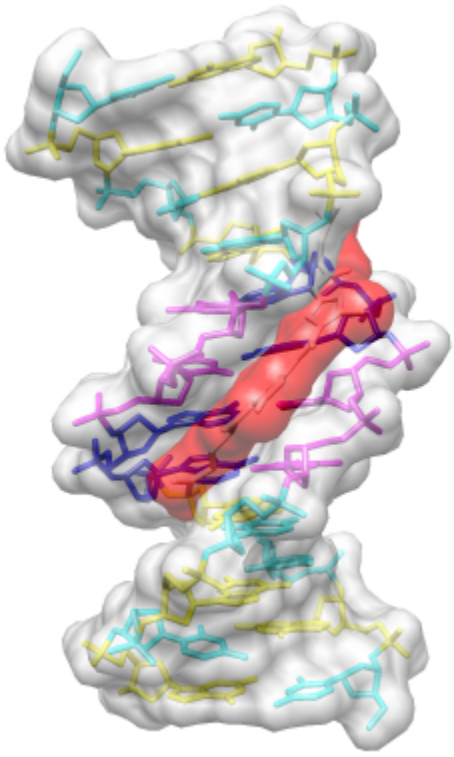
AFM's updates are in magenta. They apply to command-line operations, which begin on page 13.

UCSF Chimera - Getting Started

This tutorial provides an overview of basic features in Chimera. You can interact with Chimera using menus and/or commands. The basic features of Chimera are available either way, but not all command functions are available in menus or graphical interfaces, and not all menu or graphical interface functions are available in commands. Thus, it is useful to become familiar with both ways of interacting with Chimera.

The **Working with menus** and **Working with commands** sections are independent of each other and (for the most part) cover identical operations, accomplished in different ways. If you go through both sections, you can skip portions that cover issues you already understand. You can also go back and forth between the sections to see the correspondence between menu and command operations.



DNA helix with bound netropsin

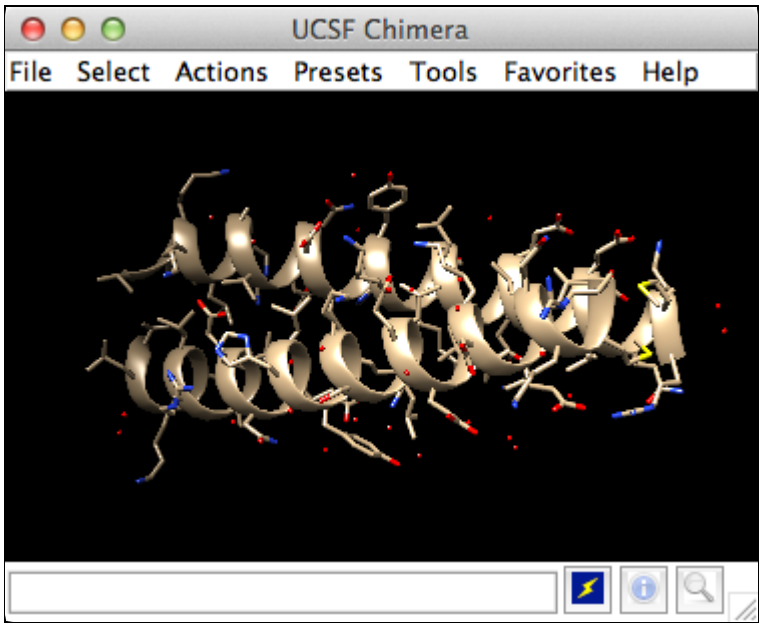
Outline:

Typographical Conventions

Item	Example	Description
Keyboard key	Ctrl	The control key
Mouse key	Btn1	Mouse button 1 (left button)
Menu action	File→Open	File Menu bar pulldown, followed by Open

Working with Menus, Part 1 - Manipulation, Selection, and Chains

← Getting started



UCSF Chimera with 1zik

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.

A splash screen will appear, to be replaced in a few seconds by the main Chimera window containing either the graphics display or the **Rapid Access** list of recently used files (it doesn't matter which, since opening a structure will automatically switch the display to the graphics window). If you like, enlarge the window by clicking and dragging its lower right corner. The window can also be moved by clicking its top bar and dragging.

Opening a structure

Now open a structure. Choose **File→Fetch by ID** from the menu and enter **1zik** as the **ID** of the structure to fetch from the **PDB**. The structure will appear in the graphics window; it 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.

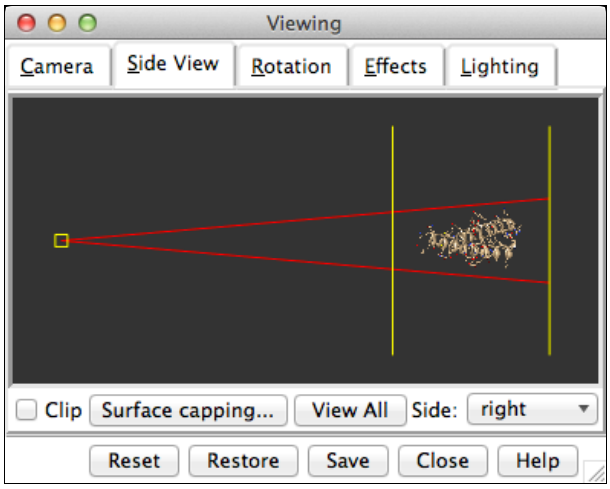
Hide ribbons to reveal the backbone atoms, then show ribbons again:

Actions→Ribbon→hide
Actions→Ribbon→show

Side View

Show the **Side View** for interactive scaling and clipping (menu: **Tools→Viewing Controls→Side View**). By default, the **Side View** is also listed in the **Favorites** menu.

It shows a tiny version of the structure. Try moving the eye position (the small square) and the clipping planes (vertical lines) by clicking and dragging 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.



Side View showing 1zik

← Using the mouse

Try manipulating the structure in the main window with the mouse. By default:

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

Default Mouse Button Assignments

Mouse button	Modifier	Action
Btn1 (left button)		Rotation
Btn2 (middle button)		XY Translation
Btn3 (right button)		Scaling
Btn1	Ctrl	Picking (selection)
Btn1	Ctrl-Shift	Addition to (removal from) selection

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**). 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. 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.

Selection with the mouse

In combination with modifier keys, the mouse buttons have additional functions. By default, ***picking*** from the screen (a type of ***selection***) is done by Ctrl-clicking an atom or bond with the left mouse button, Btn1. You can also drag out a selection area with Ctrl-Btn1 (sweep out an area before releasing). Shift-Ctrl-Btn1 adds to or toggles an existing selection. The selection is outlined in green, and placing the mouse cursor over the green magnifying glass icon  near the bottom right corner of the window reports what is selected in a pop-up "balloon."

The arrow keys can be used to broaden (↑), narrow (↓), or invert (→) a selection. The hierarchy for broadening and narrowing a selection could include (depending on the initial selection): atom/bond, residue, protein secondary structure element, bonded set of atoms, all atoms with the same chain ID, entire model. When a selection is inverted, the selected atoms become deselected and *vice versa*.

Spend some time selecting various parts of the structure. An easy way to clear the selection (deselect everything) is to use Ctrl-Btn1 in any blank space in the graphics window.

← Selection/Action

In general, operations performed with the Chimera **Actions** menu apply to the current ***selection***. Selections can be made in many ways, including with the **Select** menu or with the mouse (as described above). When nothing is selected, the **Actions** menu applies to everything.

The following will color all residues named LYS hot pink.

Select→Residue→LYS
Actions→Color→hot pink

The selection is highlighted in green, and the magnifying glass icon  near the bottom right corner 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

Actions Menu Items

Menu Item	Description
Atoms/Bonds	Controls the display and representation of atoms and bonds.
Ribbon	Controls the display and representation of ribbons.
Surface	Controls the display and representation of molecular surfaces.
Color	Colors selected objects. Color target can be limited to object types in the **all options** dialog.
Label	Labels selected atoms. The **residue** submenu labels residues containing the selected atoms.
Focus	Focuses the view on the selected atom(s), zooming and translating if necessary.
Set Pivot	Sets the center of rotation based on the selected atom(s) without adjusting the view.
Inspect	Launches the **Selection Inspector**; same as clicking  .
Write List	Writes a list of the currently selected objects to a parsable text file.
Write PDB	Writes the coordinates of the currently selected atoms to a PDB file.

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.

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

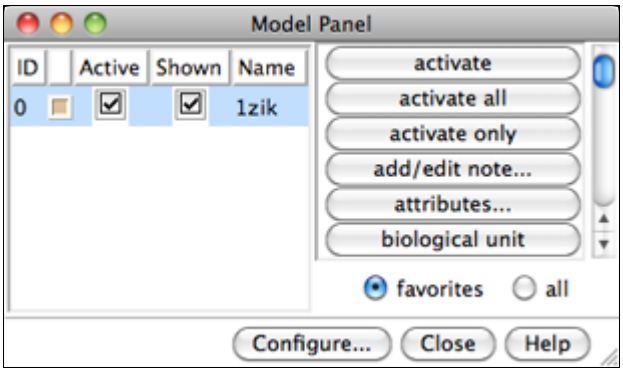
Clear the selection by **Ctrl**-clicking in empty space, as if picking “nothing.”

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).

← Models and model status



Chimera Model Panel

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** lists the current models and enables many operations upon them. Open this tool with **Tools→General Controls→Model Panel**.

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
- model name

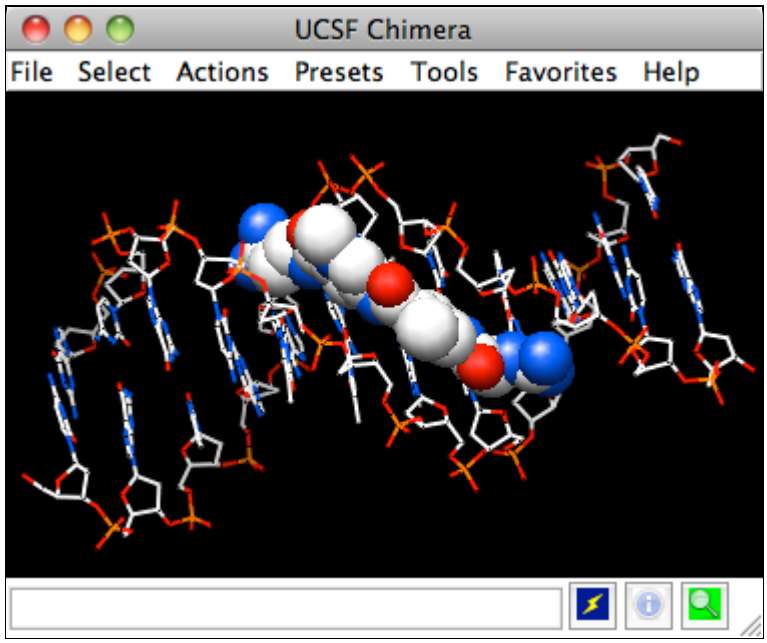
Try toggling the checkboxes to see what happens; a model that is not activated for motion cannot be rotated or translated interactively. In the list of functions on the right side of the **Model Panel** (*not* the button at the bottom), click **close** to remove model **1zik**. Use the **Close** button at the bottom to close the **Model Panel**.

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

Working with Menus, Part 2 - Molecular Representations and Surfaces

← Setup

With Chimera started as described at the beginning of Part 1, open a different structure. Choose **File→Fetch by ID** from the menu and enter **1d86** as the **ID** of the structure to fetch from the **PDB**. 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.



Chimera showing netropsin as spheres

Rotate, translate, and scale the structure as needed to get a better look (see **Using the mouse** to review how this is done). Continue moving and scaling the structure as desired throughout the tutorial.

A ***preset*** is a predefined combination of display settings. Use 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:

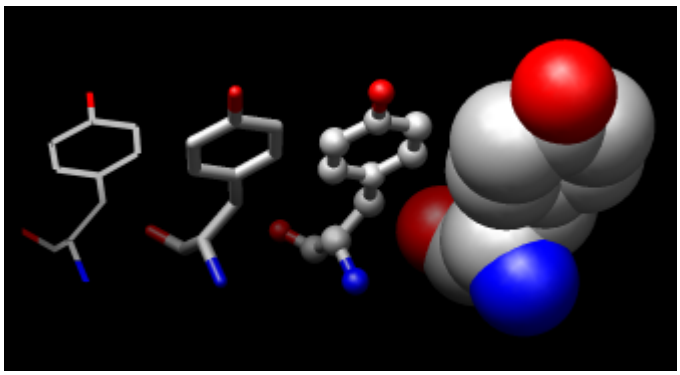
Select→Residue→DA
Actions→Color→blue

Analogously, color DC residues cyan, DG residues yellow, and DT residues magenta. Clear the selection with **Select→Clear Selection** or **Ctrl**-click in empty space.

← Representations

Next, try some different display styles, or representations.

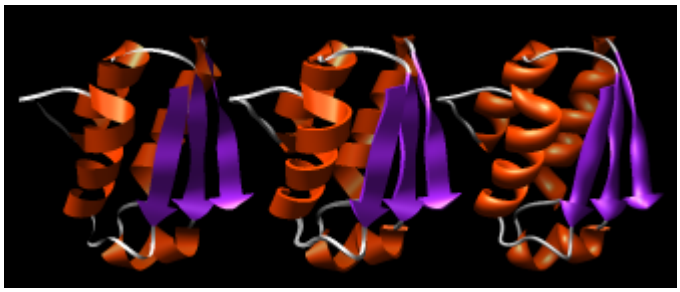
Actions→Atoms/Bonds→sphere
Select→Chain→A
Actions→Atoms/Bonds→ball & stick
Select→Clear Selection
Actions→Atoms/Bonds→stick



Atoms/Bonds: wire, stick, ball & stick, and sphere

Showing ribbon automatically hides the mainchain (backbone) atoms.

Actions→Ribbon→show
Actions→Ribbon→edged
Actions→Ribbon→rounded



Ribbon: flat, edged, and 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:

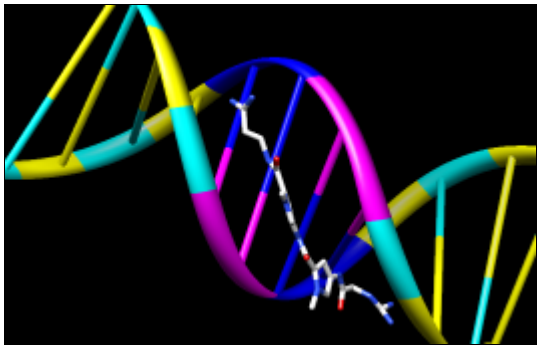
Favorites→Sequence

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**), then 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)



Ribbons and nucleotide ladder

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

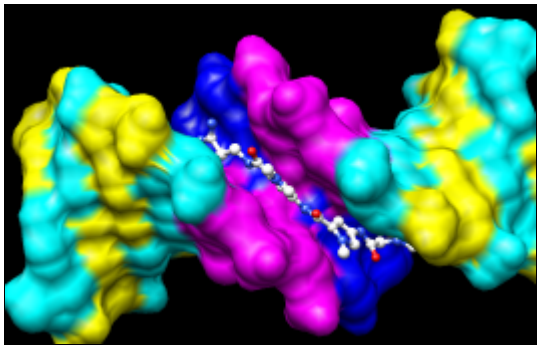
Actions→Atoms/Bonds→nucleotide objects→off

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

Actions→Ribbon→hide
Actions→Atoms/Bonds→ball & stick

← Surfaces

Finally, have some fun with molecular 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**.



Molecular surface (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-line (**Tools→General Controls→Command Line**) equivalent is much more concise, but requires some knowledge of the atom specification syntax:

Command: **surf :da.b,dt.b**

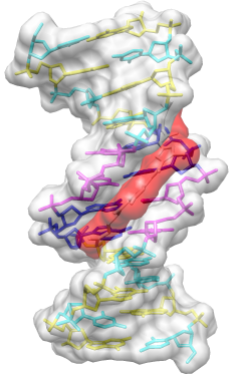
Sometimes it is helpful to make a surface transparent:

Actions→Surface→transparency→50%

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

← Front image how-to (menu)

How to recreate the image at the front of the tutorial using the menu (see commands):



DNA helix with bound netropsin

1. Choose **File→Fetch by ID** and fetch PDB entry **1d86**
2. Use the all atoms preset:
    - **Presets→Interactive 2 (all atoms)**
3. Set the display style to stick:
    - **Actions→Atoms/Bonds→stick**
4. Delete the waters:
    - **Select→Structure→solvent**
    - **Actions→Atoms/Bonds→delete**
5. Color the residues:
    - **Select→Residue→DA**
    - **Actions→Color→blue**
    - **Select→Residue→DC**
    - **Actions→Color→cyan**
    - **Select→Residue→DG**
    - **Actions→Color→yellow**
    - **Select→Residue→DT**
    - **Actions→Color→magenta**
    - **Select→Residue→NT**
    - **Actions→Color→white**
6. Broaden the selection to the whole chain and then to the whole model (both **ligand** and **main**), show surfaces, make them transparent:
    - **Select→Broaden**
    - **Select→Broaden**
    - **Actions→Surface→Show**
    - **Actions→Surface→transparency→40%**
7. Set coloring to surfaces only, make them light gray:
    - choose **Actions→Color→all options...** to show the **Color Actions** dialog, and in that dialog:
        - change the **Coloring applies to** (target) setting to **surfaces**
        - click **light gray** (keep the dialog open)
8. Select just netropsin again, make just its surface red:
    - **Select→Residue→NT**
    - in the **Color Actions** dialog:
        - click **red** (keep the dialog open)
    - **Select→Clear Selection**
9. Set coloring to background only, make it white:
    - in the **Color Actions** dialog:
        - change the coloring target to **background**
        - click **white**
        - click **Close** (which will automatically reset the coloring target back to **all of the above**)
10. Adjust the view as desired
11. Save the image:
    - **File→Save Image**

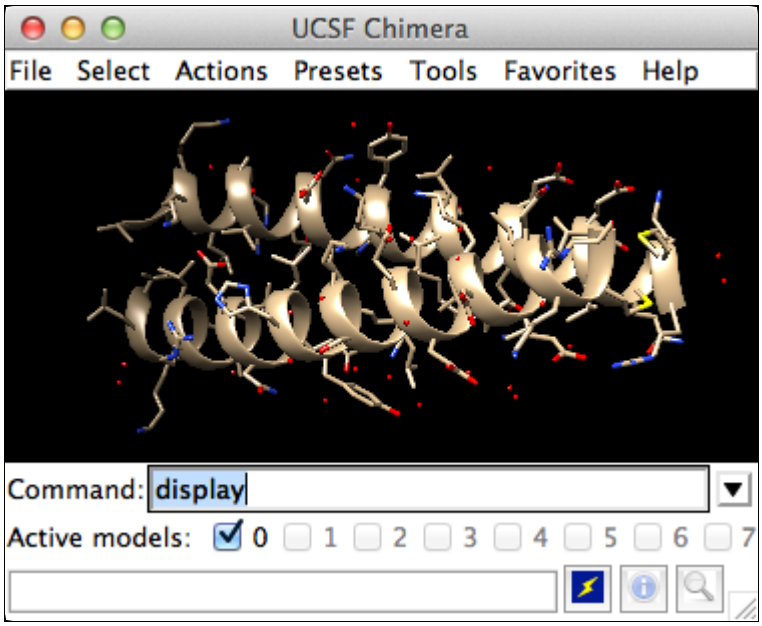
Working with Commands, Part 1 - Manipulation, Selection, and Chains

← Getting started

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.

or Dock

A splash screen will appear, to be replaced in a few seconds by the main Chimera window containing either the graphics display or the **Rapid Access** list of recently used files (it doesn't matter which, since opening a structure will automatically switch the display to the graphics window). If you like, enlarge the window by clicking and dragging its lower right corner. The window can also be moved by clicking its top bar and dragging.



Chimera with Command Line

Show the **Command Line** with **Tools→General~~Controls~~→Command Line**. By default, the **Command Line** is also listed in the ~~**Favorites**~~ menu.

The Favorites menu no longer exists, most such items are in the "Tools" menu.

Opening a structure

Now open a structure. To fetch the structure of entry **1zik** from the Protein Data Bank (PDB), use the command:

> *Command*: **open 1zik**

The structure will appear in the graphics window; it is a leucine zipper formed by two peptides.

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

> *Command*: **display**

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.

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

> *Command*: **~ribbon**
> *Command*: **ribbon**

Many commands have "**~**" versions that perform the opposite function.

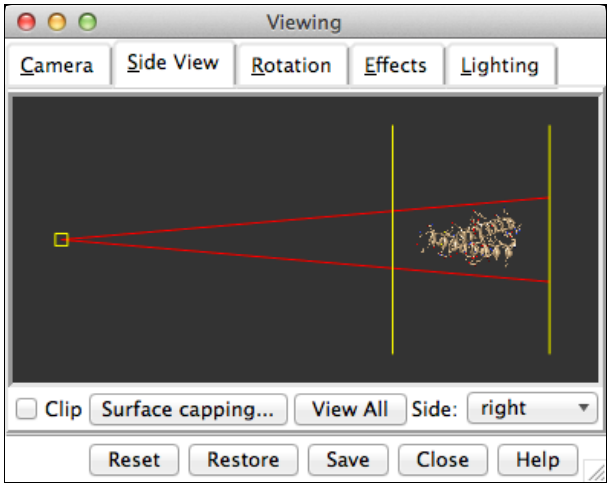
Side View

Show the **Side View** for interactive scaling and clipping:

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

By default, the **Side View** can also be started from the ~~**Favorites**~~ menu. Tools>General

It shows a tiny version of the structure. Try moving the eye position (the small square) and the clipping planes (vertical lines) by clicking and dragging 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.

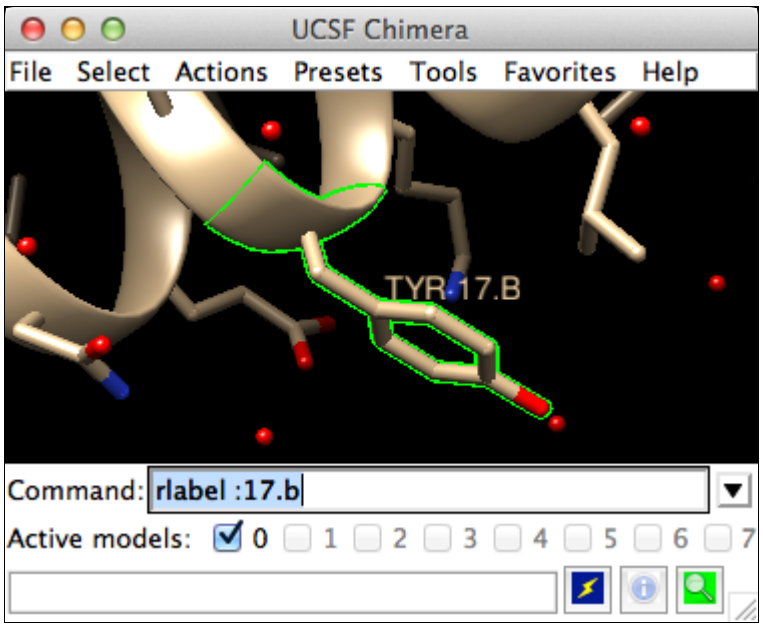


Side View showing 1zik

← Using the mouse

Try manipulating the structure in the main window with the mouse. By default:

- the left mouse button **Btn1** controls rotation
- the middle mouse button **Btn2** controls XY translation (panning)
- the right mouse button **Btn3** performs scaling (zooming)



1zik with tyrosine 17 (B chain) selected

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**).

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. For an atom, the balloon information is of the form:

~~res-name res-num.chain atom-name~~ cain name number (atom, if shown)

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.

Selection with the mouse

In combination with modifier keys, the mouse buttons have additional functions. By default, ***picking*** from the screen (a type of ***selection***) is done by **Ctrl**-clicking an atom or bond with the left mouse button, **Btn1**. Additionally pressing **Shift** adds to or toggles an existing selection. The selection is outlined in green, and placing the mouse cursor over the green magnifying glass icon near the bottom right corner of the window reports what is selected in a pop-up "balloon." Below the command line

The arrow keys can be used to broaden (↑), narrow (↓), or invert (→) a selection. The hierarchy for broadening and narrowing a selection could include (depending on the initial selection): atom/bond, residue, protein secondary structure element, bonded set of atoms, all atoms with the same chain ID, entire model. When a selection is inverted, the selected atoms become deselected and *vice versa*.

Spend some time selecting various parts of the structure. An easy way to clear the selection (deselect everything) is to use **Ctrl**-**Btn1** in any blank space in the graphics window.

← Command/Target

A Chimera command may include ***arguments*** and a ***target*** (or ***atom specification***). For example, in the following **color** command,

Command: **color hot pink :lys**

hot pink is an argument that specifies a color name, and **:lys** specifies that the target is all residues named LYS.

If no target is specified, the command acts on all applicable items. For example, the following makes everything hot pink:

Command: **color hot pink**

A basic specification may contain residue names, residue numbers, chain identifiers, and/or atom names (see the table of symbols, right). Note also that commands can be truncated to unique strings.

color <specify affected items> <color spec> <target representation>

Command: col /a:20-22 gray
Command: col /b:lys teal
Command: ~disp HOH
Command: col /a blue r
Command: disp :AMP
Command: style :AMP bs
(ball & stick)
Command: style :AMP stick
disp @S*
Command: col /a:cys@S* gold atoms
Command: ~disp @S*

Atom Specification Symbols

Symbol	Function	Usage
#	model number	# *model* (integer)
:	residue	: *residue* (name or number)
/	Chain ID	/a or /A
@	atom name	@*atom*
*	whole wildcard	matches whole atom or residue names, *e.g.*, **:*@CA** specifies the α-carbons of all residues
?	single-character wildcard	used for atom and residue names only, *e.g.*, **:G??** specifies all residues with three-letter names beginning with G
z<	zone specifier	**z<***zone* or **zr<***zone* specifies all residues within *zone* angstroms of the indicated atoms, and **za<***zone* specifies all atoms (rather than entire residues) within *zone* angstroms of the indicated atoms. Using **>** instead of **<** gives the complement.
&	intersection	intersection of specified sets
|	union	union of specified sets
~	negation	negation of specified set (when space-delimited)

Also, type 'help color'

The Chimera Quick Reference Guide lists all of the commands and gives some examples of atom specification. It can be accessed by choosing **Help→Tutorials** from the Chimera menu and clicking the “Chimera Quick Reference Guide” link.

Many other types of specifications can be used, including element symbols and built-in classifications such as **solvent**:

Command: **~disp solvent**
Command: **color blue S** color solvent blue
Command: **disp protein**

The command **help** can be used to show the manual page for any command:

Command: **help color**

As explained in the manual page, the **color** command also allows coloring only certain

These are 'targets'

representations. For example, "**,a**" in the following means atoms only (not ribbons, surfaces, *etc.*):

omit the comma, and put the target representation last. see help color.

Command: **col gold,a :glu,lys**

Restore the original coloring:

col :glu,lys gold atoms or
col :glu,lys gold target a

Command: **col tan**
Command: **col byhet**

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

Try picking two atoms in different residues (**Ctrl**-click the first, **Shift**-**Ctrl**-click the second). Unlike the **Actions** menu, commands do not automatically act on the current selection. However, the current selection can be specified as the target of a command with the word **selected**, **sel**, or **picked**. Show residue labels for the atoms you have selected:

Command: ~~**rlabel**~~ **sel**

label sel residues

(The **label** command shows atom information instead.) The 3D labels from **rlabel** and **label** move along with structures and are mainly for interactive use. For figures and movies, **2D Labels** are recommended instead.

The following command can be used to promote the selection to the entire residues:

Command: **select up**

(The keyboard up arrow ↑ also broadens a selection, but you may need to click into the graphics window first to use that approach.) Show only the selected atoms:

Command: **show sel**

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:

Command: **~rlab**
Command: **~ribbon**
Command: **disp**
Command: **col byelement**

display se

Coloring **byelement** is the same as **byhet** except it also color-codes carbons (gray).

← Models and model status

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~~. 1

~~The **Active models** line right under the **Command Line** shows which models are activated for motion. Unchecking the box for **0** makes it impossible to rotate or translate model 0 interactively. Checking the box again restores the movable state.~~ A similar row of checkboxes for toggling model display can be shown using the preferences (menu: **Favorites**→**Preferences**, category **Command Line**).

Remove the model:

Command: **close 0**

To move individual models, go to Right Mouse in the toolbar and drag model, for example.

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

Command: **stop**

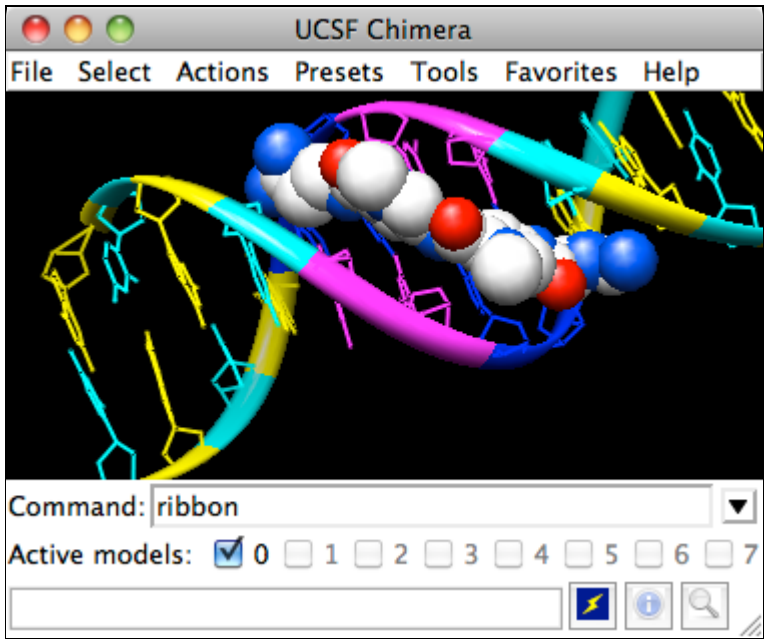
To come back later to the current state of your project, go to Home in the tool bar and Save... ChimeraX session (.cxs) but PAY ATTENTION to the destination folder and navigate as needed to save your file in a desired location.
in command line first get to the right folder via pwd
save test.cxs This saved to my desktop, even though I had defined a different working folder

Working with Commands, Part 2 - Molecular Representations and Surfaces

← Setup

With Chimera started and the **Command Line** opened as described at the beginning of **Part 1**, fetch the structure of entry **1d86** from the Protein Data Bank (PDB):

Command: **open 1d86**



Chimera with Command Line

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.

Rotate, translate, and scale the structure as needed to get a better look (see **Using the mouse** to review how this is done). Continue moving and scaling the structure as desired throughout the tutorial.

A ***preset*** is a predefined combination of display settings. Use the "all atoms" preset, which will show the DNA as wire and netropsin as spheres:

Command: **preset ~~apply int~~ 2** preset 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:

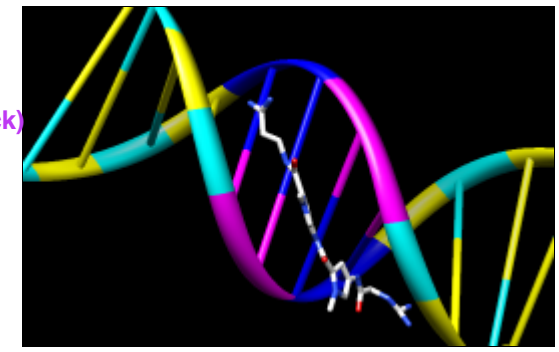
Command: **color blue :da** col :da blue
Command: **color cyan :dc** col :dc cyan
Command: **color yellow :dg** col :dg yellow
Command: **color magenta :dt** col :dt magenta

← Representations

Next, try some different display styles, or representations.

Command: **represent sphere**
Command: **repr bs :.a**
Command: **rep stick**

style shere
style /a ball **(for ball and stick)**
style stick



Ribbons and nucleotide ladder

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**

ribbon style xsection piping
ribbon style xsection oval

xsection arguments are: 'barbell', 'oval', 'piping', 'rectangle', 'round', or 'square'

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**

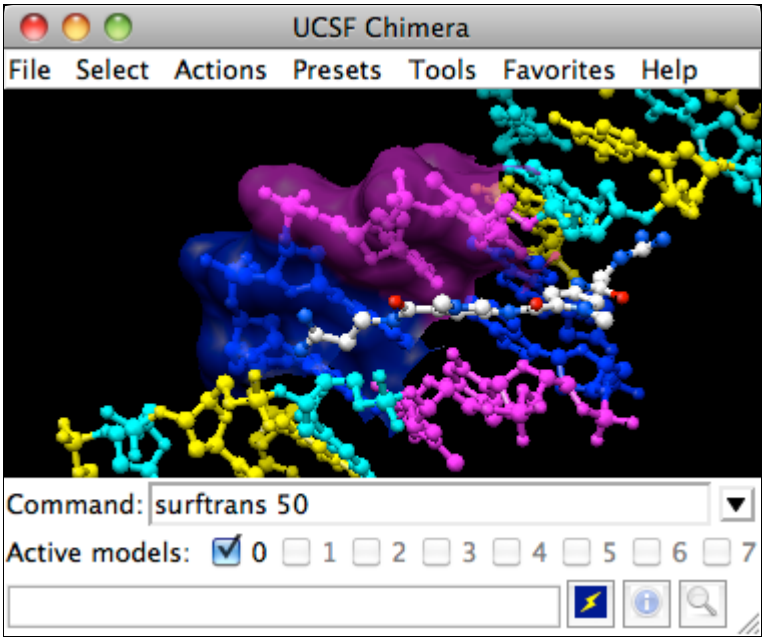
Hide the ribbons and show everything as ball-and-stick:

Command: **~ribbon**
Command: ~~**rep bs**~~

← Surfaces

Finally, have some fun with molecular surfaces. 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**



Chimera showing a transparent surface

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**

surface style mesh (mesh | solid | dot)
color ligand red surface OR color ligand red target s
surface style 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 surface transparent:

Command: **transp 50,s**

transp 50 surface or transp 50 target s

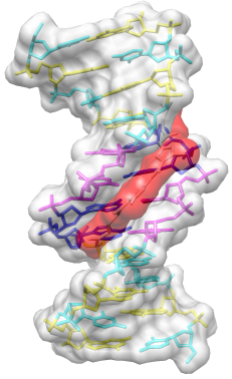
When finished, exit from Chimera:

Command: ~~**stop now**~~

Exit or Quit
Stop now is used to stop any movements occurring, such as rotation ('rolling').

← Front image how-to (commands)

How to recreate the image at the front of the tutorial using commands (see menu approach):



DNA helix with bound netropsin

1. Fetch 1d86:
    - *Command*: **open 1d86**
2. Use the all atoms preset:
    - *Command*: **preset apply int 2**
3. Set the display style to stick:
    - *Command*: **repr stick**
4. Delete the waters:
    - *Command*: **del solvent**
5. Color the residues:
    - *Command*: **color blue :da**
    - *Command*: **color cyan :dc**
    - *Command*: **color yellow :dg**
    - *Command*: **color magenta :dt**
    - *Command*: **color white :nt**
6. Show surfaces for the whole model (both **ligand** and **main**), make them transparent:
    - *Command*: **surf #0**
    - *Command*: **surftrans 40**
7. Color the **main** (DNA) surface light gray and the **ligand** (netropsin) surface red:
    - *Command*: **color light gray,s main**
    - *Command*: **color red,s ligand**
8. Change the background color to white:
    - *Command*: **set bg_color white**
9. Adjust the view as desired
10. Save the image:
    - *Command*: ~~**copy png file ~/Desktop/myfile.png**~~

save <myfiledname>.png