quit** from the menu to exit from Chimera.

---

meng@cgl.ucsf.edu / August 2008