


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.

Menus, Part 1 - Manipulation, Selection, and Chains

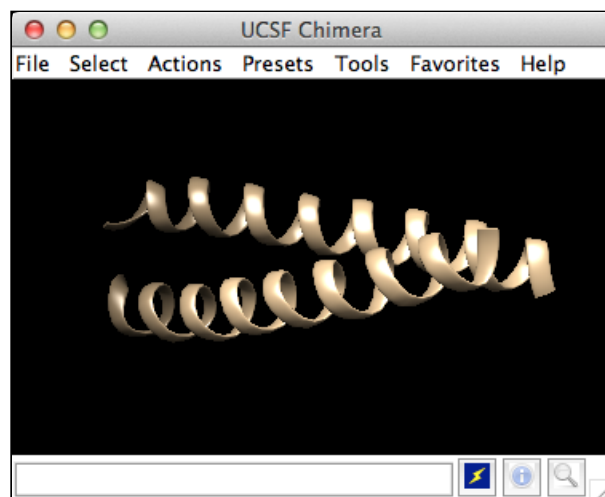
Start Chimera by clicking or doubleclicking the **Chimera** icon  (depending on its location). Typically, this icon will be present on the desktop. The Chimera executable can also be run from its installation location ([details...](#)).

A splash screen will appear, to be replaced in a few seconds by the main Chimera [graphics window](#) or [Rapid Access](#) interface. It doesn't matter which, since opening a structure will switch the display to the graphics window. If you like, resize the Chimera window by dragging its lower right corner.

Now open a structure. Choose **File... Fetch by ID** from the menu and fetch the entry with ID **1zik** from the Protein Data Bank (PDB). Alternatively, if you're not connected to the internet, you can [save](#) the PDB-format file [1zik.pdb](#) to a convenient location, then use **File... Open** in the Chimera menu to find and open it. The structure is a leucine zipper formed by two peptides.

The default initial display is ribbons. To also display atoms:

Actions... Atoms/Bonds... show



This shows all of the atoms and bonds in the structure, except that those in the peptide backbone are suppressed by the ribbon display. How to indicate specific parts of a structure for display, coloring, *etc.* is discussed [below](#). Initially, heteroatoms (atoms other than carbon) are color-coded [by element](#): oxygens red, nitrogens blue, *etc.* The carbons retain the 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)

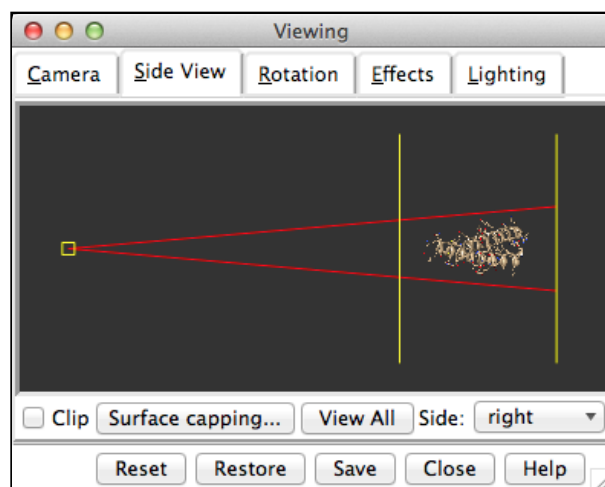
If you are using a touchpad or single-button mouse, modifier keys allow emulating the middle and right mouse buttons. These are **option** and **command** (⌘) on Mac keyboards. Multitouch gestures on a Mac touchpad are enabled by default, but can be turned off in the preferences (menu: **Favorites... Preferences**, category **Mouse**).

Hide ribbons to reveal the backbone atoms, then show ribbons again:

Actions... Ribbon... hide

Actions... Ribbon... show

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, bond, or ribbon segment without clicking any buttons will show identifying information in a pop-up “balloon.” The balloon will disappear when the cursor is moved away. For an atom, the balloon information is of the form:


res-name res-num.chain atom-name

You can see from the balloons that this structure contains two peptide chains, A and B, and water (HOH residues), also with chain identifiers A and B.

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. Several tools also provide specialized ways of making selections. The [Actions menu](#) applies to whatever is selected, but when nothing is selected, the [Actions menu](#) applies to everything. For example,

Select... Residue... LYS

Actions... Color... hot pink

will color all residues named LYS [hot pink](#). 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. Clearing the selection (deselecting) beforehand will color everything:

Select... Clear Selection

Actions... Color... hot pink

[Select menu](#) choices also include chain ID, element, and many other categories of atoms and residues. (More complicated selections can be built up by intersecting some of these choices, as shown near the end of [Part 2](#).)

Select... Chain... B
Actions... Color... cyan
Actions... Ribbon... hide
Select... Structure... solvent
Actions... Atoms/Bonds... hide
Select... Chemistry... element... N
Actions... Atoms/Bonds... sphere
Select... Clear Selection
Actions... Atoms/Bonds... stick

One way to select specific residues or ranges of residues is in the [Sequence](#) tool (menu **Favorites... Sequence**, show sequence for chain A). When the sequence window has mouse focus, placing the cursor over a residue symbol in the sequence shows information for the corresponding structure residue at the bottom of the window. Click-drag a box within the sequence window to select one or more residues (as opposed to simply clicking within the light yellow box, which will select the entire helix), then hide their atoms:

Actions... Atoms/Bonds... hide

Quit from the sequence window and display all protein atoms again:

Select... Structure... protein
Actions... Atoms/Bonds... show

Coloring can be limited to only certain representations, such as atoms only (not ribbons, surfaces, *etc.*):

Select... Residue... GLU
Actions... Color... all options

In the resulting [Color Actions](#) dialog:

1. choose to **Show all colors** (lower right)
2. change the **Coloring applies to** (target) setting to **atoms/bonds**
3. click to choose any color

Notice that only the atoms/bonds of the selected residues and not their ribbon segments change color. Clear the selection (main menu **Select... Clear Selection**), then in the [Color Actions](#) dialog:

1. change the coloring target back to **all of the above**
2. click to choose [tan](#) (colors are listed alphabetically in the all-colors section)
3. click **Close** to dismiss the dialog

Restore heteroatom color-coding:

Actions... Color... by heteroatom

Coloring by heteroatom is useful for showing functional groups, yet keeping different models distinguishable by their different carbon colors.

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 in different residues (Ctrl-click the first, Shift-Ctrl-click the second).

Show residue labels for the atoms you have selected:

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

(**Actions... Label... name** would show the atom names instead.) These 3D labels move along with structures and are mainly for interactive use. For figures and movies, [2D labels](#) are recommended instead.

Promote the selection to the entire residues with the keyboard up arrow *or* the following:

Select... Broaden

Show only the selected atoms:

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

Clear the selection by Ctrl-clicking in empty space, as if [picking](#) “nothing.”

Turn off residue labels, hide ribbon, display all atoms, and color by element:

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

Actions... Ribbon... hide

Actions... Atoms/Bonds... show

Actions... Color... by element

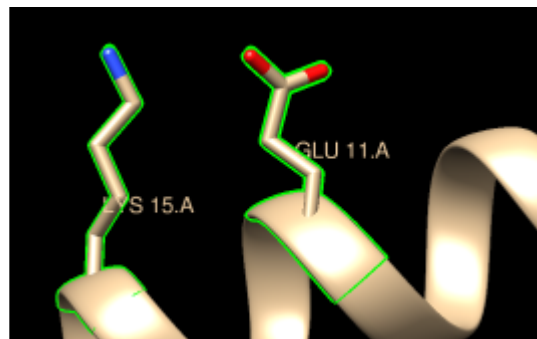
The **by element** coloring is the same as **by heteroatom** except it also color-codes carbons (gray).

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 [Model Panel](#) (open with **Tools... General Controls... Model Panel**) lists the current models and enables many operations upon them.

The columns on the left side of the **Model Panel** show:

- model ID number
- model color
- A(ctive) - whether [activated for motion](#)
- S(hown) - whether display-enabled

residue labels



coloring by element



- model name

Try toggling the checkboxes to see what happens; a model that is not activated for motion cannot be rotated or translated interactively. In the list of functions on the right side (*not* the button at the bottom), click **close** to remove model **1zik**. Use the **Close** button at the bottom to close 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 **File... Fetch by ID** from the menu and fetch the entry with ID **1d86** from the Protein Data Bank (**PDB**). (Alternatively, if you're not connected to the internet, you can [save](#) the PDB-format file [1d86.pdb](#) to a convenient location, then use **File... Open** in the Chimera menu to find and open it.)

The structure contains the molecule netropsin bound to double-helical DNA, initially shown with ribbons and stylized representations of the nucleic acid sugars and bases. [Move and scale](#) with the mouse in the graphics window and **Side View** as desired throughout the tutorial.

A [preset](#) is a predefined combination of display settings. 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.

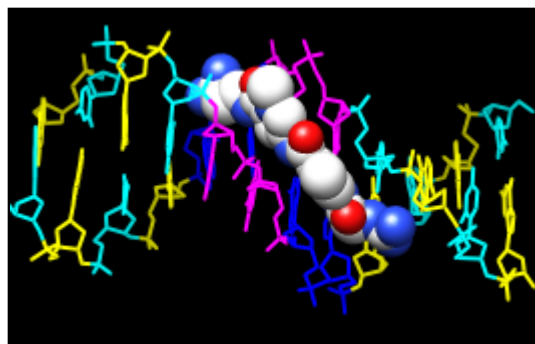
Residue names can be identified by looking in the **Select... Residue** menu or by hovering the cursor over an atom or bond to see information in a pop-up “balloon.” Color the different nucleotides different colors, for example:

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.

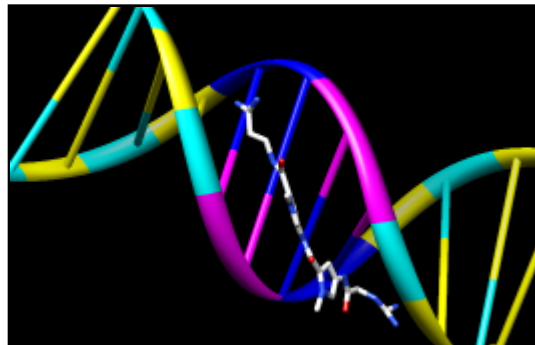


Actions... Atoms/Bonds... sphere
Select... Chain... A
Actions... Atoms/Bonds... ball & stick
Select... Clear Selection
Actions... Atoms/Bonds... stick

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**.

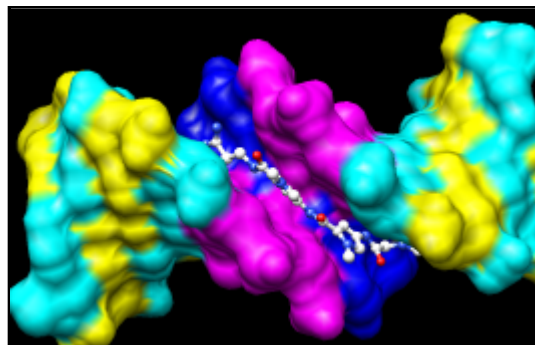
Actions... Surface... show

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:

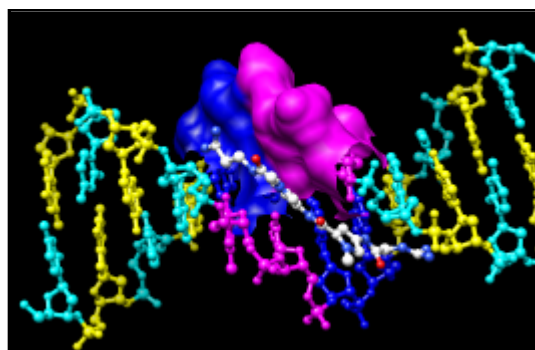
Select... Clear Selection

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 surface transparent:

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

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

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