Übung 3: Chimera, A Molecular Graphics Program

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1. Introduction

This is an introductory exercise to *Chimera (http://www.cgl.ucsf.edu/chimera/),* which is one of the more powerful programs for drawing protein structures, comparing them and performing some kinds of analyses. In future Übungen and in other courses, we will assume that you know how to play with this program and some of the things it can do.

2. Running Chimera

Start the program with */usr/local/zbh/chimera/bin/chimera &*

3. **The Chimera Tutorials**

This is a brief version of the *chimera* tutorial. The full version is available in *chimera* 's homepage (http://www.cgl.ucsf.edu/chimera/1.1872/docs/UsersGuide/indextut.html).

The Getting Started Tutorial

This is a basic tutorial in two parts command line and menu interface on the same set of operations. It covers the procedure for selecting atoms, bonds, and residues in a PDB file, and how to display molecular structure in different ways.
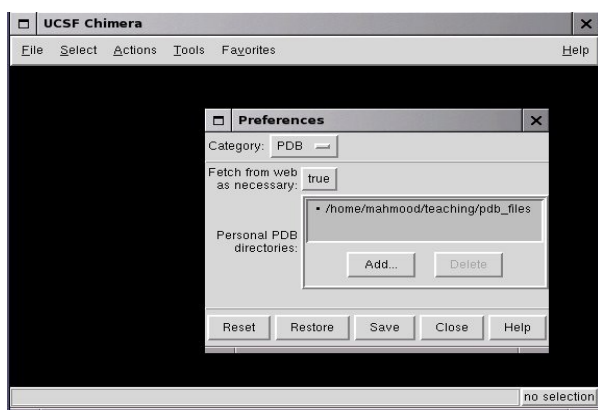
Downloading PDB Files:

Chimera can retrieve PDB files from the Protein Data Bank via the net or from local directories.

The directory containing all the PDB files used in the exercise is:

/home/mahmood/teaching/uebung1.

<u>Menu Molecular Manipulation, Selection, and Chains</u>

In the following section, you will apply the same operations to the molecules, except that you will use the menu instead of the command line interface.

Open a structure:

File»Open

In the dialog, find and select **1zik.pdb** in */home/mahmood/teaching/uebung1/* and then *Open* to dismiss the dialog.
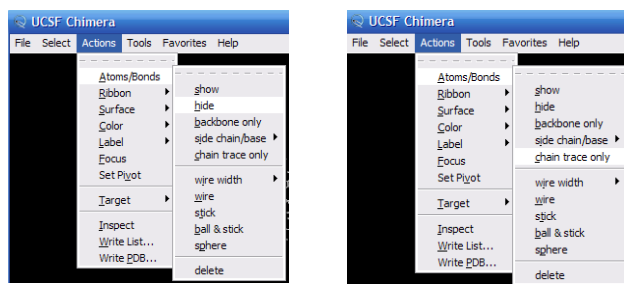
Simplify the display:

Actions»Atoms/Bonds»Hide
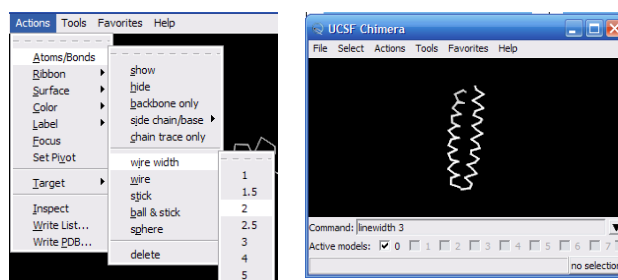
Actions»Atoms/Bonds»backbone only»chain trace

This will show only the CA atoms.

To thicken the lines:

Actions»Atoms/Bonds»wire width» 2

The Actions menu applies to whatever is selected. When nothing is selected, the Actions menu applies to everything
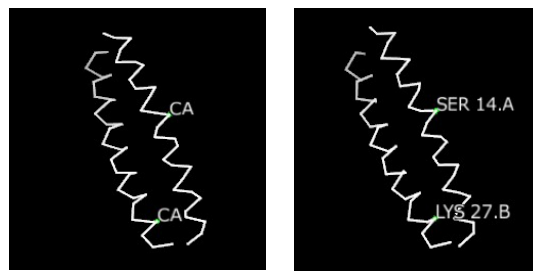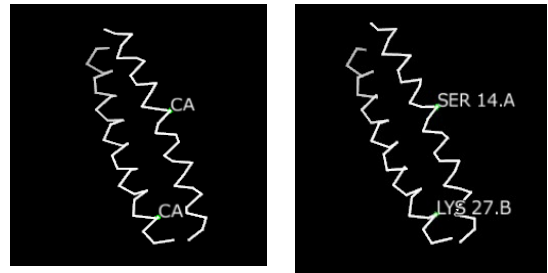
Labeling:

Pick two alpha carbons from each peptide. Label the atoms you have selected, first by atom name, and then by residue name and number:

Actions»Label»name

Actions»Label»off

Same as the last part, it is now evident that one peptide is chain A, and the other is chain B. To deselect the atoms, pick in the region of the graphics window away from any atoms or use the menu item *Select»Clear Selection.*
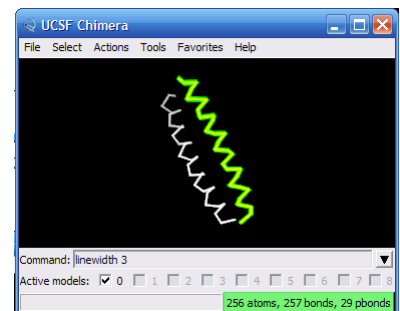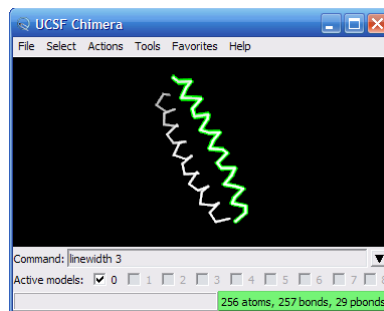
To un-display the residue labels:

Actions»Label»residue»off

Color the two chains with different colors:

Select»Chain»A

Actions»Color»yellow

Repeat the process to color chain B cyan. Another way to select an entire chain is to pick an atom or bond in the chain and then hit the up arrow key twice, once to expand the selection to the entire residue and another time to expand it to the entire chain

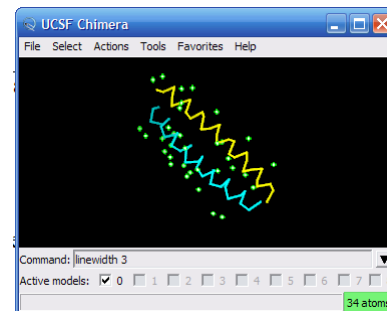Now select the water molecule as the last part:

Select»Chain»water

Actions»Atoms/Bonds»show

Select»Clear Selection

Alternatively, the water could have been selected using

Select»Structure»solvent, or

Select»Residue»name»HOH

To display all atoms of the A chain only:

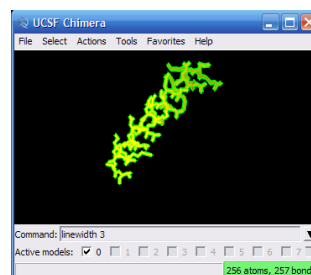*Actions»Atoms/Bonds»hide*

Select»Chain»A

Actions»Atoms/Bonds»show

Then to show the backbone only,

Actions»Atoms/Bonds»Backbone only»full

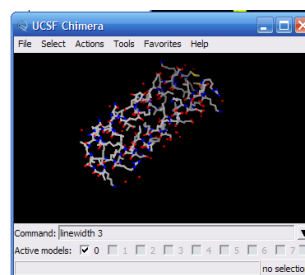Only the A chain's backbone is displayed because chain A was selected.

To display all the atoms and to color them according to element:

Select»Clear Selection
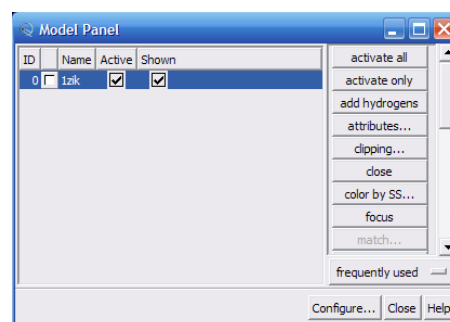
Actions»Atoms/Bonds»show

Actions»Color»by element

There is a checkbox in the Active column of the **Model Panel**

Tools»General Tools»Model Panel, or

Favorites»Model Panel

It shows that the model is activated for motion; un-checking the box inactivates the model. It can be restored by checking the box again. Close the model by highlighting **1zik.pdb** on the left side of the **Model Panel**, and then click **Close** on the right.
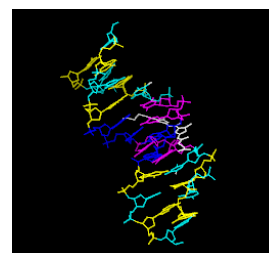
Menu Molecular Representations and Surfaces

Open another structure:

File»Open. In the resulting **dialog**, find and select *6bna.pdb*, and then *Open* to dismiss the **dialog**. Try coloring the different nucleotides with different colors. For example, color the adenosine (A) residues blue:

Select»Residue»A

Actions»Color»blue

Analogously, color cytosine (C) residues cyan, guanine (G) residues yellow, and thymine (T) residues magenta. Undisplay the water (the white dots) as you did in the last part.

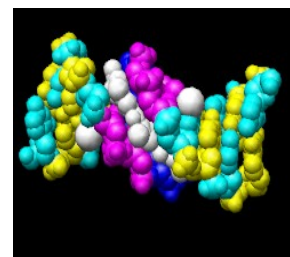Next, try some alternate representations.

Select»Clear Selection

Actions»Ribbon»show

Actions»Ribbon»hide
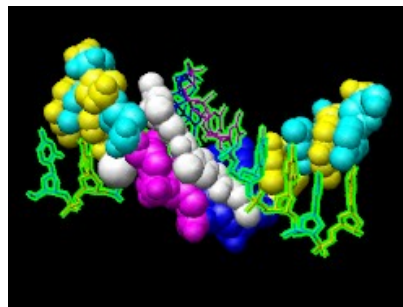
Actions»Atoms/Bonds»stick

Actions»Atoms/Bonds»sphere

Change the representation of only one of the DNA strands, chain B:

Select»Chain»B
Actions»Atoms/Bonds»stick

Next, change everything to a ball-and-stick representation:
Select»Clear Selection Actions»Atoms/Bonds»ball & stick

In this representation, pick one of the atoms in the white netropsin molecule. Label the residue by residue name:

Actions»Label»residue»name
Since it is a residue label, the label may be closer to other parts of the residue than to the selected atom. Remove the label:
Actions»Label»residue»off

The first submenu under Label controls individual atom labels, while the second controls residue labels. *Actions»Label»name* would have shown the name of the atom instead of the name of the residue. Other than the white netropsin molecule, there are two additional white atoms. They are apparently attached to cytosines, which have been colored cyan. Pick and then label these two atoms:

Actions»Label»residue»name + specifier
It shows that one DNA strand is chain A, the other strand is chain B, and each strand contains a brominated cytosine. Use *Select»Clear Selection* to deselect the atoms and then un-display the labels.

 Actions»Label»residue»off
Actions»Label»off
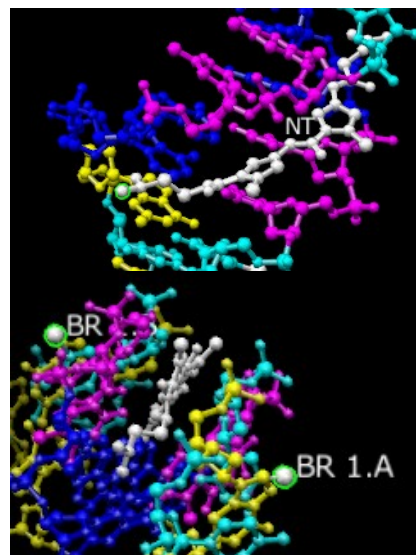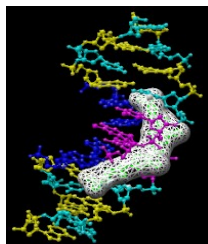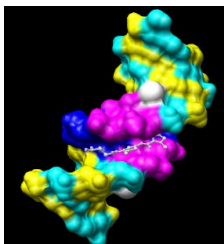Finally, have some fun with surfaces:

Actions»Surface»show
Actions»Surface»hide
Select»Structure»ligand
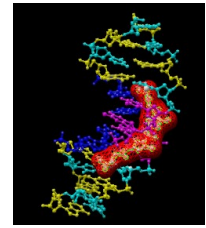*Actions»Surface»show*
Actions»Surface»mesh

By default, a surface has the same color as the corresponding atoms; however, surface color can be specified separately.

To change the surface color of only netropsin (which is still selected)

Actions»Color»surfaces to change the coloring target

Actions»Color»red

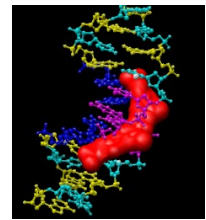*Actions»Color»all of the above* to restore the default coloring target.

Clear the selection, change back to solid surface, and then un-display the surface:

Select»Clear Selection

Actions»Surface»solid

Actions»Surface»hide

As an example of a more complicated selection process, show the surface of the adenine and thymine in chain B only:

Select»Selection Mode»append (to change selection mode)

Select»Residue»name»A

Select»Residue»name»T

Select»Selection Mode»intersect (to change selection mode)

Select»Chain»B

Action»Surface»show

To prepare for any future commands, restore the selection mode and clear the selection:
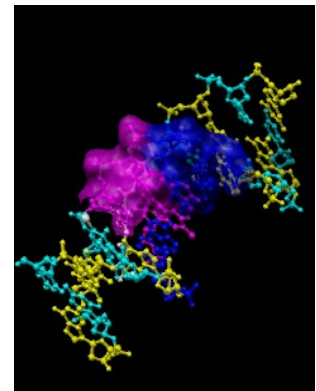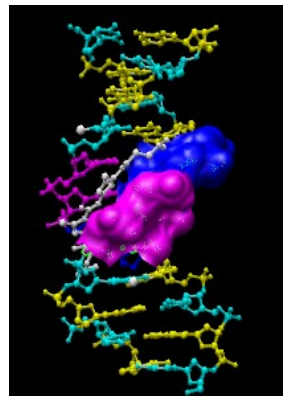
Select»Selection Mode»replace

 Select»Clear Selection

Sometimes, it is helpful to make a solid surface transparent:

Actions»Surface»transparency»50%

This is the end of this section. You can close the model. At this point, you can decide, which is easier to operate ? The menus or command-line ?

The Model Panel Tutorial

This tutorial introduces one of the most useful windows in *chimera*, and gives a little more information on how the *chimera* data-model works. The aim is to analyze a PDB file containing an ensemble of models that have been generated from NMR data.

From NMR data, one does not usually have a single structure. Instead, one often has a group (ensemble) of possible structures. This tutorial focuses on using the **Model Panel** and handling ensembles of structures (such as those determined by NMR). Note that the **Model Panel** is generally useful whether or not ensembles are being viewed.

You will work on two PDB files, which contain NMR-determined structures of a bovine prion protein fragment. 1dwz-edit4.pdb contains the first four members of an ensemble of 20 structures (present in the original PDB entry 1dwz), whereas 1dwy.pdb is a single representative minimized structure.

Make the window a convenient size, then choose the menu item *File»Open*. In the resulting **dialog**, find and select 1dwz-edit4.pdb and check the box '*Keep dialog up after Open'* so that the dialog does not disappear; next, open 1dwy.pdb, click **Close** to also dismiss the **dialog**.
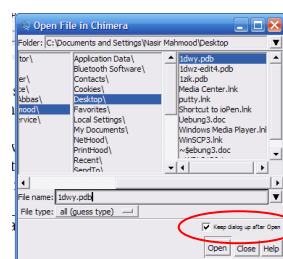
Thicken the lines: *Actions»Atoms/Bonds»wire width»3*. The structure includes all atoms, even the hydrogens. Simplify the display using *Actions»Atoms/Bonds»backbone only»full*. Now, only the N, CA, and C atoms are shown.

Open the Model Panel (*Favorites»Model Panel*). Each file of coordinates opened in *chimera* becomes a model with an associated model ID number and model-level color. Some PDB files are further subdivided into multiple structures designated with MODEL and ENDMDL records; when the input file contains more than one set of such records, sub-model numbers are assigned sequentially starting with 1. In this case, the four ensemble members in *1dwz-edit4.pdb* are sub-models 1-4 of model 0. Each sub-model (0.3, for example) can be treated as a separate model. Thus, "models" will be used to indicate sub-models and/or models that are not subdivided into sub-models. By default, the **Model Panel** shows the model-level colors behind the names. Once one or more models have been chosen within the left side, any of several functions represented by buttons on the right side may be executed. At first, most buttons are grayed out since no model has been chosen in the left side of the panel.
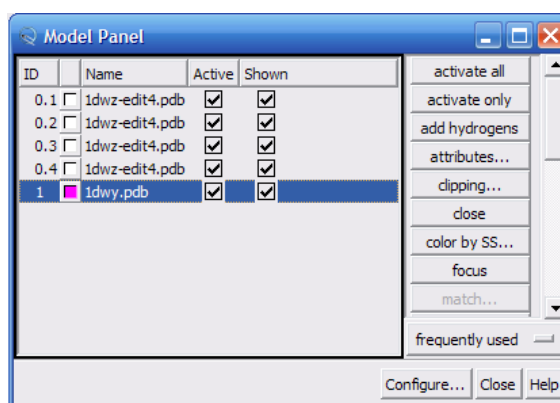
Individual models or blocks of models may be chosen (highlighted) using the left mouse button. Ctrl-Click adds to an existing choice rather than replacing it. To highlight a block of models without having to hold down the mouse button, click on the first (or last) and then Shift-Click on the last (or first) in the desired block. Click on *1dwy.pdb* in the left side of the **Model Panel** and then try various functions on the right side:

show only hide the other models

trace chains display the chain trace, which includes only CA atoms

show all atoms display all atoms

select select the entire model for further operations

Complete the follow steps in the menu:

Actions»Color»by element

Select»Chemistry»element»H

Actions»Atoms/Bonds»hide

> *Select»Clear Selection* (important, or else the invisible hydrogens will still be selected)

Back to the **Model Panel**:

sequence opens a **sequence panel** for the model; Click-Select one or a string of residues in the sequence and see how the corresponding residues of the structure become selected. Next, **Close** the panel and perform some action in the menu upon the new selection, such as:

> *Actions»Atoms/Bonds»sphere*

Select»Clear Selection
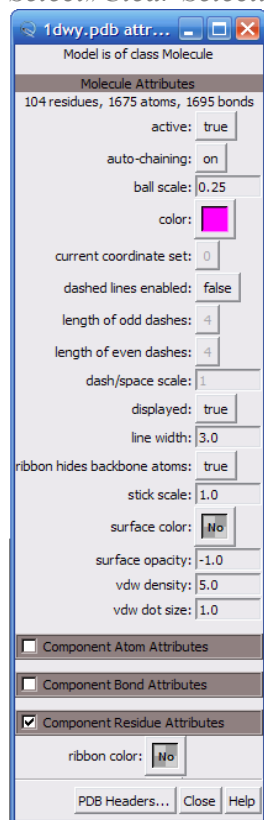
Back to the **Model Panel**:

attributes opens a **molecule model attributes panel**; Click on the **Component Residue Attributes**:

set **ribbon display** to **on**

set **ribbon cross section** to **round**

set **ribbon display** back to **off**

click **Close** to dismiss the panel

uncheck the **Shown** checkbox for *1dwy.pdb* *check* the **Shown** checkbox for *1dwy.pdb*

Note that using the **Shown** checkbox is not the same as using the command **display**, which works on individual atoms and bonds; instead, it enables/disables the whole model's display. Checking **Shown** enables the

display, but the display settings of individual atoms and bonds are not changed; in this example, the hydrogens are still un-displayed, as they were before the model was hidden. Toggling checkmarks in the **Shown** column is the same as using the **hide** and **show** buttons; toggling checkmarks in the **Active** column is the same as using **activate** and **deactivate** buttons. By default, these buttons are not included on the right side of the **Model Panel** because they are classified as **infrequently used**.
uncheck the **Active** checkbox for *1dwy.pdb* deactivate the model for motion (so it cannot be moved with the mouse) *check* the **Shown** checkbox for all of the models. Move the four sub-models of 0 so that they do not overlap with model 1 (which is deactivated and will not move). Scaling the view down with the mouse or **Side View** may be helpful.
check the **Active** checkbox for *1dwy.pd*b
Choose sub-model #0.1 in the **Model Panel**, **select** it, and use the **Action**s menu to color it. Repeat the process with the three other sub-models (choosing different colors), then clear the selection (*Select»Clear Selection*) and **Clos**e the **Model Panel**.