

## Getting Started Tutorial - Command 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 menus in the [Getting Started Tutorial - Menu Version](#) are carried out using commands 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

---

### Commands, 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.

Use the **Favorites** menu to show the [Command Line](#). Now open a structure. Enter the command:

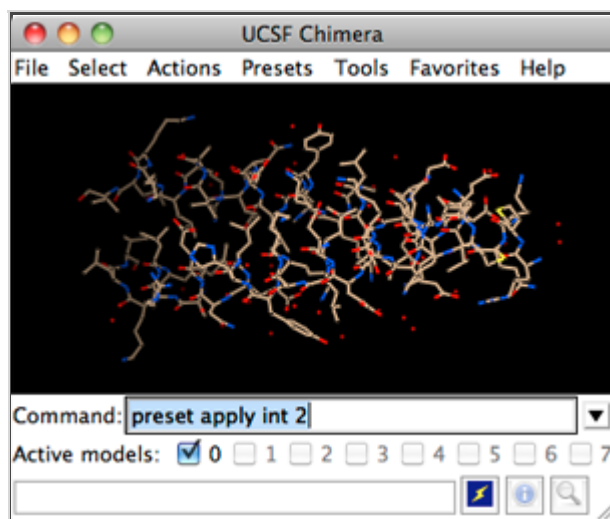
```
Command: open
```

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:

```
Command: preset apply int 2
```

This displays all atoms and color-codes atoms other than carbon [by element](#) (oxygens red, nitrogens 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

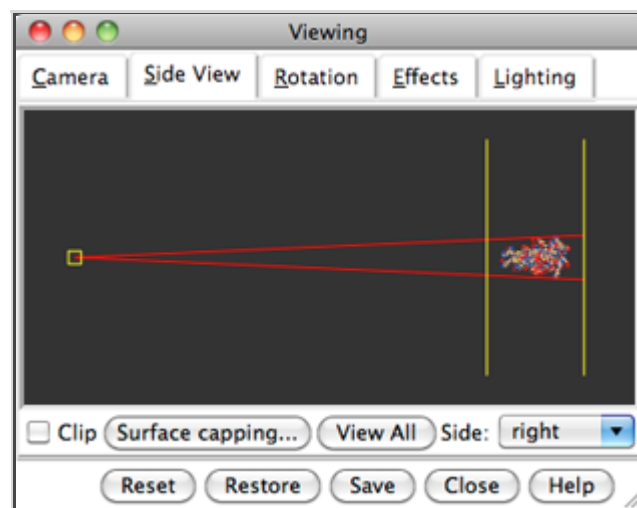
- the right mouse button performs scaling (zooming)

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.

Show the [Side View](#) for interactive scaling and clipping:

Command: [start Side View](#)

It is also listed in the **Favorites** menu by default. 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.

A Chimera command may include **arguments** and/or an [atom specification](#). For example, in the following,

Command: [color hot pink :lys](#)

the [color name hot pink](#) is an argument of the command [color](#), and [:lys](#) specifies all residues named LYS.

A blank specification is interpreted as all applicable items. For example,

Command: [color hot pink](#)

makes all atoms (and their labels, surfaces, etc.) hot pink.

Many commands have “~” versions that perform the opposite function. The following will change a structure back to its default color:

Command: [~color](#)

The command [help](#) can be used to show the manual page for any command. For example,

Command: [help color](#)


Atom Specification Symbols		
Symbol	Meaning	Usage
#	model	# <i>model</i> (model ID number)
:	residue	: <i>residue</i> (residue name or number)
::	chain	:: <i>chain</i> (chain ID)
@	atom	@ <i>atom</i> (atom name)
=	partial wildcard	matches partial atom or residue name, e.g., @C= specifies all atoms with names beginning with C
?	single-character wildcard	matches single character in atom or residue name, e.g., :G?? specifies all residues with three-letter names beginning with G

shows the manual page for the command [color](#). The [Chimera Quick Reference Guide \(PDF\)](#) lists most [commands](#) and gives some examples of command-line [atom specification](#).

Thicken the lines and display only the atoms named CA ( $\alpha$ -carbons):

```
Command: linewidth 3
Command: show @ca
-OR- (equivalently)
Command: ~display ~ @ca
```

The latter command undisplay atoms *not* named CA.

By default, [picking](#) from the screen (a type of [selection](#)) 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  $\alpha$ -carbons, one from each peptide chain (Ctrl-click the first, Shift-Ctrl-click the second). 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.

The word **selected**, **sel**, or **picked** can be used in commands to specify the current selection. Label the atoms you have selected:

```
Command: label sel
```

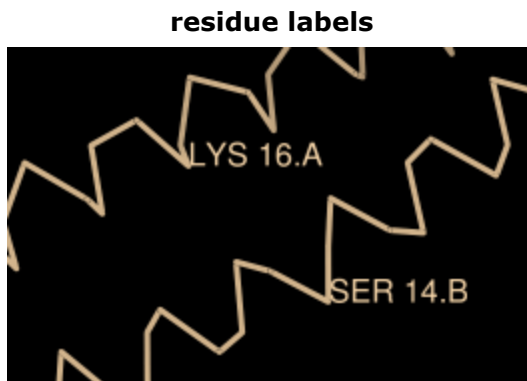
The [label](#) command shows atom information (atom name, by default). Undisplay the atom labels, then show labels for the *residues* containing the selected atoms:

```
Command: ~label
Command: rlabel sel
```

Each residue label is of the form:

***res\_name res\_number.chain***

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:

```
Command: ~rlabel
```

Color the two chains different colors; note that commands can be truncated to unique strings:

```
Command: color cyan :.a
Command: col yellow :.b
```

Residues and atoms can also be specified, along with or independent of chain:

```
Command: col orange :5-9.a,12.a,8.b
Command: col magenta :14-18
Command: disp :leu.b
```

Command: [col green :leu.b@cb](#)

The structure also includes water, which can be shown with:

Command: [disp solvent](#)

-OR- (equivalently)

Command: [disp :hoh](#)

Display the full backbone of chain A:

Command: [disp :a@n,ca,c,o](#)

Display all atoms in chain A only:

Command: [show :a](#)

Display all atoms and color them by element:

Command: [disp](#)

Command: [col byelement](#)

Coloring **byelement** is the same as **byhet** 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. The **Active models** line right under the **Command**

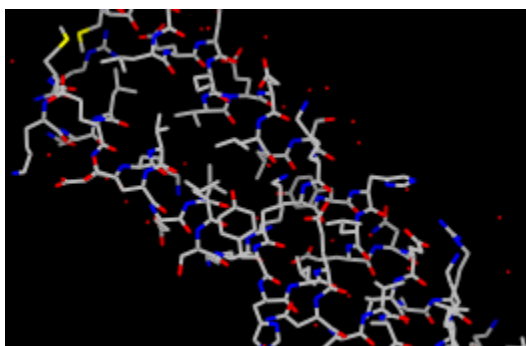
**Line** shows which models are [activated for motion](#). The checkbox for **0** is activated. Unchecking the box makes it impossible to move model 0. Checking the box again restores the movable state.

Command: [close 0](#)

closes the model. Go on to **Part 2** below, **OR** exit from Chimera with the following command:

Command: [stop](#)

coloring by element



---

## Commands, Part 2 - Molecular Representations and Surfaces

With Chimera started and the [Command Line](#) opened 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:

Command: [preset apply int 2](#)

Color carbons white, then undisplay the water:

Command: **color white C**

Command: **~disp solvent**

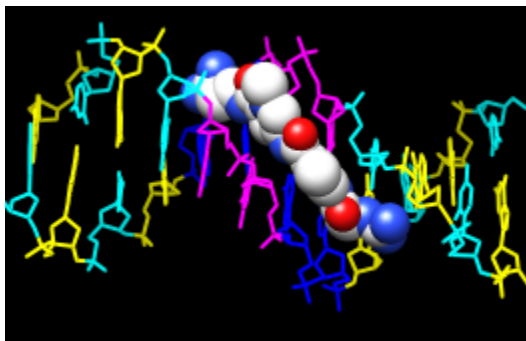
Residue names can be identified by looking in the **Select... Residue** menu or by hovering the cursor over an atom or bond to see information in a pop-up "balloon." Color the different nucleotides different colors, specifying them by residue name:

Command: **color blue :da**

Command: **color cyan :dc**

Command: **color yellow :dg**

Command: **color magenta :dt**



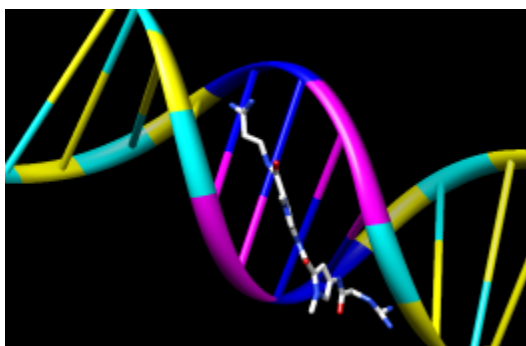
Next, try some different [display styles](#), or representations.

Command: **represent sphere**

Command: **repr bs :.a**

Command: **rep stick**

Notice that commands (but not necessarily their keyword arguments) can be truncated to unique strings. For example, the command **represent** can be shortened to **repr** or **rep** but not **re** (because other commands also start with **re**), whereas its keywords **stick**, **sphere**, etc. cannot be truncated. If the truncation is not unique, one of the corresponding commands will be executed, but it may not be the one intended.



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

Command: **ribbon**

Command: **ribrep edged**

Command: **ribr rounded**

DNA can be shown with special [nucleotide objects](#). We will show "lollipops," boxes with orientation bumps, and then a ladder. You can copy and paste into the **Command Line**. The command-line contents can be edited, and past commands can be accessed using the up and down arrow keys or **Ctrl-p** (previous) and **Ctrl-n** (next).

Command: **nuc side tube/slab shape ellipsoid orient false style skinny**

Command: **nuc side tube/slab shape box orient true style skinny :8-10.a**

Command: **nuc side ladder radius 0.3**

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

Command: **~nuc**

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

Command: **~ribbon**

Command: [rep bs](#)

Finally, have some fun with the **surface** command. There are [built-in categories](#) within structures such as **main** and **ligand**; when nothing is specified, [surface](#) shows the surface of **main**.

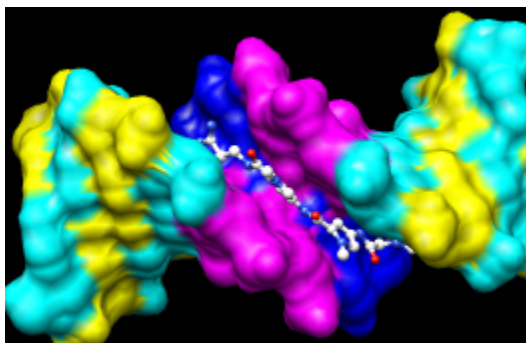
Command: [surface](#)

Command: [~surf](#)

Command: [surf ligand](#)

-OR- (equivalent)

Command: [surf :nt](#)



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. Show the ligand surface as red mesh:

Command: [surfrep mesh](#)

Command: [color red,s ligand](#)

Command: [surfrep solid](#)

Parts of a surface can be shown:

Command: [~surf](#)

Command: [surf :da,dt](#)

Command: [~surf](#)

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

Sometimes it is helpful to make a solid surface transparent:

Command: [surftrans 50](#)

When finished, exit from Chimera:

Command: [stop now](#)

