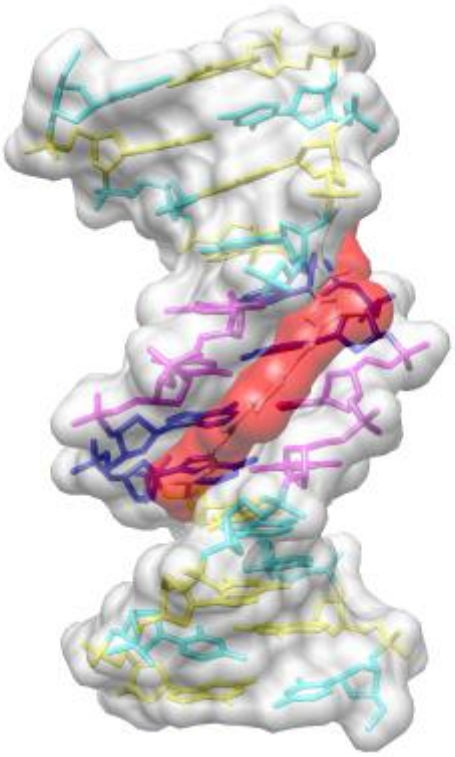
UCSF Chimera - Getting Started



DNA helix with bound netropsin

This tutorial provides an overview of basic features in Chimera for displaying and manipulating structures. You can interact with Chimera by using the menus and/or by entering commands. The basic features of Chimera are available either way, but several tools are not available as commands, and several command operations (and scripting) are not available through the menus. Thus, it is useful to become familiar with both ways of interacting with Chimera.

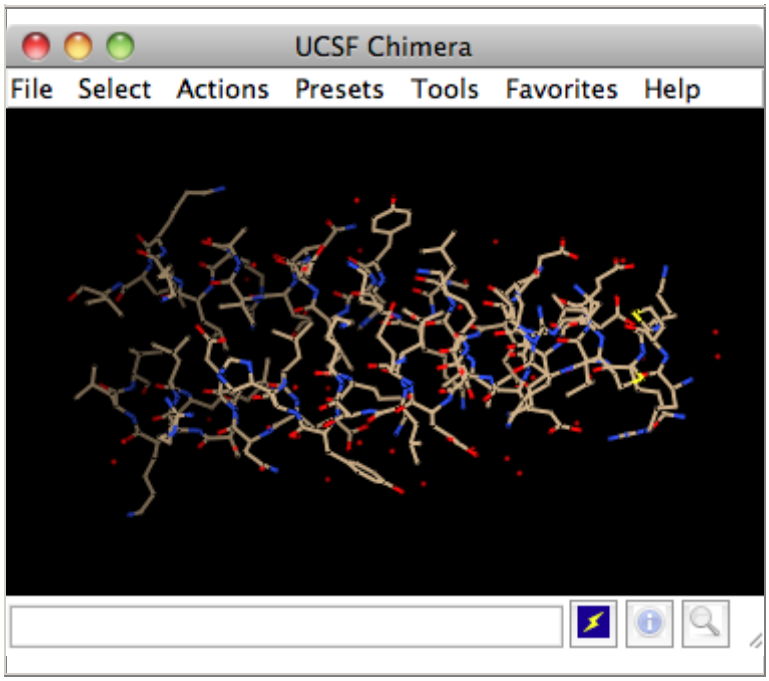
The **Working with menus** and **Working with commands** sections were designed to be independent of each other. They cover (for the most part) identical operations, accomplished in different ways. If you go through both sections, you can skip portions that cover issues you already understand. You can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

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
Filename (or file path)	`1zik`	File 1zik

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



UCSF Chimera with 1zik

Getting started

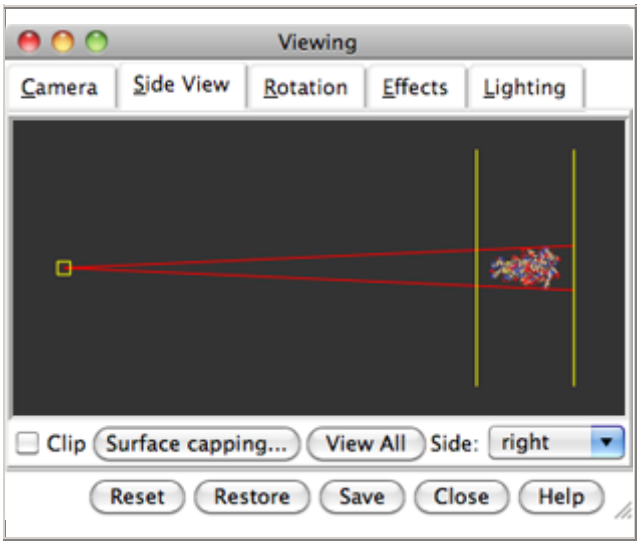
On **Linux**, run the executable "chimera" in the bin directory of your Chimera installation. If Chimera is installed in `/usr/local/chimera`, run `/usr/local/chimera/bin/chimera` from a shell.

On **Windows**, start Chimera by doubleclicking the Chimera icon in the directory called **bin** in your Chimera installation. If Chimera is installed in `\Program Files` the executable will be in the directory `\Program Files\Chimera\bin`. By default, a Chimera icon will also be placed on your desktop.

On **Mac**, start Chimera by clicking the Chimera icon or by doubleclicking the Chimera application in the Finder window.

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 does not matter which, the following instructions will work with either; the **Rapid Access** interface reverts to the graphics display as soon as something is opened). If you like, enlarge the main window by clicking and dragging its lower right corner. Chimera includes a number of tools and dialogs that can be present on the screen at the same time. Each Chimera window or tool can be moved to a convenient location by clicking its top bar and dragging.

Opening a structure



Side View showing 1zik

Now open a structure. Choose **File→Fetch by ID** and type `1zik` in the **PDB ID** field. The structure will appear in the main graphics window; it 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 (oxygens red, nitrogens blue, *etc.*); carbons are left in the initial model color, in this case tan.

Side View

Scaling and clipping operations can be performed with the **Side View**. There are several ways to start this tool; one is to choose **Tools→Viewing Controls→Side View** from the menu. By default, the **Side View** is also listed in the **Favorites** menu. The **Side View** 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.

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, and the right mouse button controls scaling. 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.

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

Continue moving and scaling the structures 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 combination with the control (**Ctrl**) key, the mouse buttons have additional functions. 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 (**Btn1**) while holding down the **Ctrl** key. To add to an existing selection, also hold down the **Shift** key. The selection is highlighted in green, and placing the mouse cursor over the green magnifying glass icon  near the bottom right corner of the window pops up a "balloon" that reports what is selected.

You can also drag out a selection area with **Ctrl**-**Btn1** (sweep out an area before releasing). All atoms and bonds within that area will be selected. As before, **Ctrl**-**Shift**-**Btn1** can be used to add to an existing selection, either by clicking or by dragging.

The arrow keys can be used to broaden, narrow, or invert a selection. Each press of the ↑ key will broaden a selection to the next available level. The selection hierarchy could include (depending on the initial selection): atom/bond, residue, bonded set of atoms, all atoms with the same chain ID, entire model. Similarly, the selection scope can be narrowed using the ↓ key. The → key inverts the selection so that selected atoms become deselected and *vice versa*.

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

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 indicated by the radio buttons.
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**.
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.

Selection/Action

In general, operations performed with the Chimera **Actions** menu affect 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 current selection is highlighted in green in the structure(s), and the magnifying glass icon  near the bottom right corner of the window is also green when a selection exists.

Changing the display

Select and hide the water (red dots):

Select→Structure→solvent
Actions→Atoms/Bonds→hide

Alternatively, the water could have been selected using **Select→Residue→HOH**. Even though the water is hidden, it is still selected.

Clear the selection and display only the chain trace:

Select→Clear Selection
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.

Try picking two α-carbons, one from each peptide (using **Ctrl**-**Btn1** for the first, **Ctrl**-**Shift**-**Btn1** for 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

Each residue label is of the form:

res_name res_number.chain

One peptide is chain A and the other is chain B. Clear the selection and undisplay the residue labels:

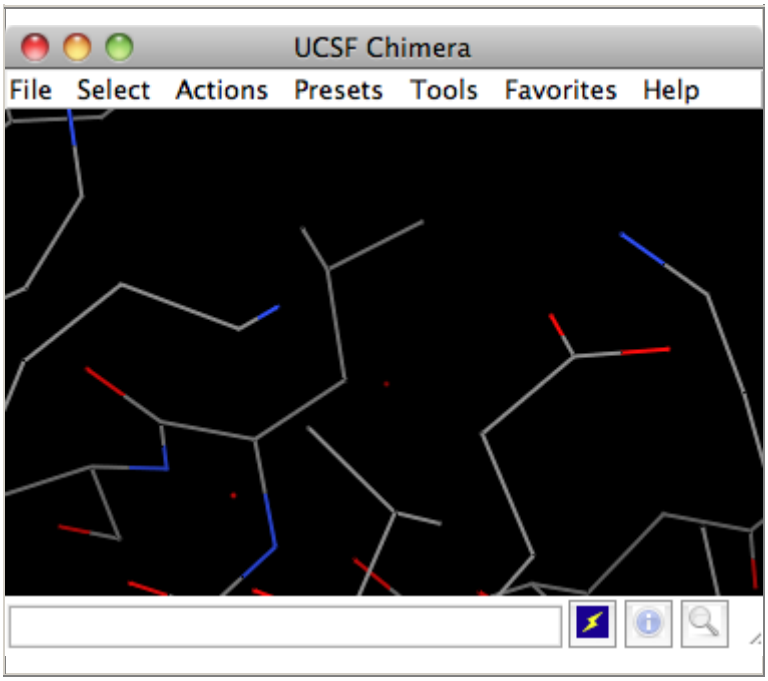
Select→Clear Selection
Actions→Label→residue→off

(Another way to clear a selection is to **Ctrl**-**Btn1** click in empty space.)

Color the two chains different colors:

Select→Chain→A
Actions→Color→cyan

Repeat the process to color chain B yellow.



1zik colored by element

Select chain A by picking any atom or bond in the chain, then hitting the ↑ 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):

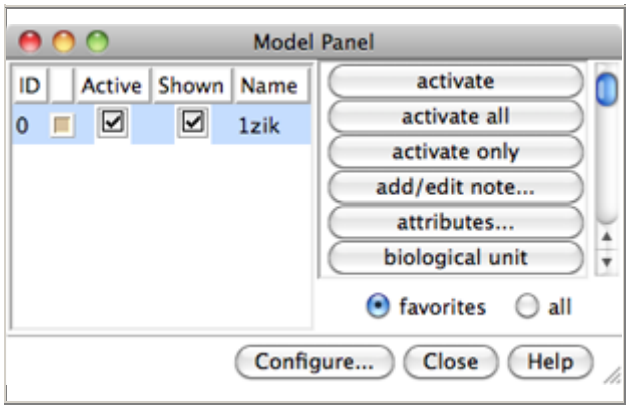
Actions→Atoms/Bonds→show only

Display all atoms and color them by element:

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

The **by element** coloring applies to all elements including carbon (gray), whereas **by heteroatom** coloring (as in the preset used near the beginning of the tutorial) leaves carbons unchanged. Heteroatom-only coloring is useful for keeping different structures distinguishable by their different carbon colors.

Models and model status



Chimera Model Panel

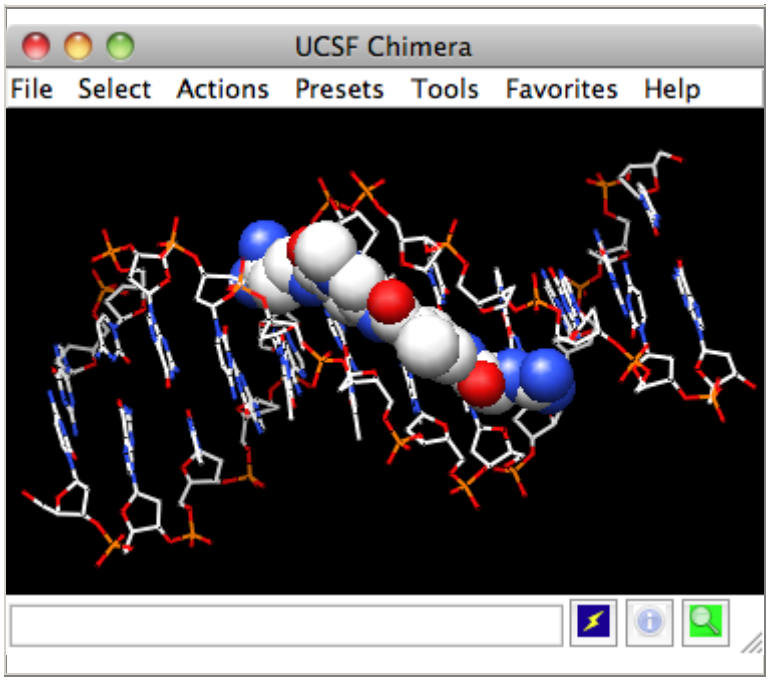
Generally, each file of coordinates opened in Chimera becomes a ***model*** with an associated model ID number. Models are assigned successive numbers starting with 0. The **Model Panel** shows the current models and enables many operations upon them. Open this tool with **Tools→General Controls→Model Panel**. By default, the **Model Panel** is also listed in the **Favorites** menu.

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. Checking the box again restores the movable state. Make sure the line for `1zik` 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. 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



Chimera showing netropsin as spheres

With Chimera started and the **Side View** opened as described at the beginning of Part 1, open a different structure. Choose **File→Fetch by ID** and type `1d86` in the **PDB ID** field. The structure contains the molecule netropsin bound to double-helical DNA.

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 until the selection is cleared or replaced with a new selection.

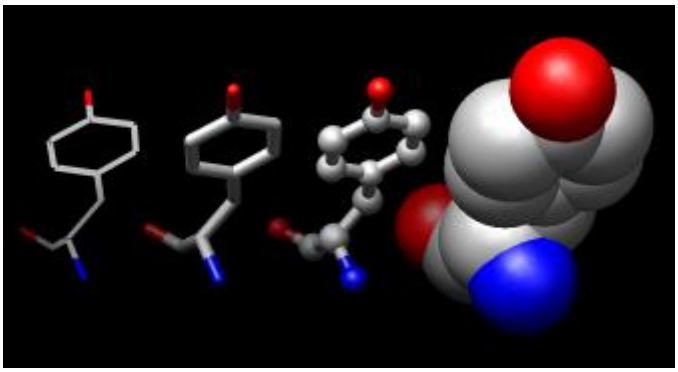
Color the different nucleotides different colors. For example, color the adenine deoxynucleotides blue:

Select→Residue→DA
Actions→Color→blue

Analogously, color cytosine deoxynucleotides (DC residues) cyan, guanine deoxynucleotides (DG residues) yellow, and thymine deoxynucleotides (DT residues) magenta. Clear the selection with **Select→Clear Selection** or by picking in empty space.

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.

Representations



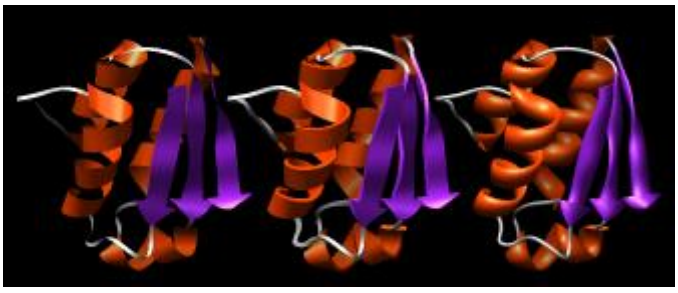
Atoms/Bonds: wire, stick, ball & stick, and sphere

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



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"

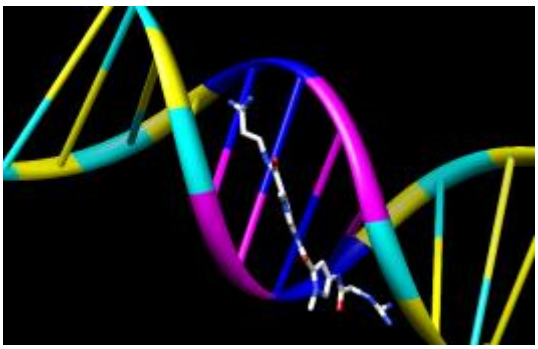
Nucleotide settings can be applied to just the selected residues (not necessarily all of the DNA). One way to select specific residues is in the **Sequence** tool:

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:



Ribbons and nucleotide 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)

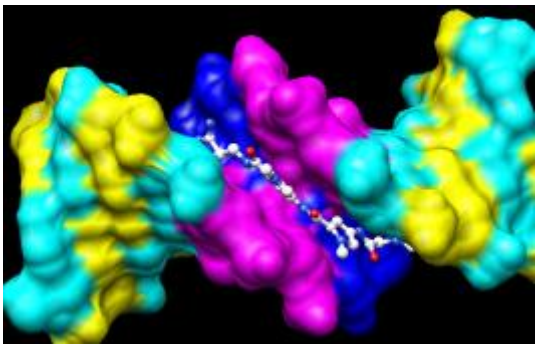
To return to more general display styles, turn off the nucleotide objects:

Actions→Atoms/Bonds→nucleotide objects→off

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

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

Surfaces



Molecular surface (main)

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**.

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

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

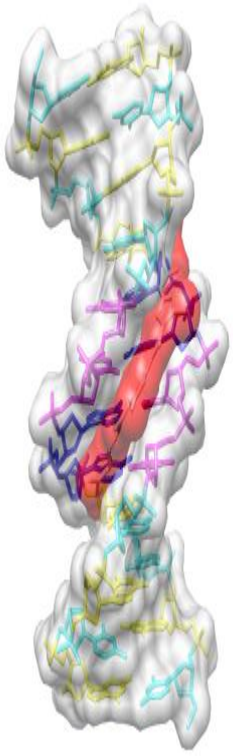
Command: **surf :da.b,dt.b**

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):

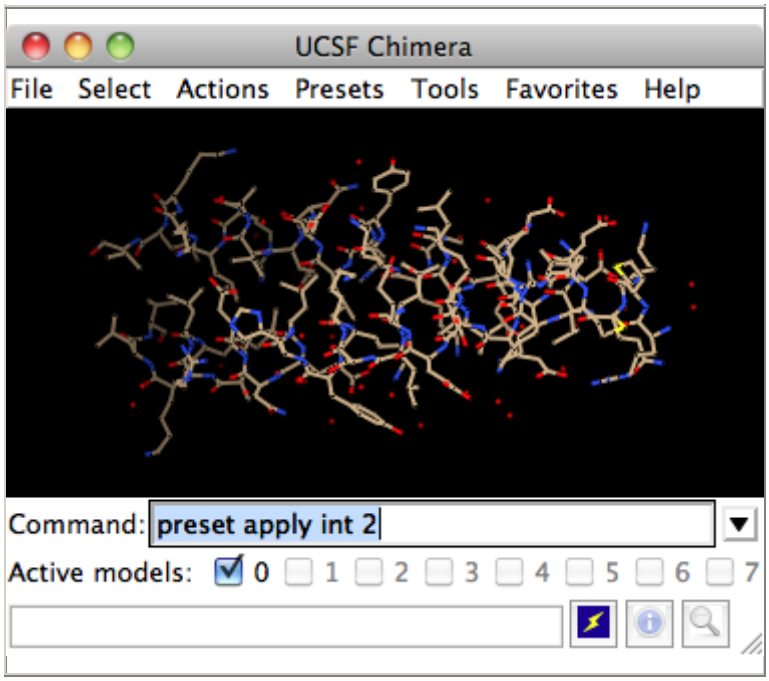


DNA helix with bound netropsin

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



Chimera with Command Line

Getting started

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On **Windows**, start Chimera by doubleclicking the Chimera icon in the directory called **bin** in your Chimera installation. If Chimera is installed in `\Program Files` the executable will be in the directory `\Program Files\Chimera\bin`. By default, a Chimera icon will also be placed on your desktop.

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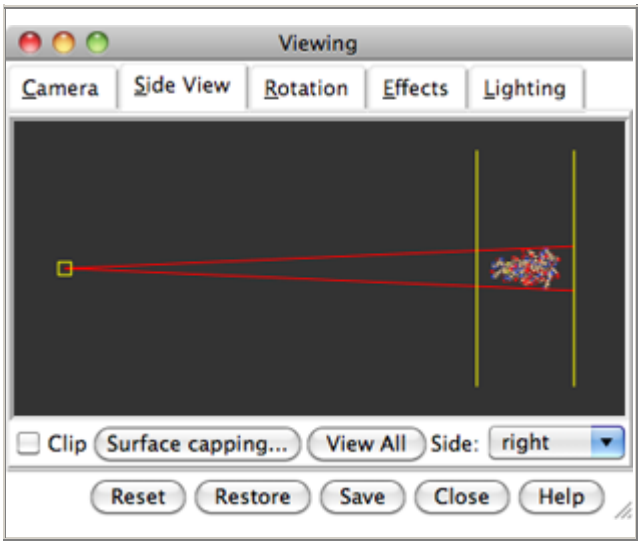
Show the **Command Line** with **Tools→General Controls→Command Line**. By default, the **Command Line** is also listed in the **Favorites** menu.

Opening a structure



Side View showing 1zik

Now open a structure. To fetch the structure directly from the PDB, use the command:

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

The structure will appear in the main graphics window; it 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.

Side View

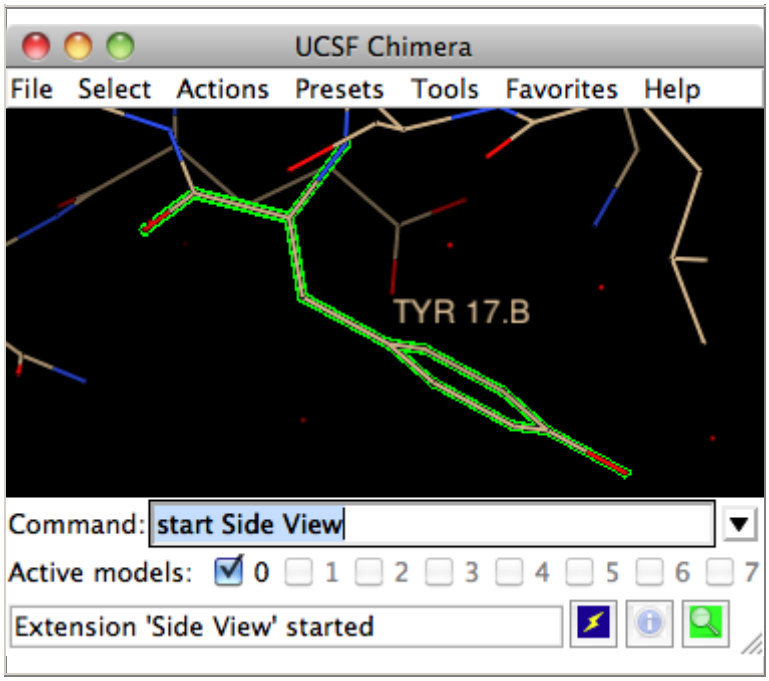
Show the **Side View**:

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

By default, the **Side View** can also be started from the **Favorites** menu.

The **Side View** allows interactive scaling (zooming) and clipping. 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.

Using the mouse



1zik with tyrosine 17 (B chain) selected

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**) button controls XY translation, and the right mouse button (**Btn3**) controls scaling. 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.

Continue moving and scaling the structures 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 combination with the control (**Ctrl**) key, the mouse buttons have additional functions. 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 (**Btn1**) while holding down the **Ctrl** key. To add to an existing selection, also hold down the **Shift** key. The selection is highlighted in green, and placing the mouse cursor over the green magnifying glass icon near the bottom right corner of the window pops up a "balloon" that reports what is selected.

The arrow keys can be used to broaden (↑), narrow (↓), or invert (→) a selection. The hierarchy for broadening and narrowing a selection may include (depending on the initial selection): atom/bond, residue, 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 model. An easy way to deselect everything is to use **Ctrl**-**Btn1** in any blank space in the graphics window.

Command/Target

Atom Specification Symbols		
Symbol	**Function**	**Usage**
#	model number	# *model* (integer)
:	residue	: *residue* (name or number)
:.	chain ID	:.*chain*
@	atom name	*@atom*
*****	whole wildcard	matches whole atom or residue names, *e.g.*, **:*@CA** specifies the α-carbons of all residues
=	partial wildcard	matches partial atom or residue names, *e.g.*, **@C=** specifies all atoms with names beginning with C
?	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)

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 the target **:lys** specifies all residues named LYS. (To see the built-in colors and their names, choose **Actions→Color→all colors** from the menu.)

If no target is specified, the command acts on all applicable items. For example,

`Command:` **color hot pink**

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

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**.

Many commands have "~" versions that perform the opposite function. For example, change the 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**
shows the manual page for the command **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.

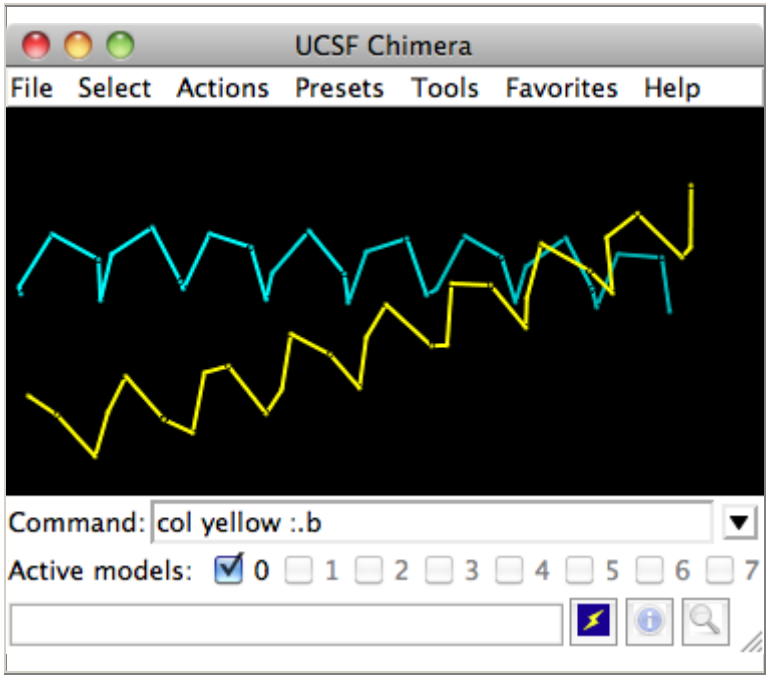
Changing the display

Display only the atoms named CA (α-carbons):

`Command:` **show @ca**

Try picking two α-carbons, one from each peptide (using **Ctrl**-**Btn1** for the first, **Ctrl**-**Shift**-**Btn1** for the second). 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**



1zik with chain traces in different colors

Each residue label is of the form:
res_name res_number.chain
One peptide is chain A and the other is chain B. Clear the selection and undisplay the residue labels:
Command: **~select**
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- (equivalent)
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: **color byelement**
The **byelement** coloring applies to all elements including carbon (gray), whereas **byhet** coloring (as in the preset used near the beginning of the tutorial) leaves carbons unchanged. Heteroatom-only coloring is useful for keeping different structures distinguishable by their different carbon colors.

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. The **Active models** line in the

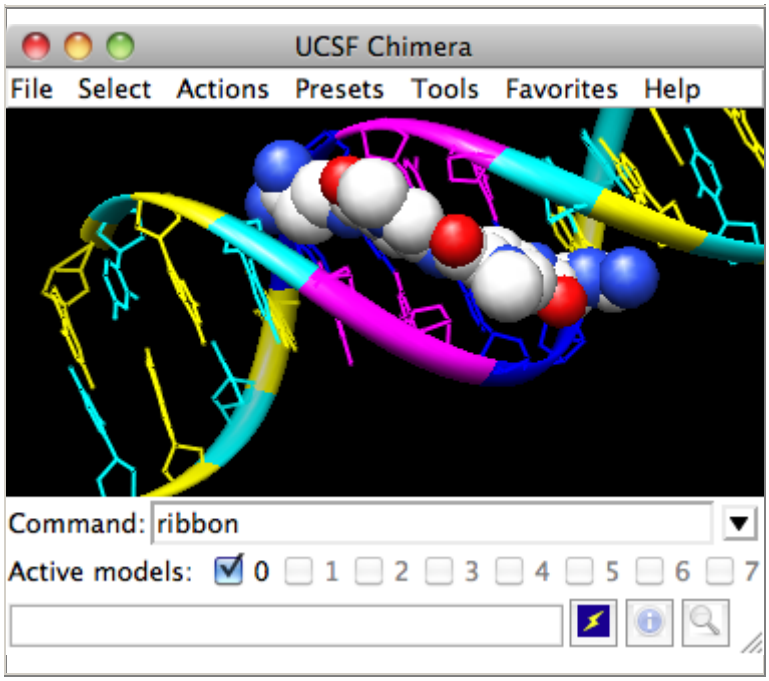
Command Line tool shows which models are activated for motion. The checkbox for **0** (currently the leucine zipper) is activated. Unchecking the box makes it impossible to move model 0. Checking the box again restores the movable state.

Command: **close 0**

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

Working with Commands, Part 2 - Molecular Representations and Surfaces

Setup



Chimera with Command Line

With Chimera started and the **Command Line** and **Side View** opened as described at the beginning of **Part 1**, open a different structure. Fetch the structure directly from the PDB:

`Command:` **open 1d86**

The structure contains the molecule netropsin bound to double-helical DNA.

Use 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:

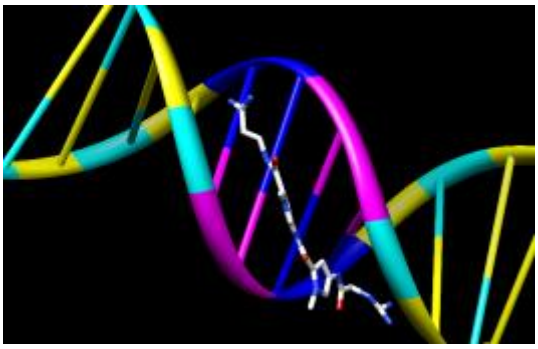
`Command:` **color white C**
`Command:` **~disp solvent**

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 magenta :dt**
`Command:` **color yellow :dg**
`Command:` **color cyan :dc**

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.

Representations



Ribbons and nucleotide ladder

Next, try some different display styles, or representations.

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

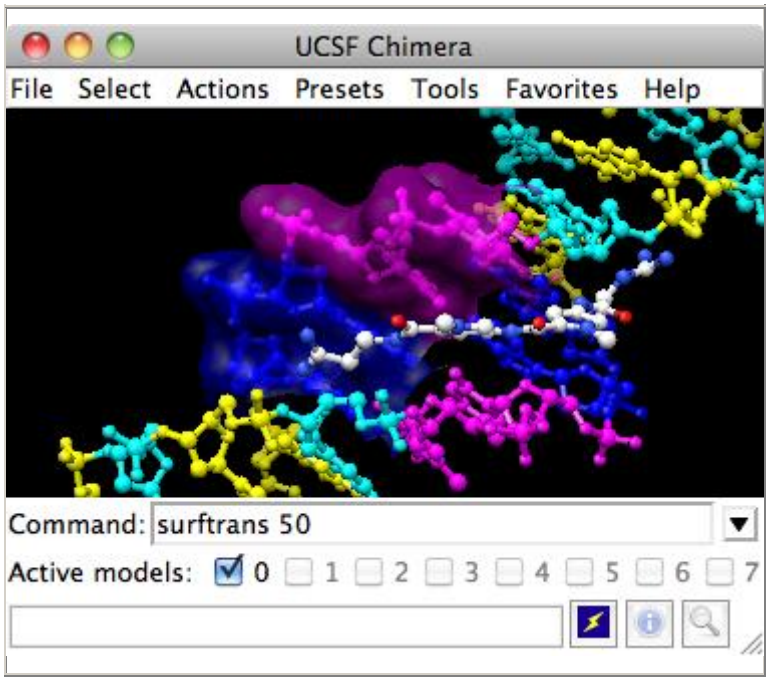
Notice that commands (but not necessarily their keyword arguments) can be truncated to unique strings. For example, the command **represent** can be shortened to **repr** or **rep** but not **re** (because other commands also start with **re**), whereas the keywords **stick**, **sphere**, *etc.* cannot 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**

Surfaces



Chimera showing a transparent surface

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
```

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 surface transparent:

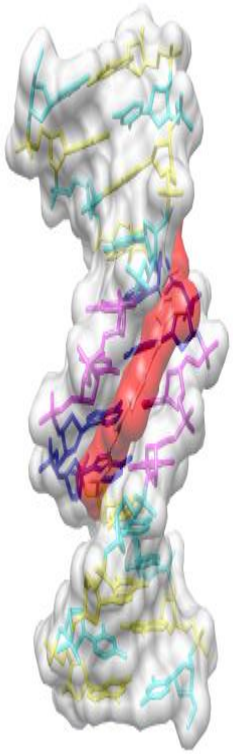
```
Command: transp 50,s
```

When finished, exit from Chimera:

```
Command: stop now
```

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**