

Getting Started Tutorial - Menu Version

Many tasks in Chimera can be accomplished in multiple ways. For example, colors and [display styles](#) can be changed with the [Actions menu](#) or by entering [commands](#). In general, commands are more concise and powerful, but menus allow easy access to features without knowledge of commands and their syntax.

In this tutorial, many of the same tasks performed with commands in the [Getting Started Tutorial - Command Version](#) are carried out using the menus instead.

To follow along, first [download](#) the PDB files included with this tutorial to a convenient location on your computer:

- [1zik.pdb](#) - leucine zipper
- [1d86.pdb](#) - DNA and netropsin

Menus, Part 1 - Manipulation, Selection, and Chains

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

```
unix: chimera
```

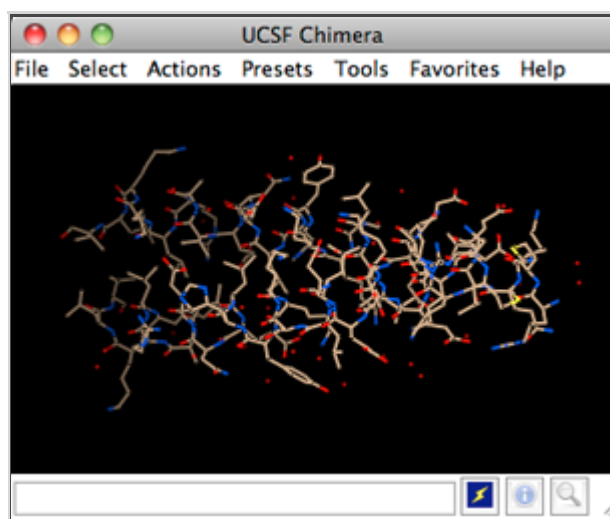
A splash screen will appear, to be replaced in a few seconds by the main Chimera [graphics window](#) or [Rapid Access](#) interface (it does not matter which, the following instructions will work with either). If you like, resize the Chimera window by dragging its lower right corner.

Now open a structure. Choose **File... Open** from the menu and use the resulting [file browser](#) to locate and open the previously [downloaded](#) file [1zik.pdb](#). The structure is a leucine zipper formed by two peptides.

A [preset](#) is a predefined combination of display settings. Apply interactive preset #2:

Presets... Interactive 2 (all atoms)

This displays all atoms and color-codes atoms other than carbon [by element](#) (oxygen red, nitrogen blue, etc.); carbons are left in the initial model color, in this case tan.



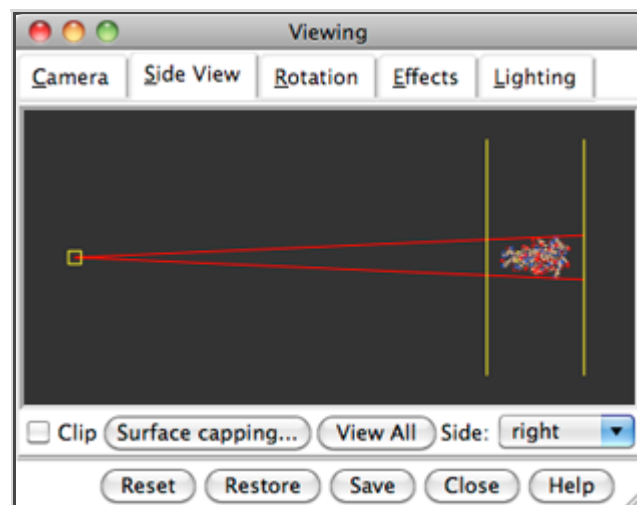
Try [moving the structure with the mouse](#) in the main graphics window. By default:

- the left mouse button controls rotation

- the middle mouse button controls XY translation
- the right mouse button performs scaling (zooming)

If you are using a touchpad or single-button mouse, modifier keys allow emulating the middle and right mouse buttons. These are **option** and **command** (⌘) on Mac keyboards.

Use the **Favorites** menu to show the **Side View** for interactive scaling and clipping. It shows a tiny version of the structure. Within the **Side View**, try moving the eye position (the small square) and the clipping planes (vertical lines) with the left mouse button. The **Side View** will renormalize itself after movements, so that the eye or clipping plane positions may appear to “bounce back,” but your adjustments have been applied.




Continue moving and scaling the structure with the mouse in the graphics window and **Side View** as desired throughout the tutorial. When the mouse focus is in the graphics window (you may need to click into it if you have been interacting with a different window), hovering the mouse cursor over an atom or bond (without clicking any buttons) will show identifying information in a pop-up “balloon.” The balloon will disappear when the cursor is moved away.

In Chimera, **selection** specifies atoms, bonds, residues, *etc.* for subsequent operations with the **Actions menu**. Ways to make a **selection** include using the **Select menu** or **picking** from the screen. The **Actions menu** applies to whatever is selected, but when nothing is selected, the **Actions menu** applies to everything.

Select the water (red dots):

Select... Structure... solvent

Another way to make the same selection is with **Select... Residue... HOH**. The selection is highlighted in green, and the magnifying glass icon near the bottom right of the window is also green: , indicating that something is selected. Hide the selected atoms:

Actions... Atoms/Bonds... hide

Even though the water atoms are hidden, they are still selected. Clear the selection, thicken the lines, and display only the chain trace:

Select... Clear Selection

Actions... Atoms/Bonds... wire width... 3

Actions... Atoms/Bonds... backbone only... chain trace

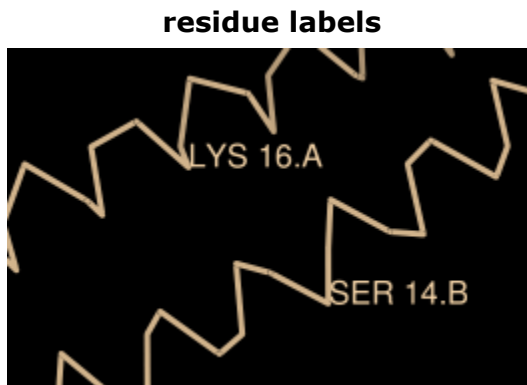
The chain trace includes just the α -carbons (atoms named CA), connected in the same way

that the residues are connected.

By default, [picking](#) from the screen is done by clicking on the atom or bond of interest with the left mouse button while pressing the **Ctrl** key. To add to an existing selection, also press **Shift**. Try picking two atoms, one from each peptide chain (Ctrl-click the first, Shift-Ctrl-click the second).

Label the atoms you have selected, first by atom name and then by residue name and number:

Actions... Label... name
Actions... Label... off
Actions... Label... residue... name + specifier



The specifier includes residue number and chain ID. One peptide is chain A and the other is chain B. Use the **Favorites** menu to show the [Preferences](#), change to **Category: Background**, and adjust the **Label font** and size as you wish. Click **Save** before closing the preferences if you want the settings to apply to later uses of Chimera.

Clear the selection by Ctrl-clicking in empty space, as if [picking](#) "nothing." Turn off the labels:

Actions... Label... residue... off

Color the two chains different colors:

Select... Chain... A
Actions... Color... cyan

Repeat the process to color chain B yellow.

Select chain A by [picking](#) any atom or bond in the chain, then pressing the up arrow key twice, once to [expand the selection](#) to the entire residue and another time to expand it to the entire chain. Display its full backbone:

Actions... Atoms/Bonds... backbone only... full

Display all atoms of chain A only (which is still selected):

Actions... Atoms/Bonds... show only

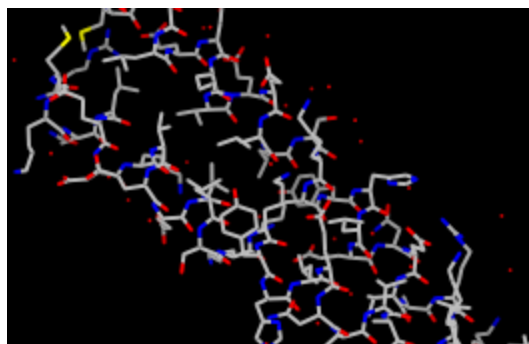
Display all atoms and color them by element:

coloring by element

Select... Clear Selection
Actions... Atoms/Bonds... show
Actions... Color... by element

The **by element** coloring is the same as **by**

heteroatom except it also color-codes carbons (gray). Heteroatom-only coloring is useful for keeping different structures distinguishable by their different carbon colors.



Generally, each file of coordinates opened in Chimera becomes a model with an associated model ID number. Models are assigned successive numbers starting with 0. Models are listed in the left side of the **Model Panel** (**Tools... General Controls... Model Panel**). A checkbox in the **A**(ctive) column of the **Model Panel** shows that the model is [activated for motion](#); unchecking the box makes it impossible to move the model. Checking the box again restores the movable state. Make sure **1zik.pdb** is highlighted on the left side of the **Model Panel** (if not, click on it) and then click **close** in the list of functions on the right side. Next, use the **Close** button at the bottom to dismiss the **Model Panel**.

Go on to **Part 2** below, **OR** exit from Chimera with **File... Quit**.

Menus, Part 2 - Molecular Representations and Surfaces

With Chimera started as described at the beginning of [Part 1](#), choose the menu item **File... Open**. Use the resulting [file browser](#) to locate and open the previously [downloaded](#) file [1d86.pdb](#). It contains the molecule netropsin bound to double-helical DNA.

[Move and scale](#) the structure with the mouse in the graphics window and **Side View** as desired throughout the tutorial.

Apply the "all atoms" preset, which will show the DNA as wire and netropsin as spheres:

Presets... Interactive 2 (all atoms)


Color carbons white, then undisplay the water:

Select... Chemistry... element... C

Actions... Color... white

Select... Structure... solvent

Actions... Atoms/Bonds... hide

Remember that hiding atoms does not deselect them; they remain selected, as indicated by the green magnifying glass icon  near the bottom right of the window, until the selection is cleared or replaced with a new selection.

Color the different nucleotides different colors. For example, color the adenine deoxynucleotides blue:

Select... Residue... DA

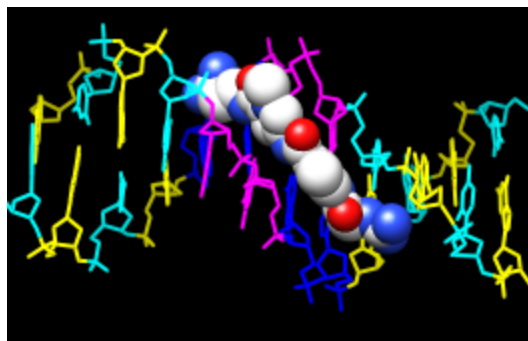
Actions... Color... blue

Analogously, color DC residues cyan, DG residues yellow, and DT residues magenta. Clear

the selection with **Select... Clear Selection** or by [picking](#) (Ctrl-click) in empty space.

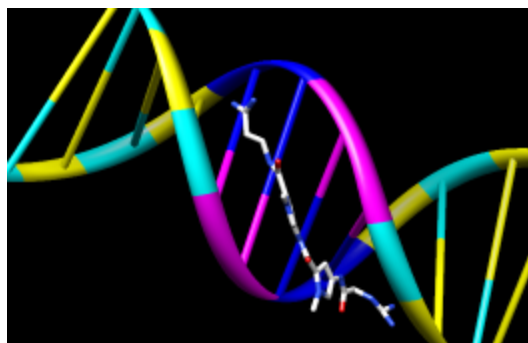
Next, try some different [display styles](#), or representations.

Actions... Atoms/Bonds... sphere
Select... Chain... A
Actions... Atoms/Bonds... ball & stick
Select... Clear Selection
Actions... Atoms/Bonds... stick



Showing ribbon automatically hides the [mainchain](#) (backbone) atoms.

Actions... Ribbon... show
Actions... Ribbon... edged
Actions... Ribbon... rounded



DNA can be shown with special [nucleotide objects](#). We will show "lollipops," boxes, and a ladder.

Actions... Atoms/Bonds... nucleotide objects... settings...

In the resulting **Nucleotides** dialog:

1. set **Show side (sugar/base) as** to **tube/slab**
2. set **Show base orientation** to **false**
3. click **Slab Style** tab, set slab style to **skinny**
4. click **Slab Options** tab, set **Slab object** to **ellipsoid**
5. click **Apply**; these are the "lollipops"

Nucleotide settings can be applied to just the selected residues (not necessarily all of the DNA). One way to select specific residues is in the [Sequence](#) tool:

Favorites... Sequence

Show the sequence of chain A and select one or a few residues in the sequence window with the mouse; this selects the corresponding part of the structure. **Quit** from the sequence window. In the **Nucleotides** dialog (also under **Tools... Depiction** in the menu):

1. set **Show base orientation** to **true**
2. set **Slab object** to **box**
3. click **Apply**; base orientations are shown with "bumps"

Clear the selection (**Select... Clear Selection** or Ctrl-click in empty space) and use **Nucleotides** to show the DNA as a ladder:

1. set **Show side (sugar/base) as** to **ladder**

2. in the **Ladder Options**, set **Rung radius** to **0.3 Å**
3. click **OK** (which will also dismiss the dialog)

To return to more general display styles, turn off the nucleotide objects:

Actions... Atoms/Bonds... nucleotide objects... off

Hide the ribbons and show everything as ball-and-stick:

Actions... Ribbon... hide

Actions... Atoms/Bonds... ball & stick

Finally, have some fun with surfaces. There are [built-in categories](#) within structures such as **main** and **ligand**; when nothing is [selected](#), **Actions... Surface... show** displays the surface of **main**.

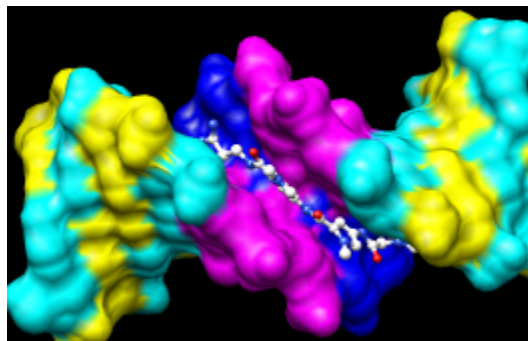
Actions... Surface... show

Actions... Surface... hide

Select... Structure... ligand

Actions... Surface... show

Actions... Surface... mesh



Surface color can be specified separately from the colors of the underlying atoms. The ligand surface is tan and white because the original model color (tan) is used for surfaces of atoms not explicitly recolored by the user, and above, only the carbon atoms were changed to white. With the ligand still selected, choose **Actions... Color... all options...** to open the [Color Actions](#) dialog. In that dialog,

1. change the **Coloring applies to** (target) setting to **surfaces**
2. click **red**
3. click **Close** (which will automatically reset the coloring target back to **all of the above**)

Clear the selection, change back to a solid surface, and then undisplay the surface:

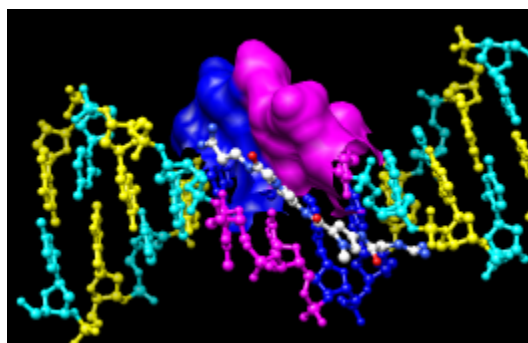
Select... Clear Selection

Actions... Surface... solid

Actions... Surface... hide

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

1. change the selection mode: **Select... Selection Mode... append**
2. **Select... Residue... DA**
3. **Select... Residue... DT**
4. change the selection mode: **Select... Selection Mode... intersect**



5. **Select... Chain... B**
6. **Actions... Surface... show**

To prepare for any subsequent operations, restore the selection mode and clear the selection:

Select... Selection Mode... replace
Select... Clear Selection (or Ctrl-click in empty space)

The [command](#) equivalent is much more concise, but requires some knowledge of the [atom specification syntax](#):

Command: **[surf](#) :da.b,dt.b**

Sometimes it is helpful to make a solid surface transparent:

Actions... Surface... transparency... 50%

Choose **File... Quit** from the menu to terminate the Chimera session.

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