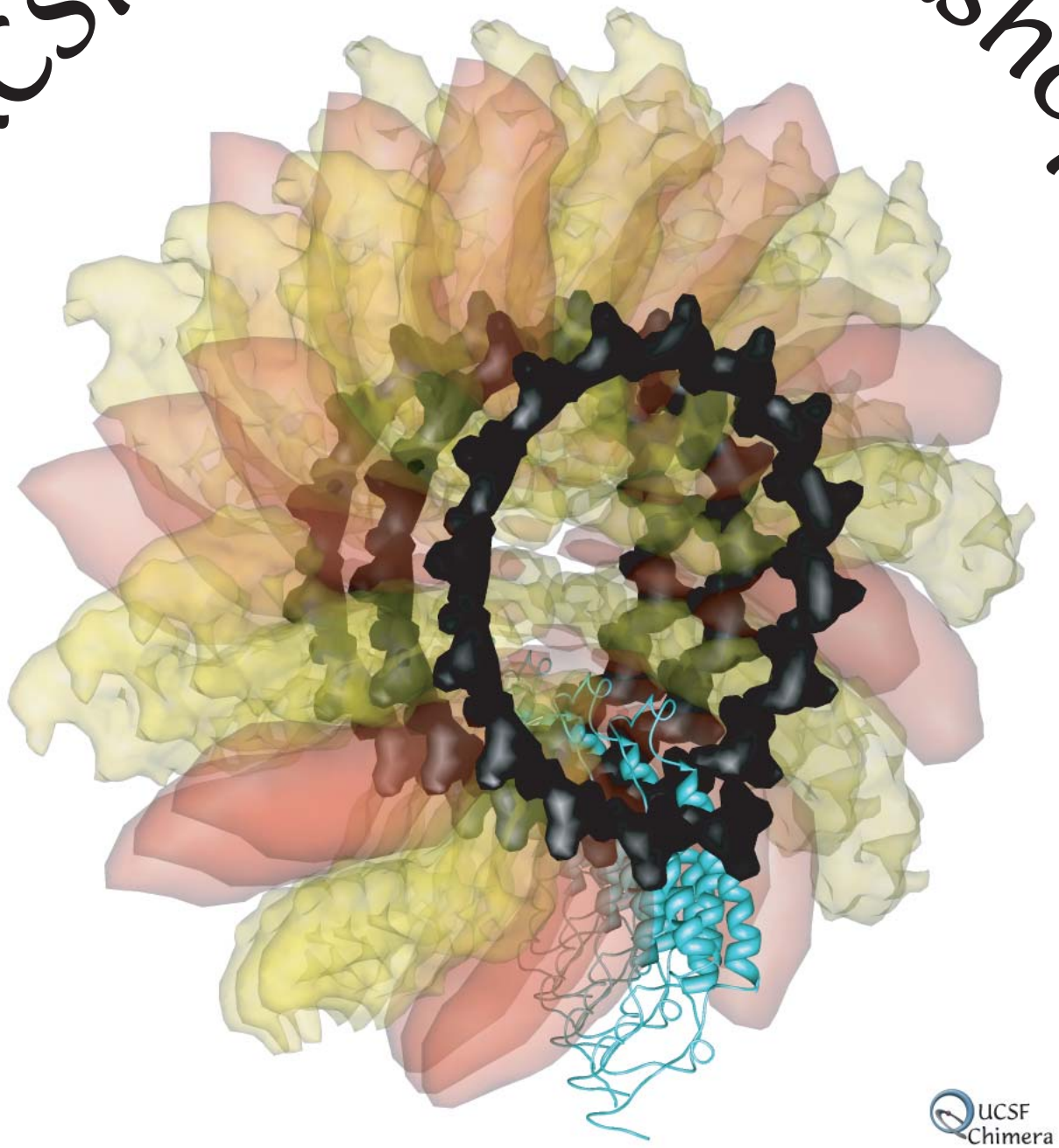
UCSF Chimera Workshop



University of California, San Francisco
November 17-18, 2005

UCSF Chimera Workshop
UC San Francisco Mission Bay
November 17-18, 2005

Agenda

Day 1 - November 17

9:00	-	10:45	Introduction to UCSF Chimera
10:45	-	11:00	Break
11:00	-	12:00	Exploring sequence-structure relationships with MultAlign viewer tool
12:00	-	1:30	Lunch
1:30	-	2:15	Screening docked ligands using ViewDock
2:15	-	3:15	MD trajectories and structural ensembles
3:15	-	3:45	Break
3:45	-	4:30	Displaying, defining, and calculating attributes
4:30	-	5:30	General lab

Day 2 - November 18

9:00	-	10:00	Large molecular assemblies
10:00	-	10:30	Break
10:30	-	11:30	Volume data
11:30	-	1:00	Lunch
1:00	-	2:00	Producing images and movies
2:00	-	3:00	Chimera scripts and demos
3:00	-	3:30	Break
3:30	-	??	Panel

UCSF Chimera Workshop
UC San Francisco
November 17-18, 2005

Day 1 Agenda

9:00 - 10:45 Introduction to UCSF Chimera
- Welcome & overview
- Introductory tutorial
- Hands-on session

10:45 - 11:00 Break

11:00 - 12:00 Exploring sequence-structure relationships with MultAlign viewer tool
- Presentation/Demo
- Hands-on session

12:00 - 1:30 Lunch

1:30 - 2:15 Screening docked ligands using ViewDock
- Presentation/Demo
- Hands-on session

2:15 - 3:15 MD trajectories and structural ensembles
- Presentation/Demo
- Hands-on session

3:15 - 3:45 Break

3:45 - 4:30 Displaying, defining, and calculating attributes
- Presentation/Demo
- Hands-on session

4:30 - 5:30 General lab
- Get help working with data of your choice

UCSF Chimera Workshop
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Day 2 Agenda

9:00 - 10:00 Large molecular assemblies
- Presentation/Demo
- Hands-on session

10:00 - 10:30 Break

10:30 - 11:30 Volume data
- Presentation/Demo
- Hands-on session

11:30 - 1:00 Lunch

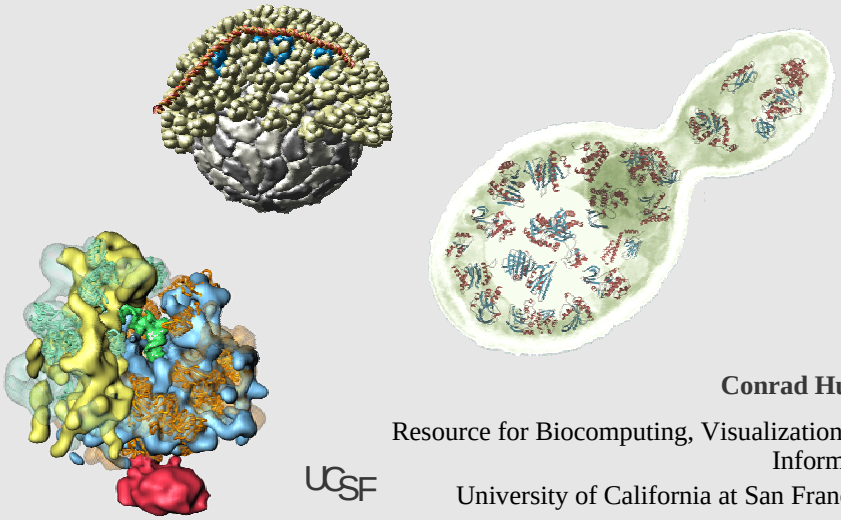
1:00 - 2:00 Producing images and movies
- Presentation/Demo
- Hands-on session

2:00 - 3:00 Chimera scripts and demos
- Presentation/Demo
- Hands-on session

3:00 - 3:30 Break

3:30 - ?? Panel
- Chimera Futures
- Q&A

UCSF Chimera Workshop, Fall 2005



Conrad Huang

Resource for Biocomputing, Visualization, and Informatics

University of California at San Francisco

Overview

- General format:
  - Short presentation/demonstration
  - Hands-on tutorial
- Topics may be domain-specific
  - Attend the topics of interest

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Today's Agenda

Time	Topic	Presenter
9:00-10:45	Introduction to UCSF Chimera	Eric
10:45-11:00	Break	
11:00-12:00	Exploring sequence-structure relationships with MultAlignViewer	Elaine
12:00-1:30	Lunch	
1:30-2:15	Screening docked ligands using ViewDock	Elaine
2:15-3:15	MD Trajectories and structural ensembles	Eric
3:15-3:45	Break	
3:45-4:30	Displaying, defining and calculating attributes	Conrad
4:30-5:30	General lab	Team

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Tomorrow's Agenda

Time	Topic	Presenter
9:00-10:00	Large molecular assemblies	Tom
10:00-10:30	Break	
10:30-11:30	Volume data	Tom
11:30-1:00	Lunch	
1:00-2:00	Producing images and movies	Greg
2:00-3:00	Chimera scripts and demos	Greg
3:00-3:30	Break	
3:30-??	Panel discussion	Team

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Today's Presenters

- Conrad Huang — Chimera Developer
- Eric Pettersen — Chimera Developer
- Elaine Meng — Scientific Advisor
- Tom Goddard — Chimera Developer
- Greg Couch — Chimera Developer
- Scooter Morris — Executive Director, RBVI

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Further information:
–www.cgl.ucsf.edu/chimera

- Staff:
  - Dr. Tom Ferrin, Dr. Conrad Huang, Tom Goddard, Greg Couch, Eric Pettersen, Dan Greenblatt, Al Conde, Dr. Elaine Meng, Dr. John "Scooter" Morris
- Collaborators (partial list):
  - Patricia Babbitt, UCSF
  - Wah Chiu and Steven Ludtke, Baylor
  - John Sedat and David Agard, UCSF
  - David Konerding and Steven Brenner, UCB

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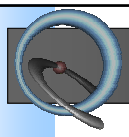


Chimera: the basics plus a few tips

- A whirlwind tour of the basics
  - With focus on a few things to make your life easier
- Hands-on experience
  - “Getting started” tutorial
    - Fleshes out the basics for those who haven’t used Chimera before — and a good refresher for others

Chimera Basic Usage Reminder Sheet

Open/Save Dialogs

- drop-down menus for recently used files/directories
- File Type filter controls type of files shown
- multi-select by:
  - mouse drag (contiguous)
  - control click (non-contiguous)
- Windows will have drive selection menu under leftmost browser column
- double-click to choose one item and open/save it

Model Manipulation

- left mouse:
  - rotate like grabbing trackball (center of screen)
  - Z axis rotation (edge of screen)
- middle mouse translates
- right mouse scales
- *Mac* ➙ alt=middle, apple=right
- "active" models respond to mouse motion -- controlled in Model Panel or command line
- clip planes controlled with Side View tool
  - grab and drag with mouse
  - grab with middle button will move planes parallel (near plane) or together/apart (far plane)

Making Selections

- *Action/Selection paradigm*
  - Actions menu works on whatever is selected
  - if nothing is selected, Actions work on everything
- *Mouse*
  - control-left click to select
  - control-left drag to region select
  - control-shift-left click/drag to toggle selection status
  - control-click on nothing to deselect everything
- up arrow increases selection to residue/chain/molecule
  - down arrow reverses
- left arrow undoes last selection change
  - shift left arrow clears selection
- right arrow inverts selection (in models with selections)
  - shift right arrow inverts selection in all models
- *Select menu*
  - change Selection Mode to compose more complicated selections
    - *remember to change back when done!*
  - selections can be named so that they are:
    - saved in sessions
    - usable in typed commands
    - retrievable from Named Selections submenu

Working with Selections

- Actions menu allows coloring, labeling, *etc*. of selections
- Focus action centers selection in view and makes it center of rotation
- *Selection Inspector*
  - invoked from Actions menu or button at bottom right of main window
  - shows details of items
  - allows modification of selected items' attributes
- contents of selection can be written to a file from Actions menu or inspector

Color Wells/Color Editor

- gray squares with sunken square centers are color wells
- color wells control the color of an item
- clicking on a color well with bring up the color editor
- *Color Editor*
  - has red/green/blue sliders for controlling color
  - color names that Chimera knows can be typed into text area
  - where appropriate, an Opacity button brings up an opacity slider
  - opacity controls transparency (inversely)
  - No Color button (if present) unsets the items color
- colors can be dragged and dropped between wells or from editor to well

Tool Shortcuts

- tools can be put in the Favorites menu or on a toolbar for quick access
- use Favorites...Add to Favorites/Toobar... menu item
- remember to use Save button to preserve your changes

Command Line

- up arrow retrieves previous command (down arrow the reverse)
- buttons control "activity" (response to mousing) of models

Problems/Questions

- full documentation in Help Menu (User's Guide)
- search documentation with Help...Search Documentation
- use Help menu's Report A Bug/Contact Us items to report problems/ask questions

Distances/Torsions

- tool in Structure Analysis category
- select two atoms or one bond
- shortcuts to set up distance/torsion:
  - *distance*
    - select one atom
    - select second atom (control left shift) but with *double* click
    - choose Show Distance from popup context menu
  - *torsion*
    - select bond but with *double* click
    - choose Rotate Bond from popup context menu

Sequence

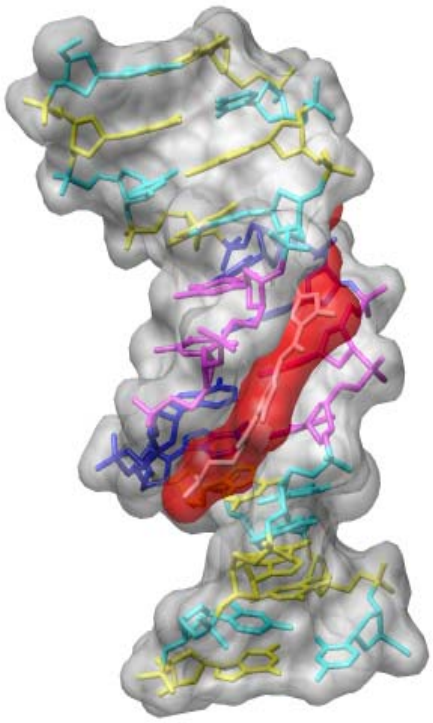
- sequences can be viewed/searched with Tools...Structure Analysis...Sequence

Hydrogen Bonds

- use FIndHBond tool in Structure Analysis category
- creates *pseudobonds* between atoms to depict H-bonds
- use Pseudobond Panel to fine tune depiction or remove the pseudobonds
- ~hbonds command will also remove H-bonds
- Pseudobond Panel is in General Controls category

UCSF Chimera - Getting Started

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.



DNA helix with bound netropsin (6bna)

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.

To follow the tutorial, you will need to access the Protein Data Bank (PDB) files `1zik` and `6bna`. If you have Internet access, these can be fetched directly from the Protein Data Bank, as described below. If you do not have Internet access, you can use the files included in the Chimera distribution. To do so,

1. start Chimera as described below
2. choose **Help→Tutorials** from the Chimera menu
3. click the link for either **Getting Started** tutorial
4. use the links to `1zik.pdb` and `6bna.pdb` to download the files to a convenient location on your computer
5. carry on with the tutorial

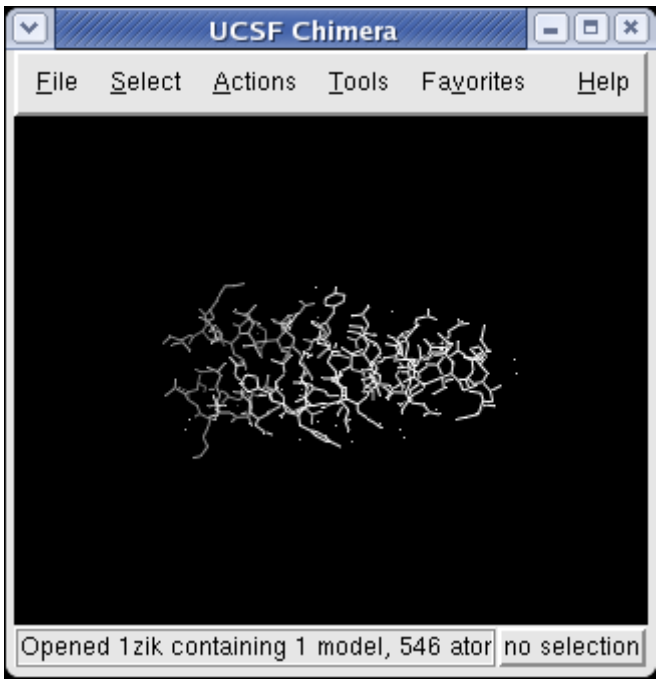
Outline:

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.pdb`	File 1zik.pdb

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

Getting started



UCSF Chimera with 1zik loaded

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.

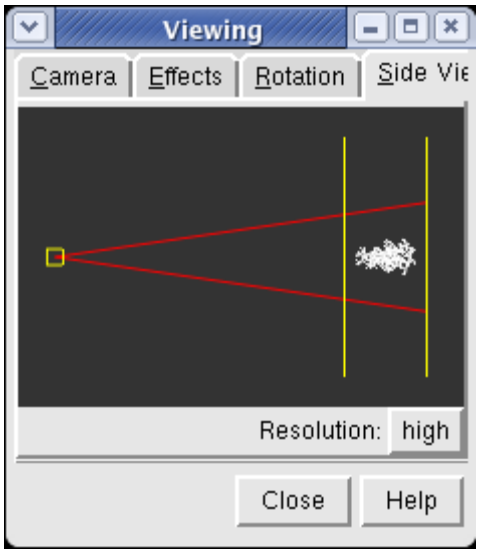
On **Windows**, start Chimera by doubleclicking the Chimera icon in the directory called **bin** in your Chimera installation. If Chimera is installed in `\Program Files` the executable will be in the directory `\Program Files\Chimera\bin`. By default, a Chimera icon will also be placed on your desktop.

On **Mac**, start the Apple X server found in `/Applications/Utilities/X11`, then doubleclick the Chimera application to start. The X server is necessary for running Chimera on the Mac. It is not automatically included in the Mac OS, but can be downloaded (as freeware) from Apple.

A basic Chimera window should appear after a few seconds. Chimera includes a number of tools and dialogs that can be present on the screen at the same time. The basic Chimera window provides the main interactive workspace for displaying and manipulating structures. The default Chimera graphics window is pretty small, so if you like, resize the main Chimera window by placing the cursor on any corner and dragging with the left mouse button.

Opening a structure

Now open a structure. If `1zik.pdb` was downloaded to your machine, choose the menu item **File→Open**. Locate the file `1zik.pdb` in the resulting dialog and open it (the **File type** should be set to **all (guess type)** or **PDB**). If you want to fetch directly from the PDB instead, 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.



Side View showing 1zik

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; scales the view) and the clipping plane positions (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" after you have adjusted them; however, your adjustments have been applied to the main display.

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. On a **Mac** with a one-button mouse, the middle and right buttons can be emulated by combining mouse action with the **option** and ■ (apple) keys, respectively.

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.

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 its contents are reported on the button near the lower right corner of the graphics window.

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. Chimera maintains a hierarchy of objects from atoms to residues to chains to models. If an atom is selected, the ↑ key will broaden the selection to the residue containing that atom. If an entire residue is selected, the ↑ key will broaden the selection to the chain containing that residue. If a chain is selected, the ↑ key will broaden the selection to the 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.

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 its contents are reported on the button near the lower right corner of 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.
Target	Restricts target of the action to certain selected or unselected object types.
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.

Changing the display

To simplify the display, use **Actions→Atoms/Bonds→hide** to undisplay the model followed by **Actions→Atoms/Bonds→chain trace only** to display only the chain trace. The chain trace includes just the α-carbons (atoms named CA), connected in the same way that the residues are connected.

Next, thicken the lines to make them more visible:

Actions→Atoms/Bonds→wire width→3

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

It is now evident that one peptide is chain A, and the other is chain B. To deselect the atoms, pick in a region of the graphics window away from any atoms or use the menu item **Select→Clear Selection**.

Undisplay the residue labels:

Actions→Label→residue→off

Color the two chains different colors:

1zik colored by element

Select→Chain→A
Actions→Color→cyan

Repeat the process to color chain B yellow. As described above, another way to select an entire chain is to pick an atom or bond in the chain and then hit the ⇑ key twice, once to expand the selection to the entire residue and another time to expand it to the entire chain.

There is actually another "chain" in this model, not currently displayed: water. This chain ID was assigned automatically when the structure was read in.

Select→Chain→water
Actions→Atoms/Bonds→show

Alternatively, the water could have been selected using **Select→Structure→solvent** or **Select→Residue→HOH**

To display all atoms of the A chain only:

Select→Clear Selection
Actions→Atoms/Bonds→hide
Select→Chain→A
Actions→Atoms/Bonds→show

Then to show the backbone only,

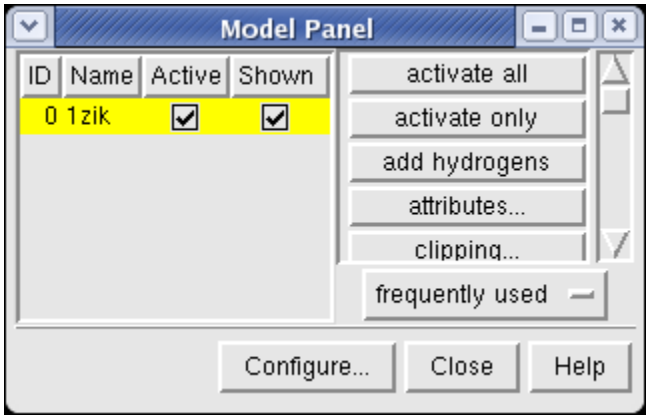
Actions→Atoms/Bonds→backbone only

Only the A chain's backbone is displayed because the A chain was selected when the action was performed.

To display all the atoms and color them according to element:

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

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 (zero). The **Model Panel** shows the current models and enables many operations upon them. Open this tool with **Tools→General Controls→Model Panel**.

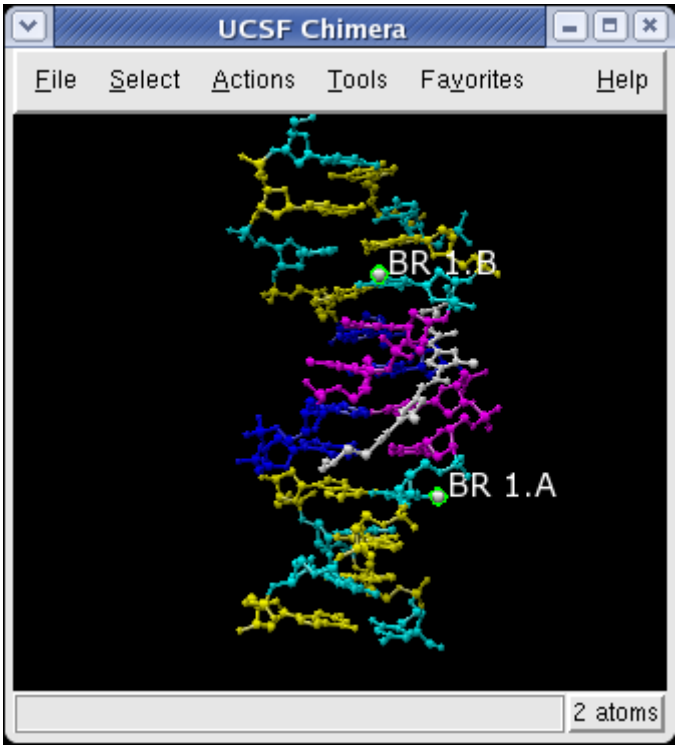
A checkbox in the **Active** column of the **Model Panel** shows that the model is activated for motion; unchecking the box makes it impossible to move. Checking the box again restores the movable state. Make sure the line for `1zik.pdb` (or `1zik`) is highlighted on the left side of the **Model Panel** (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 terminate the Chimera session. A Chimera session may be ended using **File→Quit**.

Working with Menus, Part 2 - Molecular Representations and Surfaces

Setup

With Chimera started and the **Side View** opened as described at the beginning of Part 1, open a different structure. If `6bna.pdb` was downloaded to your machine, choose the menu item **File→Open**. Locate the file `6bna.pdb` in the resulting dialog and open it (the **File type** should be set to **all (guess type)** or **PDB**). If you want to fetch directly from the PDB instead, choose **File→Fetch by ID** and type `6bna` in the **PDB ID** field. The structure contains the molecule netropsin bound to double-helical DNA.



Chimera showing ball & stick (6bna)

Thicken the lines to make them more visible:

Actions→Atoms/Bonds→wire width→3

Color the different nucleotides different colors. For example, color the adenosine residues (adenine nucleotides) blue:

Select→Residue→A
Actions→Color→blue

Analogously, color cytosine nucleotides (C residues) cyan, guanine nucleotides (G residues) yellow, and thymine nucleotides (T residues) magenta. Clear the selection by using **Select→Clear Selection** or picking in a region of the graphics window away from any atoms.

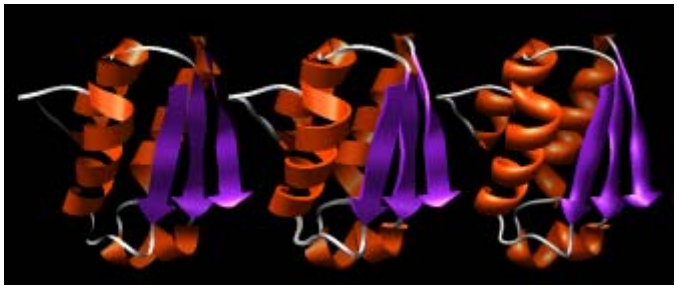
Rotate, translate, and scale the structure as needed to get a better look (see **Using the mouse** to review how this is done). Continue moving and scaling the structure as desired throughout the tutorial. There are still many white atoms, including the netropsin molecule in the minor groove of the DNA and water. Undisplay the water:

1. pick one of the white dots with **Ctrl**-**Btn1** (the white dots are water oxygens; if you cannot see them, first change to a stick representation with **Actions→Atoms/Bonds→stick**)
2. hit the ↑ key once to expand the selection to the entire "chain" water; only one click is needed because the picked atom is equivalent to an entire residue
3. **Actions→Atoms/Bonds→hide**

Representations and labels

Before proceeding, clear the selection. Otherwise, the water will remain selected, potentially causing confusion when menu **Actions** have no visible affect (they affect only the selection, currently the invisible waters).

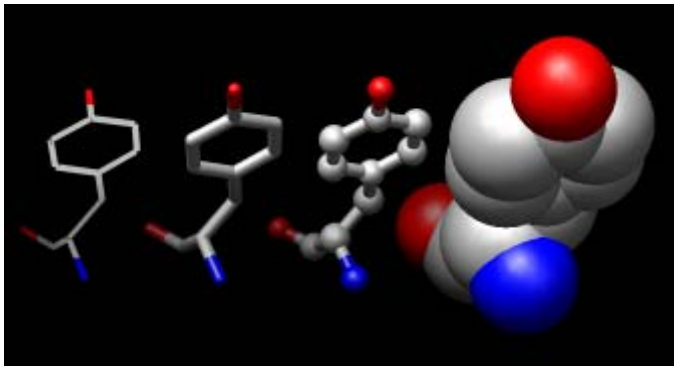
Select→Clear Selection



Ribbon: flat, edged, and round

Now that nothing is selected, the **Actions** menu will affect everything. Try some different molecular representations. They can be translated, rotated, and scaled interactively. Multiple representation types can be combined with each other and with surfaces (more on surfaces below).

Actions→Ribbon→show
Actions→Ribbon→round
Actions→Ribbon→hide
Actions→Atoms/Bonds→stick
Actions→Atoms/Bonds→sphere



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

Change the representation of only one of the DNA strands, chain B:

Select→Chain→B
Actions→Atoms/Bonds→stick
Select→Clear Selection

Next, change everything to a ball-and-stick representation:

Actions→Atoms/Bonds→ball & stick

In this representation, pick one of the atoms in the white netropsin molecule. Label the residue,

Actions→Label→residue→name + specifier

showing that it is named NT and is part of chain het (assigned automatically when the structure was read in). The residue label might not be near the selected atom. Remove the residue label:

Actions→Label→residue→off

The first submenu under **Label** controls individual atom labels, while the second controls residue labels. **Actions→Label→name** would have shown the name of the atom instead of the name of the residue.

Two white atoms that are not part of netropsin are displayed. They are apparently attached to cytosines, which were previously colored cyan. Pick the two atoms and label their residues,

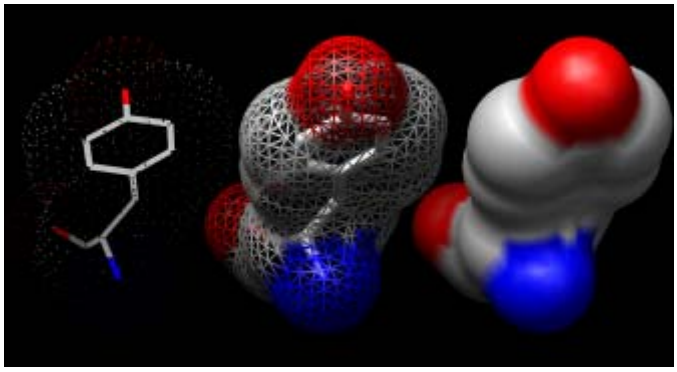
Actions→Label→residue→name + specifier

showing that one DNA strand is chain A, the other strand is chain B, and each strand contains a brominated cytosine. Use **Select→Clear Selection** to deselect the atoms, then undisplay the residue labels:

Actions→Label→residue→off

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**. Surfaces can be translated, rotated, and scaled interactively.



Surface: dot, mesh, and solid

Actions→Surface→show
Actions→Surface→hide
Select→Structure→ligand
Actions→Surface→show
Actions→Surface→mesh

By default, a surface has the same color as the corresponding atoms; however, surface color can be specified separately. To change the surface color only of netropsin only (which is still selected):

1. change the coloring target: **Actions→Color→surfaces**
2. **Actions→Color→red**
3. restore the default coloring target: **Actions→Color→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 nucleotides in chain B only:

1. change the selection mode: **Select→Selection Mode→append**
2. **Select→Residue→A**
3. **Select→Residue→T**
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 :a.b,t.b**

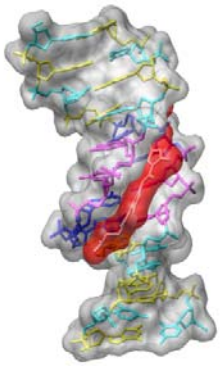
Sometimes it is helpful to make a solid surface transparent:

Actions→Surface→transparency→50%

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

Front image how-to (menu)

Here are the steps to recreate the image at the front of the tutorial:



DNA helix with bound netropsin (6bna)

1. Read in `6bna.pdb` (or fetch `6bna`)
2. Set the representation to "stick":
    - **Actions→Atoms/Bonds→stick**
3. Undisplay the waters:
    - **Select→Chain→water**
    - **Actions→Atoms/Bonds→hide**
4. Color the residues:
    - **Select→Residue→A**
    - **Actions→Color→blue**
    - **Select→Residue→C**
    - **Actions→Color→cyan**
    - **Select→Residue→G**
    - **Actions→Color→yellow**
    - **Select→Residue→T**
    - **Actions→Color→magenta**
    - **Select→Clear Selection**
5. Add a surface to the DNA, color the surface light gray, and make surfaces transparent:
    - **Actions→Surface→show**
    - **Actions→Color→surfaces**
    - **Actions→Color→light gray**
    - **Actions→Surface→transparency→50%**
6. Add a surface to netropsin, color the surface red (it will already be transparent):
    - **Select→Structure→ligand**
    - **Actions→Surface→Show**
    - **Actions→Color→red**
    - **Select→Clear Selection**
7. Rotate and translate as desired
8. Change the background to white:
    - **Actions→Color→background**
    - **Actions→Color→white**
    - **Actions→Color→all of the above**
9. Save the image:
    - **File→Save Image**

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

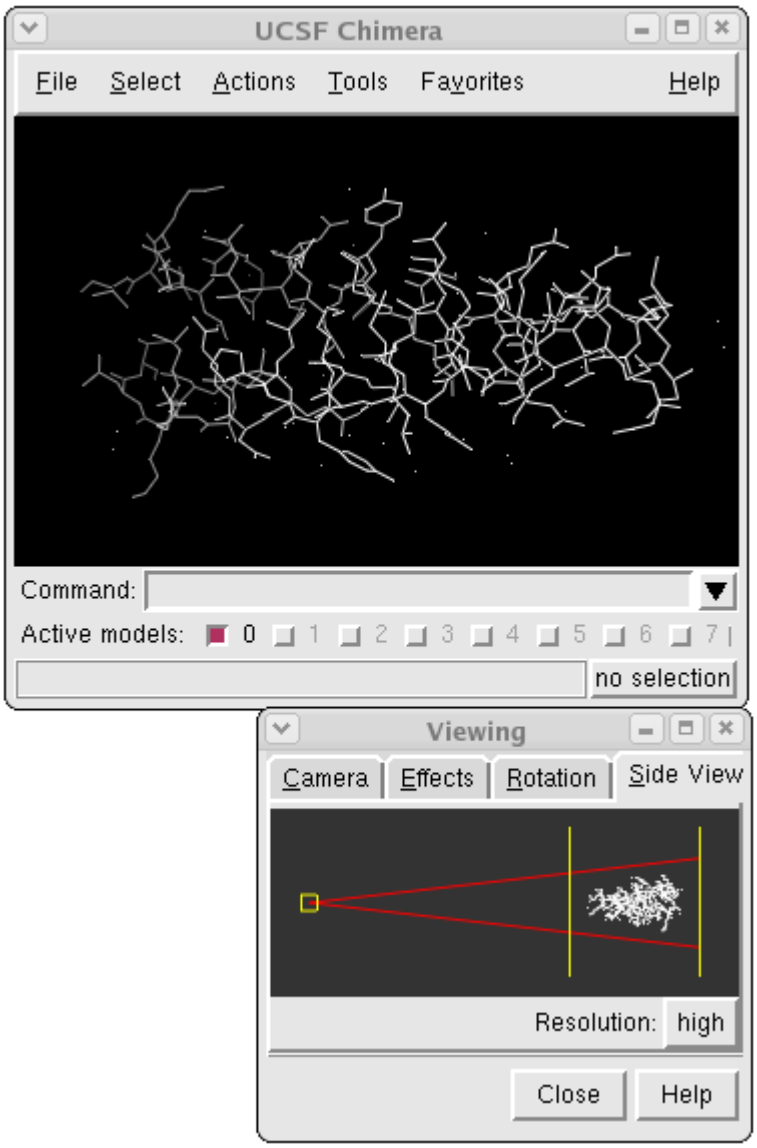
Getting started

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 the Apple X server found in `/Applications/Utilities/X11`, then doubleclick the Chimera application to start. The X server is necessary for running Chimera on the Mac. It is not automatically included in the Mac OS, but can be downloaded (as freeware) from Apple.

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



Chimera with Command Line and Side View

Opening a structure

A local file can be opened from the command line if it is in the working directory (or if the entire pathname is entered):

> *Command*: **open 1zik.pdb**

If the file has been downloaded but is not in the working directory, use **File→Open** instead, as described in **Part 2**.

Alternatively, to fetch 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.

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; scales the view) and the clipping plane positions (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" after you have adjusted them; however, your adjustments have been applied to the main display.

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. On a **Mac** with a one-button mouse, the middle and right buttons can be emulated by combining mouse action with the **option** and ■ (apple) keys, respectively.

Continue moving and scaling the structures with the mouse in the graphics window and **Side View** as desired throughout the tutorial.

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 its contents are reported on the button near the lower right corner of the graphics window.

The arrow keys can be used to broaden (↑), narrow (↓), or invert (→) a selection. The hierarchy for broadening and narrowing selections contains atoms, residues, chains, and models, in that order. 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

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**

would color all atoms, bonds, ribbons, and molecular surfaces 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**.

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.

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 ressidue 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??** selects all residues with three-letter names beginning with G
z<	zone specifier	**z<***zone* or **zr<***zone* spcifies all residues within *zone* angstroms of the indicated atoms, and **za<***zone* specifies all atoms (rather than entire residues) within *zone* angstromgs 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)

Changing the display

To simplify the display:

> *Command*: **chain @ca**

This command shows only the atoms named CA (α-carbons) and connects them in the same way that the residues are connected. Next, thicken the lines:

> *Command*: **linewidth 3**

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**

Each residue label is of the form:

> ***res_name res_number.chain***

It is now evident that one peptide is chain A, and the other is chain B. To deselect the atoms, pick in a region of the graphics window away from any atoms or use the menu item **Select→Clear Selection**. Undisplay the residue labels:

> *Command*: **~rlabel**

Color the two chains different colors:

> *Command*: **color cyan :.a**
> *Command*: **color yellow :.b**

There is actually another "chain" in this model, not currently displayed: water. This chain ID was assigned automatically when the structure was read in.

> *Command*: **disp :.water**

displays the water (only the oxygens are visible in the X-ray structure);

> *Command*: **show :.a**

gets rid of everything except the A chain, but displays all of its atoms;

> *Command*: **chain :.a@n,ca,c**

shows the backbone of the A chain only. If the chain specification "**:.a**" had been omitted, then the backbones of both chains would have been displayed.

Command: **disp**
Command: **color byelement**

displays all the atoms and colors them according to element.

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 (zero). 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** terminate the Chimera session. A Chimera session may be ended using the following command:

Command: **stop**

Working with commands, Part 2 - Molecular Representations and Surfaces

Setup

With Chimera started and the **Command Line** and **Side View** opened as described at the beginning of **Part 1**, open a different structure. If `6bna.pdb` was downloaded to your machine, choose the menu item **File→Open**. Locate the file `6bna.pdb` in the resulting dialog and open it (the **File type** should be set to **all (guess type)** or **PDB**). Alternatively, fetch the structure directly from the PDB:

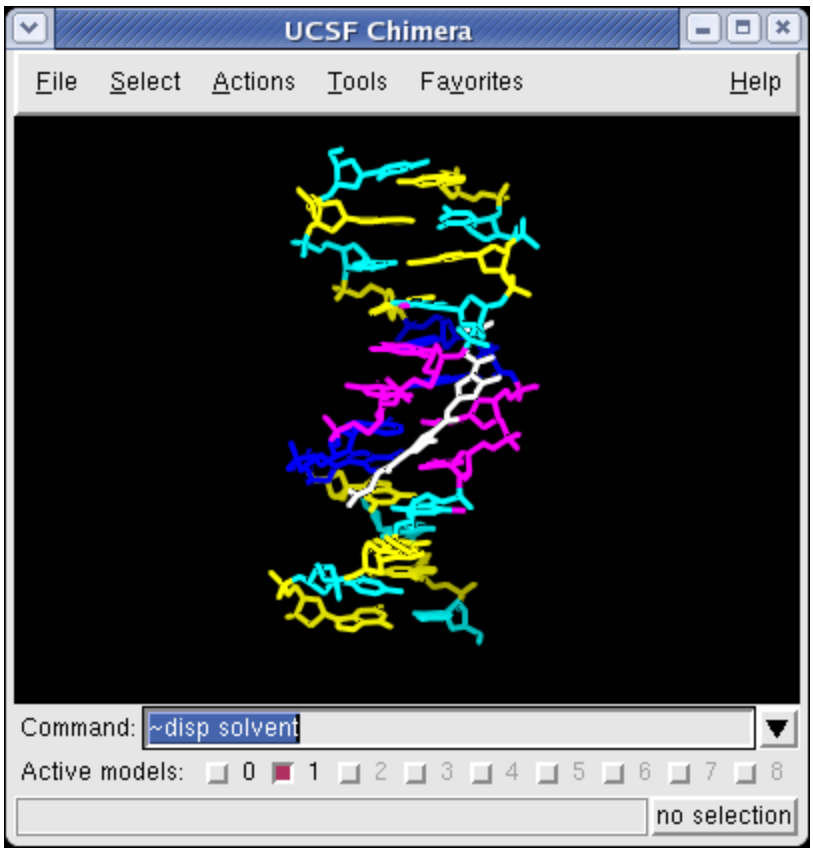
Command: **open 6bna**

The structure contains the molecule netropsin bound to double-helical DNA. Thicken the lines to make them more visible:

Command: **linewidth 3**

Color the different nucleotides different colors, specifying them by residue name:

Command: **color blue :a**
Command: **color magenta :t**
Command: **color yellow :g**
Command: **color cyan :c**



Chimera with Command Line, showing 6bna

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. There are still many white atoms, including the netropsin molecule in the minor groove of the DNA and water. Undisplay the water:

Command: **~disp :.water**
`-`**OR**`- (these are equivalent)`
Command: **~disp solvent**

Representations and labels

Next, try some different molecular representations. They can be translated, rotated, and scaled interactively. Multiple representation types can be combined with each other and with surfaces (more on surfaces below).

Command: **ribbon**
Command: **ribrepr round**
Command: **~ribbon**
Command: **represent stick**
Command: **repr sphere**
Command: **rep stick :.b**

The latter command changes only chain B to the stick representation, with the rest remaining in the sphere representation.

Note that commands (but not their keyword arguments) can be truncated to unique identifiers. 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.

Next, change everything to a ball-and-stick representation:

Command: **repr bs**

In this representation, pick one of the atoms in the white netropsin molecule. Label the residue,

Command: **rlabel picked**

showing that it is named NT and is part of chain het (assigned automatically when the structure was read in). The residue label might not be near the selected atom. Remove the residue label:

Command: **~rlabel**

Two white atoms that are not part of netropsin are displayed. They are apparently attached to cytosines, which were previously colored cyan. Pick the two atoms and label their residues,

Command: **rla picked**

showing that one DNA strand is chain A, the other strand is chain B, and each strand contains a brominated cytosine. Use **Select→Clear Selection** to deselect the atoms, then undisplay the residue labels:

Command: **~rla**

Surfaces

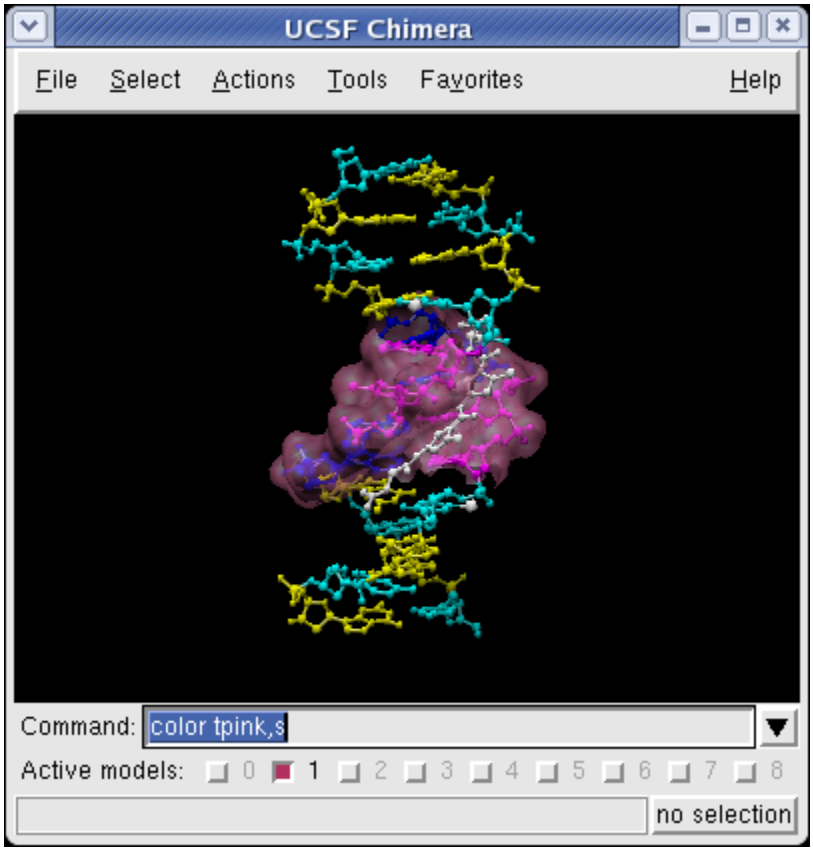
Finally, have some fun with molecular surfaces. There are built-in categories within structures such as **main** and **ligand**; when nothing is specified, **surface** shows the surface of **main**. Surfaces can be translated, rotated, and scaled interactively.

Command: **surface**
Command: **~surface**
Command: **surface ligand**

-**OR**- (these are equivalent)
Command: **surface :nt**
-**OR**-
Command: **surface :.het**

By default, a surface has the same color as the corresponding atoms; however, surface color can be specified separately:

Command: **surfrepr mesh**
Command: **color red,s ligand**
Command: **surfrepr solid**
Command: **~surf**
Command: **surf :a.b,t.b**
Command: **surf :a,t**
Command: **color green,s :t**



Chimera showing a transparent surface (6bna)

Sometimes it is helpful to make a solid surface transparent. One way to do this is to define a transparent color and then use the new color in a command:

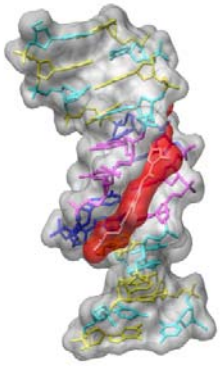
Command: **colordef tpink 1. .5 .7 .4**
Command: **color tpink,s**

The numbers in the **colordef** command refer to red, green, blue, and opacity components, respectively.

Use the command **stop** to terminate the Chimera session.

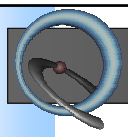
Front image how-to (commands)

Here are the steps to recreate the image at the front of the tutorial:



DNA helix with bound netropsin (6bna)

1. Fetch 6bna:
    - *Command*: **open 6bna**
2. Set the representation to "stick":
    - *Command*: **repr stick**
3. Undisplay the waters:
    - *Command*: **~disp solvent**
4. Color the residues:
    - *Command*: **color blue :a**
    - *Command*: **color cyan :c**
    - *Command*: **color yellow :g**
    - *Command*: **color magenta :t**
5. Add a surface to the DNA, color the surface transparent light gray:
    - *Command*: **surf**
    - *Command*: **colordef tgray .827 .827 .827 .5**
    - *Command*: **color tgray,s**
6. Add a surface to netropsin, color the surface transparent red:
    - *Command*: **surf ligand**
    - *Command*: **colordef tred 1 0 0 .5**
    - *Command*: **color tred,s ligand**
7. Rotate and translate as desired
8. Change the background to white:
    - *Command*: **set bg_color white**
9. Save the image:
    - *Command*: **copy png file ~/Desktop/myfile.png**



Exploring sequence-structure relationships

- Demo of selected tools in the Structure Comparison category
  - Multalign Viewer - sequence alignment viewer with many features, including crosstalk to and from associated structures
  - MatchMaker - constructs pairwise sequence alignments and matches structures accordingly (demo: 1jta, 1bn8, 2pec)
  - Match -> Align - constructs pairwise or multiple sequence alignments based on pre-existing structural superpositions
- Hands-on experience
  - Sequences and Structures tutorial (the online version can be accessed from the Chimera Help menu)

1

Sequences and Structures Tutorial

This tutorial focuses on looking at sequences and structures together using the **Multalign Viewer** extension. Members of the enolase superfamily of enzymes are used to illustrate these features of Chimera. The enolase superfamily has been described in several publications, including:

> P.C. Babbitt, M.S. Hasson, J.E. Wedekind, D.R. Palmer, W.C. Barrett, G.H. Reed, I. Rayment, D. Ringe, G.L. Kenyon, and J.A. Gerlt, "The Enolase Superfamily: A General Strategy for Enzyme-Catalyzed Abstraction of the Alpha-Protons of Carboxylic Acids" *Biochemistry* **35**:16489 (1996).

To follow along with the tutorial, you will first need to download the MSF file super8.msf into your working directory. This file contains a sequence alignment of the barrel domains of eight enolase superfamily members.

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

```
unix: chimera
```

A basic Chimera window should appear after a few seconds. Choose the menu item **Tools... Structure Comparison... Multalign Viewer**. In the resulting dialog, locate and open super8.msf (the file type is **MSF**). A **Multalign Viewer** window containing the alignment will appear. **Multalign Viewer** has its own preferences; choose **Preferences... Layout** from the **Multalign Viewer** menu and change the font size and the sequence-wrapping behavior as desired. Size and place the sequence window and main Chimera window so that both are visible. If the sequence window becomes obscured at any point, it can be raised from the Chimera **Tools** menu (**Tools... MAV - super8.msf... Raise**).

When the mouse focus is in the sequence window, the **Page Down** key (or **space**) moves the alignment view down and **Page Up** (or **Shift-space**) moves the alignment view up. The names of the sequences are shown on the left; a **Consensus** sequence and **Conservation** histogram are shown above the multiple alignment. The superfamily is very diverse; there are very few positions in the alignment in which all the sequences have the same residue (indicated with a red capital letter in the consensus sequence).

The first sequence in the alignment, named **mr**, corresponds to the barrel domain of mandelate racemase from *Pseudomonas putida*. The next-to-the last sequence in the alignment, named **enolyeast**, corresponds to the barrel domain of enolase from *Saccharomyces cerevisiae*. There are multiple structures in the Protein Data Bank for each of these sequences; **2mnr** (mandelate racemase) and **4enl** (enolase) are used in this tutorial.

To open the structures, choose **File... Fetch by ID** from the Chimera menu. In the resulting dialog, check the **PDB ID** option (if it is not already checked) and the option to **Keep dialog up after Fetch**. Enter **2mnr** in the blank marked **PDB ID** and click **Fetch**. Repeat the process to fetch **4enl**, and then click **Close** to dismiss the dialog. Chimera will attempt to find the files within a local installation of the Protein Data Bank. If a file is not found locally, Chimera will try to retrieve it from the Protein Data Bank web site. If this procedure does not work, it may be that you do not have internet connectivity; instead, download the files 2mnr.pdb and 4enl.pdb included with this tutorial and open them in that order as local files (with **File... Open**).

The view is initially centered on a protein colored white, the mandelate racemase structure. Off to the side (and possibly out of view) is the enolase structure, which is colored magenta. Readjust the view to focus on both structures:

Actions... Focus

The structures are not matched in any way; the coordinates are taken straight from the Protein Data Bank. Rotate, translate, and scale the structures as needed to get a better look (see mouse manipulation to review how this is done). If you like, open the **Side View**; choosing **Tools...Viewing Controls... Side View** is one way to do this. Continue moving and scaling the structures as desired throughout the tutorial.

Notice that in the sequence window, the sequence names **mr** and **enolyeast** are now shown in bold within boxes colored white and magenta, respectively. This means that the sequences have been compared with the sequences in the structures, found to match sufficiently well, and automatically associated with the structures. The colors indicate which sequence has been associated with which structure.

The alignment includes just the barrel domains, so it will be simplest to display only a chain trace of these portions. First, open the **Command Line**; choosing **Tools... General Controls... Command Line** is one way to do this. Next, find out which residue numbers in the *structures* correspond to the beginning and end of the alignment. In general, these numbers will not be the same as the numbers marked on the alignment. However, placing the cursor over any residue in a sequence that is associated with a structure gives the corresponding structure residue number near the bottom of the sequence window. In each of the two structure-associated sequences, find out the starting and ending residue numbers by placing the cursor over the first and last residues in the alignment. Doing this reveals that the residue ranges are 134-317 in the mandelate racemase structure and 151-400 in the enolase structure. Display the alpha-carbon chain traces of the barrel domains and increase the linewidth (review atom specification syntax if desired):

```
Command: chain #0:134-317@ca
Command: chain #1:151-400@ca
Command: linewidth 2
```

The sequence alignment can be used to guide a structural match. From the **Multalign Viewer** menu, choose **Structure... Match...** and make 2mnr the reference structure and 4enl the structure to match. Click **Apply** without checking any boxes. This causes the match to use all pairs of alpha-carbons of residues aligned in the sequence alignment. Readjust the view to focus on the structures:

Actions... Focus

The match is fairly rough; the RMSD is 8.4 angstroms (match values are written to the **Reply Log**, **Tools... Utilities... Reply Log**). It is evident that not all of the residues aligned in the sequence alignment are really structurally equivalent. Some loops in enolase (magenta) are much longer than those in mandelate racemase (white). Try the structure matching again, but this time, check the box marked **Iterate by pruning...** and edit the angstrom value to **1.0** before clicking **OK**. This will superimpose only the pairs that collectively match very well in space. Visually, the match is improved; the dissimilar loops were not used in the match.

Next, we will see where some of the conserved residues are within the structures. In the sequence window, use the mouse to drag a column containing the first completely conserved residue in the alignment (the aspartate, D, at alignment position 99). This selects the residues in the associated structures, which then can be displayed:

Actions... Atoms/Bonds... show

Open the **Region Browser** (**Tools... Region Browser** in the **Multalign Viewer** menu). If a sequence region is created by mistake, it can be deleted by clicking on its line and then **Delete** within the **Region Browser**. Create another region (this time, press **Ctrl** along with the mouse button to start a *new* region) for the next

completely conserved residue. This is a glutamate, E, at alignment position 148; display it too:

Actions... Atoms/Bonds... show

The displayed residues point into the center of the barrel, ligating a catalytically important metal ion. Display the Mn++ ion in mandelate racemase:

Select... Chemistry... element... other... Md-Ni... Mn
Actions... Atoms/Bonds... show
Actions... Atoms/Bonds... sphere
Actions... Color... yellow
Select... Clear Selection

Sequence regions can be created automatically. From the **Multalign Viewer** menu, choose **Structure... Secondary Structure... show actual**. This creates regions in the structure-associated sequences named **structure helices** and **structure strands** colored goldenrod and lime green, respectively (yes, these are really named colors). The region names are listed in the **Region Browser**. Clicking on a region in the sequence window (or clicking the **Active** checkbox for that region in the **Region Browser**) will select the corresponding residues in any associated structures. For sequences not associated with structures, **Structure... Secondary Structure... show predicted** creates regions named **predicted helices** and **predicted strands** colored gold and light green, respectively. The GOR method is used for prediction. **Close** the **Region Browser** if it is open.

A structure can be colored according to the conservation in an associated sequence alignment. First, close one of the structures, clear any selections, and show a ribbon for the other structure:

```
Command: close 1
Command: ~select
Command: ribbon
```

Choose **Structure... Render by Conservation** from the **Multalign Viewer** menu. The resulting **Render by Attribute** tool shows a histogram of the residue attribute **mavPercentConserved**, the percent conservation of the most prevalent residue at the corresponding position in the alignment. Adjust the coloring sliders on the histogram (and their **Color** values, if desired) before clicking **Apply**. Coloring the structure by **mavPercentConserved** shows the high conservation of the metal-binding residues and the low conservation of most residues around the outside of the barrel.

The residue attribute **mavConservation** is also listed in the **Render by Attribute** dialog. Its values are those shown in the **Conservation** line in the sequence window. Several different methods for calculating conservation are available. The **Multalign Viewer** **Analysis** preferences (**Preferences... Analysis**) control which method is used. If you wish, try using and visualizing different measures of conservation. After changing any conservation parameters, it is necessary to **Refresh... Histogram/List** in the **Render by Attribute** tool before clicking **Apply**. When finished, **Close** the **Multalign Viewer** preferences and **Render by Attribute**.

See the **Multalign Viewer** documentation for a full description of its many functions, including alignment editing. A number of sequence alignment formats can be read in and (with or without prior editing) written out.

When finished, end the Chimera session:

```
Command: stop
```

Screening docked ligands

- Demo of selected tools in the Surface/Binding Analysis category
  - ViewDock - facilitates screening of ligands output by the program DOCK
  - FindHBond - identifies hydrogen-bonding interactions based on atom types and geometrical relationships
- Hands-on experience
  - ViewDock tutorial (the online version can be accessed from the Chimera Help menu)

1

ViewDock Tutorial

The program DOCK calculates possible binding orientations, given the structures of ligand and receptor molecules. The structure of a physiologically important target molecule can be used to find other molecules that may bind it and modulate (usually inhibit) its function. Generally, one searches a large database of commercially available compounds with DOCK, treating each as a possible "ligand," against the structure of a target protein, treated as the "receptor." Simple scoring methods are used to identify the most favorable binding modes of a given molecule, and then to rank the molecules according to these best orientations. The output consists of a large number of candidate ligands in the binding orientations considered most favorable by DOCK. It is then up to human users to look through the molecules and decide which ones are worth pursuing in the real world. Please consult the DOCK web site for more details.

ViewDock facilitates the selection of compounds by a human user from the output of **DOCK** (versions 3, 3.5, the variant 3.5.x developed in the Shoichet laboratory, 4, and 5). In this tutorial, the results of docking a small database of 30 compounds to the protein H-ras (from Protein Data Bank entry 121P) are used to illustrate the workings of **ViewDock**. See the **ViewDock** manual page for a more formal description of the program.

To follow along with the tutorial, you first need to download the files ras.pdb (the structure of the receptor, H-ras), gto.pdb (the ligand GTO bound to H-ras in the original PDB file, for comparison with docked molecules), ras.mol2 (the docked molecules output by DOCK 4, in Mol2 format), and setup.com (a file containing commands that set up the viewing context) into your working directory.

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

```
unix: chimera
```

A basic Chimera window should appear after a few seconds. If you like, resize it by placing the cursor on any corner and dragging with the left mouse button. Commands are entered into the **Command Line** and scaling and clipping operations can be performed with the **Side View**. One of several ways to start these tools is with **Tools... General Controls... Command Line** and **Tools... Viewing Controls... Side View** in the menu. Tools can be moved to a convenient location on the screen by dragging with the left or middle mouse button when the cursor is placed on the top bar.

First, open the (previously downloaded) structures of the receptor and its co-crystallized ligand. Choose **File... Open**. In the resulting dialog, check the option to **Keep dialog up after Open**. Make sure the **File type** is set to **all (guess type)** or **PDB**, then locate the files. Choose ras.pdb and click **Open**; after that structure appears, open gto.pdb in the same way. Click **Close** to dismiss the dialog.

Next, start **ViewDock** (**Tools... Surface/Binding Analysis... ViewDock**); this brings up a dialog requesting the file of docked ligands (also previously downloaded). Choose and open ras.mol2 (the **File type** is **Dock 4 or 5**). The **ViewDock ListBox** will appear, along with a thicket of molecules in the graphics window. Move the **ListBox** aside if it is obstructing the graphics window or any of the other tools.

Now the receptor is in model 0, GTO is in model 1, and the docked molecules are in model 2 (the lowest available model is used for each successive structure opened, and the file of docked molecules was opened last).

In most cases, one is focusing on a particular target protein and will be viewing many different files of docked molecules; thus, many **ViewDock** sessions will be initiated with the same protein. It can be tedious to set up the same view over and over. One approach is to save a session with the target protein displayed as desired, and then repeatedly restart that session before opening different files of docked ligands with **ViewDock**. Another approach (used in this tutorial) is to put the necessary commands in a file and simply execute the command file as needed.

The command file (setup.com) used in this tutorial contains:

```
color aquamarine #0
chain #0@ca
disp #0 & #2 z<5
color orange #0@o=
color medium blue #0@n=
repr bs #1
color magenta #1
color byatom #2
```

These commands color the receptor (model #0) aquamarine, simplify it to an alpha-carbon trace, and then display all atoms for only the residues within 5 angstroms of any docked molecule. Oxygen atoms in the receptor are colored orange, nitrogens medium blue. The co-crystallized ligand GTO (#1) is shown in magenta ball-and-stick and the docked molecules (#2) are colored by atom type.

If setup.com is in the working directory, enter the following in the **Command Line** (indicated here by *Command*:):

```
Command: open setup.com
```

If setup.com is not in the working directory, use **File... Open**, uncheck the box to **Keep dialog up after Open**, set the file type to **all (guess type)** or **Chimera commands**, and browse to the file and open it. Opening the command file executes its contents; this may take a few seconds.

Throughout the tutorial, adjust the view as desired with the mouse and **Side View**. Show the docked molecules as sticks to make them more prominent:

```
Command: repr stick #2
```

Most of the compounds are docked into the active site, as indicated by the co-crystallized ligand GTO (magenta). Undisplay GTO:

```
Command: ~disp #1
```

The docked compounds are enumerated in the top part of the **ViewDock ListBox**. If the **ListBox** has become obscured by other windows, it can be resurrected with **Tools... ViewDock** (near the bottom of the menu, below the horizontal line)**... Raise**. Since in this case **Name** is not very informative, it may be helpful to add other descriptors to the listing. Use the **Column** menu to show **Description** and **Energy score**, and to hide **Name** and **Number**.

Clicking on a line ***chooses*** the corresponding compound: the line is highlighted, just the chosen compound is shown in the main graphics window, and more detailed information is shown in the lower part of the **ListBox**. Try clicking various lines in the **ListBox** to choose different docked molecules. Multiple compounds may be chosen at once. **Ctrl**-click adds to an existing choice rather than replacing it. To choose a block of compounds without having to hold down the mouse button,

click on the first (or last) and then **Shift**-click on the last (or first) in the desired block.

The listing can be sorted by any column, by clicking on the header. Make sure the list is sorted by **Energy score**, with the most negative values (which are the most favorable) at the top. Scroll down to the lowest line in the top panel of the **ListBox** and click on it to choose the worst-scoring molecule. The following command can be used to locate this molecule if it is outside the view:

```
Command: window
```

This compound is not docked in the active site like the others, and its docking scores are zero.

There are three mutually exclusive states that can be assigned to docked compounds. **Viable** compounds are interesting (or have not been looked at yet), **Deleted** compounds are less interesting but may deserve another look, and **Purged** compounds are definitely not interesting. The **S** column shows **V**, **D**, and **P** to indicate these states. Viable and deleted but not purged molecules are included when **File... Rewrite** is used. Change the status of the worst-scoring molecule to purged by clicking the **Purged** checkbox near the bottom of the **ListBox**. Note that its listing disappears; make it reappear by checking the box next to **List Purged** in the **Compounds** menu.

Normally, a user will click on successive lines, examine the compounds in the binding site, and change the status of less interesting compounds to deleted or purged. Compounds can also be chosen by descriptor values and then changed in status collectively. Several sessions may be needed to whittle the list down sufficiently.

As an example, choose compounds based on their hydrogen-bonding interactions with the receptor. **HBonds... Add Count to Entire Receptor** will bring up the **FindHBond** tool; make sure the **inter-model** mode is set and increase the **Line width** to 3 (the detected hydrogen bonds will be shown as lines). Click **OK**. When the calculation is finished, new columns of descriptors will appear in the **ListBox**. Again, individual compounds can be examined by clicking on their respective lines in the **ListBox**. Use the **Column** menu to hide the descriptors **HBond Ligand Atoms** and **HBond Receptor Atoms** (the numbers of ligand and receptor atoms, respectively, participating in the detected ligand-receptor hydrogen bonds).

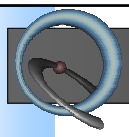
Compounds... Choose by Value opens an interface with several sections. Choose from **Viable** compounds and uncheck the boxes next to **Description** and **Energy score** to collapse the corresponding sections. In the **HBonds (all)** section, move the sliders to include 0-1 hydrogen bonds. A message near the top of the **Choose by Value** dialog will report that 17 of the 29 viable compounds meet the criteria. Click **OK** to choose the compounds and dismiss the dialog. The 17 viable compounds with 0-1 hydrogen bonds to the receptor will be chosen in the **ListBox** and displayed in the main Chimera window. Change these compounds to purged by clicking the **Purged** checkbox near the bottom of the **ListBox**. Uncheck the box next to **List Purged** in the **Compounds** menu to remove the purged compounds from the listing.

Finally, we will flip through the remaining listed compounds with the **Movie** feature. First, place a surface on the binding site (receptor residues within 7 angstroms of GTO; this may take a minute):

```
Command: surf #0 & :gto z<7
```

The surface can be made transparent with **Actions... Surface... transparency... 60%** (in the main Chimera menu). **Movie... Play** (back in the **ListBox** menu) flips through all of the listed compounds, in the order in which they are listed, regardless of status. It is possible to change the view and move

the molecules around while the movie is playing. The movie will loop continuously through the list until halted with **Movie... Stop**. The length of time each compound is shown can be controlled with **Movie... Options**. If molecules are "unlisted" using the checkboxes in the **Compounds** menu, they are not included in the movie; in addition, the order of display depends on how the molecules are sorted. No matter how the molecules are sorted in the **ListBox**, however, they remain in the original order (minus any purged compounds) in output files created with **File... Rewrite**. Once you have seen enough, stop the movie and exit from Chimera.



MD trajectories and structural ensembles

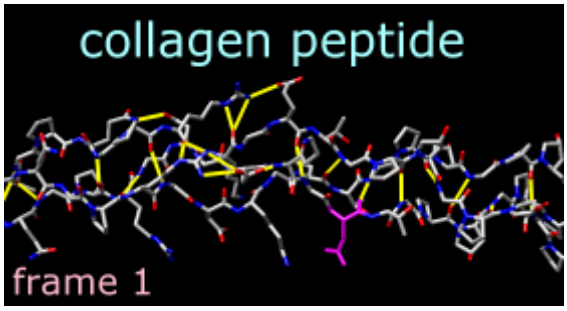
- MD Movie (this tool is in the MD/Ensemble Analysis category)
  - Demo: trajectory playback/recording, holding structural elements “steady”, RMSD calculations, generation of occupancy maps
- Hands-on experience
  - Trajectory and Ensemble Analysis tutorial (the online version can be accessed from the Chimera Help menu)

1

Trajectory and Ensemble Analysis Tutorial

This tutorial focuses on visualization and analysis of molecular dynamics (MD) trajectories and other structural ensembles with the **MD Movie** tool. Part 1 uses an MD trajectory of a collagen peptide, and Part 2 uses an NMR ensemble of Met-enkephalin.

Part 1 - Collagen Peptide



We will view an MD trajectory of the nonmutant collagen peptide described in:

> R. J. Radmer and T. E. Klein, "Severity of Osteogenesis Imperfecta and Structure of a Collagen-like Peptide Modeling a Lethal Mutation Site" *Biochemistry* **43**:5314 (2004).

(Thanks to the authors for providing the data!) To follow along, download the data files:

- leap.top - AMBER parameter/topology file
- md01.crd - AMBER trajectory file
- collagen.meta - metafile specifying these input files for **MD Movie**

Click the **chimera** icon; a basic Chimera window should appear after a few seconds. Show the **Command Line** (**Tools... General Controls... Command Line**) and start **MD Movie** (**Tools... MD/Ensemble Analysis... MD Movie**). In the resulting dialog, the inputs can be specified in two different ways:

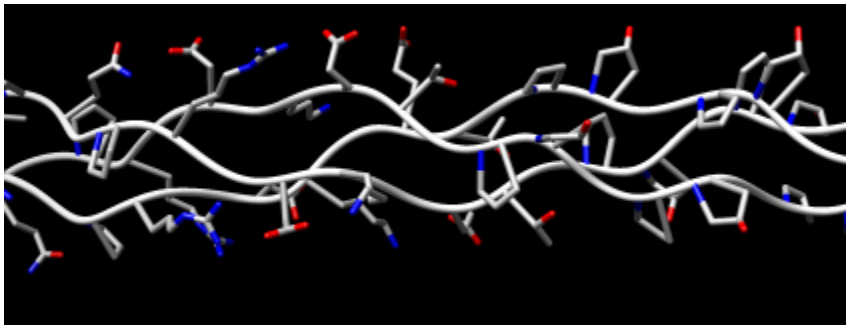
- by setting the **Trajectory format** to **Amber** and browsing to the **Prmtop** file leap.top and the **Trajectory** file md01.crd
- by setting the **Trajectory format** to **metafile** and browsing to the file collagen.meta (it must be in the same directory or folder as the other two files). It contains the following lines, which simply specify the options and filenames that would otherwise be entered into the dialog:

```
amber
leap.top
md01.crd
```

Once the inputs have been specified, click **OK**. The first set of coordinates will be displayed and the **MD Movie** controller will appear. Show the structure with sticks and ribbons, color by element, and

undisplay the hydrogens:

```
Command: repr stick
Command: ribbon
Command: ribrepr smooth
Command: col byelement
Command: ~disp H
```



Move and scale the structure as desired throughout the tutorial. The structure contains three chains. Each chain is in a left-handed polyproline II helix conformation, and together the chains form the right-handed triple helix characteristic of fibrillar collagen. The ribbons are narrow because the peptides are not in a standard alpha-helical conformation.

MD Movie controller buttons

Use the **MD Movie** controller to play the trajectory. From left to right, the buttons mean: play backward continuously; go back one step; stop; go forward one step; and play forward continuously. The rate of continuous play can be adjusted with the **Playback speed** slider. The **Frame** number is reported and can also be entered directly to view a specific frame. **Frame** number and **Step size** changes take effect when return (**Enter**) is pressed. If the controller becomes obscured by other windows, it can be raised using its instance in the **Tools** menu (near the bottom of the menu, below the horizontal line).

Show the sequence with **Tools... Structure Analysis... Sequence**. Fibrillar collagen typically contains many -Gly-X-Y- repeats, where X is often Pro (proline) and Y is often Hyp (hydroxyproline). Both Pro and Hyp are shown as P in the sequence panel. Mousing over the sequences shows that the residues in the peptides are numbered 1-34, 35-68, and 69-102, respectively. Selecting residues highlights both the sequences and the structures:

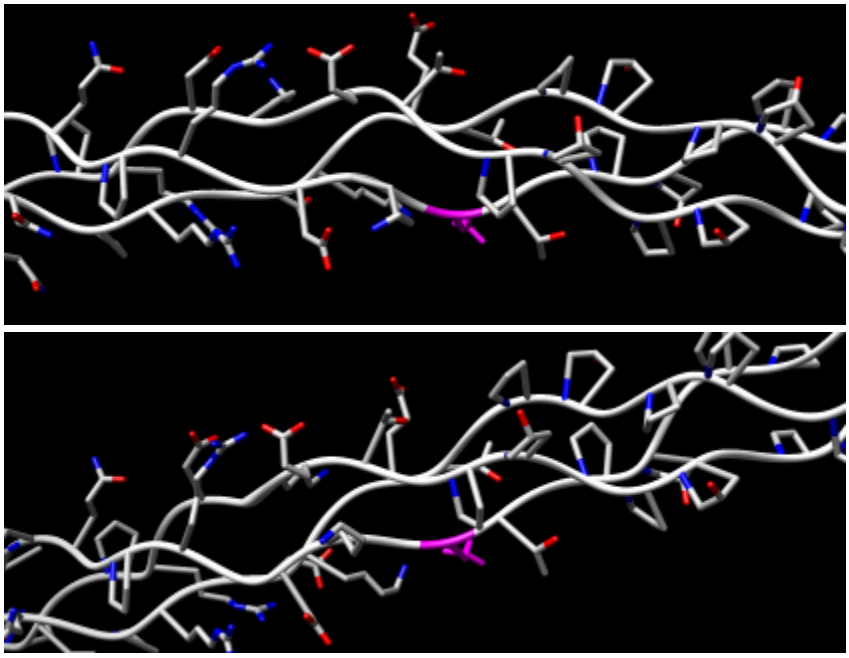
```
Command: sel :gly
Command: sel :pro
Command: sel :hyp
```

Close the sequence panel.

It may be useful to hold certain atoms steady during trajectory playback. For example, hold Glu-86 steady to view its interactions:

Command: **sel :86**
(from the controller menu) **Actions... Hold selection steady**
Command: **color magenta sel**
Command: **~sel**

Residue 86 held steady



Even though it is no longer selected, residue 86 will be held steady during playback (as possible; there will still be internal motions) until **Hold selection steady** with a different selection or **Stop holding steady** is used. The structure can still be moved with the mouse, however. Try playing the trajectory with residue 86 held steady and then without holding any atoms steady (from the controller menu, choose **Actions... Stop holding steady**).

We will create a short movie of several frames in the trajectory. The following procedure is just one example; there are many possibilities of what to show, how to show it, whether to use a script, and so on.

Adjust the Chimera window to the dimensions desired for the movie. If needed, use the **Side View** (**Tools... Viewing Controls... Side View**) to adjust the clipping planes. Turn off the ribbon to reveal the backbone atoms:

Command: **~ribbon**

Use **2D Labels** to add a title (**Tools... Utilities... 2D Labels**). When the **Mouse** setting in the **2D Labels** dialog is **labeling**, the left mouse button (button 1) is reassigned to labeling: clicking starts a new 2D label and previously created 2D labels can be repositioned by dragging. Click in the Chimera window where you would like to start a title and type in the title text; drag the text if you want to reposition it. Adjust the **Font size** and **Color** (click the color well, use the **Color Editor**) to your liking. Changing the **Mouse** setting to **normal** returns the left mouse button to its previous function (by default, rotation of models).

Create another 2D label, this time using the **2dlabels** command so that the label will have a name:

Command: **2dlabels create mylabel text temp**

This label will be used to display the frame number. Make sure that the **Mouse** setting in the **2D Labels** dialog is **labeling**, then drag the temporary text to near the lower left corner of the Chimera window. Adjust its **Font size** and **Color** to your liking, then **Close** the **2D Labels** dialog.

Next, define a script to execute at each frame. Halt any playback. From the **MD Movie** controller menu, choose **Per-Frame... Define script**. Enter a script to be interpreted as **Chimera commands**:

```
findhbond linewidth 2 color yellow
2dlabels change mylabel text "frame <FRAME>"
```

Uncheck the option to **Use leading zeroes...** This script will calculate the hydrogen bonds in each frame, show them as yellow lines, and display the current frame number in the label named **mylabel**. Click **OK** to dismiss the dialog with the script. Play a few steps by clicking the button to go forward or backward one step at a time. The number and arrangement of H-bonds vary somewhat from step to step. (Although the number of H-bonds cannot be accessed in **Chimera commands**, a **Python** script could be used to display this information. For example, hbcount.py would show the H-bond count instead of the frame number in **mylabel**.)

Halt any playback, but move the **Playback speed** slider all the way to the right. From the controller menu, choose **File... Record movie**. If a dialog with an MPEG license agreement appears, click **Accept** since the movie will not be used for commercial purposes. In the dialog for recording, choose a **File type** you will be able to play back on your computer (the choices are MPEG-1, MPEG-2, MPEG-4, and Quicktime). Change the **Ending frame** to 25, specify a convenient name and location for the output file, and click **Record**. Frames 1-25 will then be played, saved as images, and automatically assembled into a movie file. (***Do not obscure any parts of the Chimera window while this is occurring***.) View the resulting 1-second movie with the appropriate application on your computer.

Click **Quit** on the controller to close the trajectory and exit from **MD Movie**. Go on to **Part 2** below, **OR** terminate the Chimera session:

```
Command: stop
```

Part 2 - Met-Enkephalin

We will view an NMR ensemble of Met-enkephalin in negatively charged bicelles, as described in:

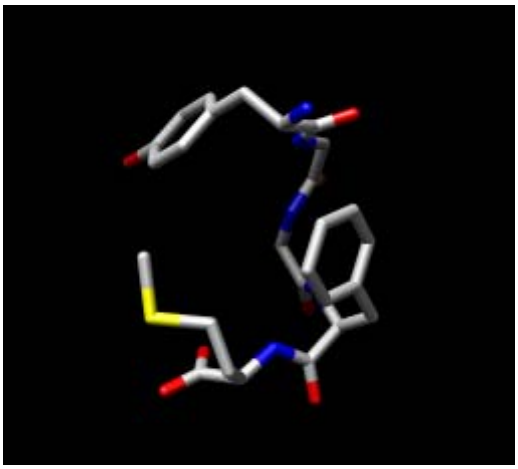
> I. Marcotte, F. Separovic, M. Auger, and S. M. Gagne, "A Multidimensional ^{1}H NMR Investigation of the Conformation of Methionine-Enkephalin in Fast-Tumbling Bicelles" *Biophys J* **86**:1587 (2004).

To follow along, download the data file 1plx.pdb.

With Chimera started and the **Command Line** shown (as in Part 1), choose **Tools... MD/Ensemble Analysis... MD Movie**. In the resulting dialog, choose **PDB** as the **Trajectory format** and indicate that the frames are contained in a **single file**. Browse to the file 1plx.pdb, then click **OK** (alternatively, a metafile in the same directory as 1plx.pdb could have been used).

The first set of coordinates will be displayed and the **MD Movie** controller will appear. Show the structure with sticks colored by element:

```
Command: repr stick
Command: col byelement
```



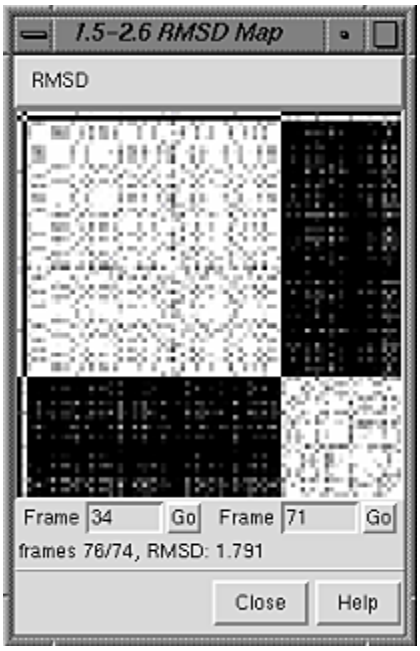
Move and scale the structure as desired throughout the tutorial. This structure is Met-enkephalin, with the sequence Tyr-Gly-Gly-Phe-Met. Enkephalins are neuropeptides that activate opioid receptors. Different subtypes of opioid receptors mediate different but overlapping responses in the body. For example, molecules that selectively activate μ-opioid receptors are more effective for treating severe pain than molecules that selectively activate δ-opioid receptors, but are also more likely to cause constipation. The conformations of molecules that bind opioid receptors (enkephalins, morphine, *etc.*) are of interest because they influence the selectivity of receptor binding and thus the physiological response.

Use the **MD Movie** controller to flip through the different conformations, as described above. The frames do not reflect time ordering, as this is an NMR ensemble rather than a trajectory. If desired, simplify the view by undisplaying hydrogens:

```
Command: ~disp H
```

It is thought (see the reference and papers cited therein) that a conformation of enkephalin in which the Tyr and Phe rings point in different directions (like frames 1 and 25) binds to μ-opioid receptors and a conformation in which they point toward each other (like frames 2 and 80) binds to δ-opioid receptors.

One way to analyze the ensemble is to calculate root-mean-square deviations (RMSDs) between pairs of frames. From the controller menu, choose **Analysis... RMSD map**. Click **Apply** on the RMSD parameters dialog to perform the calculation without closing the dialog. This will compute all pairwise RMSDs between frames and show the result as a map in grayscale. After the initial calculation, the map will be recolored to enhance contrast.



In the RMSD map, the axes are frame numbers; lighter squares reflect pairs of frames with lower RMSDs (more similar structures) and darker squares reflect pairs of frames with higher RMSDs (less similar structures). Mousing over the map shows the RMSD values and the numbers of the frames being compared. Clicking on the map enters the corresponding pair of **Frame** numbers below the map. Clicking **Go** then displays that frame in the main Chimera window.

Roughly, the upper left block of white in the map represents conformations more similar to to a μ-binding conformation, and the lower right block of white represents conformations more similar to a δ-binding conformation. Similar conformations are mostly grouped together in this ensemble, but will not necessarily be grouped together in ensembles in general. Also, ensembles usually contain many more groups of conformations, especially for larger structures with more degrees of freedom.

All atoms were used in the RMSD calculation, because although the parameter **Restrict map to current selection, if any** was set to **true**, nothing was selected. Select the nonhydrogen backbone atoms only,

> *Command*: **sel** **@n,ca,c,o**

and this time click **OK** to dismiss the RMSD parameters dialog and perform the calculation. Although the two maps span different ranges in RMSD, they reveal essentially the same groups of conformations. **Close** both maps.

Another way to analyze the ensemble is to calculate spatial occupancy maps for atoms of interest. From the controller menu, choose **Analysis... Calculate occupancy**. The resulting dialog will show the warning message "No atoms being held steady." This means you have not previously selected a set of atoms and chosen **Actions... Hold selection steady** from the controller menu for this ensemble.

Why might it be useful to hold atoms steady while calculating occupancy? The contents of different frames may move around enough to obscure certain spatial patterns. Even if the structure as a whole is held fairly steady, one may want to hold a particular set of atoms (such as a sidechain) steady to examine local interactions. However, if the structure or region of interest is already sufficiently steady, the "hold steady" step can be omitted.

One approach to analyzing the relative positions of the aromatic rings is to hold the Phe ring atoms steady and map the occupancy of the Tyr ring atoms:

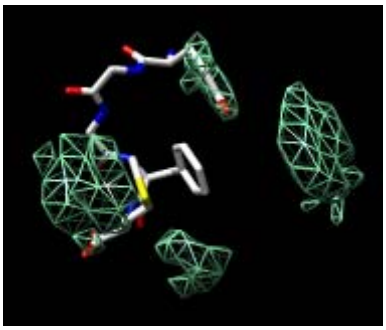
1. Select the six Phe ring atoms. One way is to pick them from the screen (Ctrl-click on one, Shift-Ctrl-click on each of the other five). Another way is with the command:

   ```
   Command: sel :phe & aromatic ring
   ```

   (the intersection of PHE residues with aromatic ring atoms)
2. Choose **Actions... Hold selection steady** from the controller menu.
3. Select the six Tyr ring atoms, by picking or with the command:

   ```
   Command: sel :tyr & aromatic ring
   ```

4. If the occupancy dialog is not already up, choose **Analysis... Calculate occupancy** from the controller menu.
5. Click **OK** on the occupancy dialog.



When the map has been computed, the **Volume Viewer** tool will appear. This tool shows a histogram of the values in the map; the slider controls what contour level is displayed.

Clear the selection in Chimera (**Select... Clear Selection**). In the **Volume Viewer** tool, change from **surface** to **mesh** and move the slider to a value of approximately 2. Use the **Side View** (**Tools... Viewing Controls... Side View**) to move the clipping planes so that all of the mesh is visible. Optionally, change the color of the mesh surface by clicking the color well below the histogram and using the **Color Editor**. (**Volume Viewer** is complex tool with many features. For more on this tool, see the **Volume Viewer** manual page and the Chimera tutorials on the web.)

You will see four main blobs or volumes representing probable positions of the Tyr ring relative to the Phe ring (similar to the upper image, which also shows frame 2). The two larger volumes represent μ-type conformations and the two smaller volumes represent δ-type conformations. The volume pairs are related by approximately 180-degree flips of the Phe ring. Although the atom pairs CD1/CD2 and CE1/CE2 in the Phe ring are chemically equivalent, each atom is distinguishable by name and is treated as distinct for holding steady.

If desired, flip through the ensemble (still holding the Phe ring steady) to verify that the volumes show areas occupied by the Tyr ring. To delete the volume display, choose **File... Close data** from the **Volume Viewer** menu.

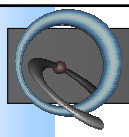
Finally, calculate a map without holding any atoms steady. Choose **Actions... Stop holding steady** from the controller menu. Since this ensemble maintains the Tyr ring in roughly the same place, simply map the occupancy of the Phe ring atoms. Select the Phe ring atoms (as above), choose **Analysis... Calculate occupancy**, and click **OK**. This time, the conformations are not as well separated; two lobes of occupancy are apparent at a contour level of approximately 2 (similar to the lower image, which also shows frame 2). One lobe represents μ-type conformations and the other represents δ-type conformations.

When finished with the Met-enkephalin ensemble, quit from Chimera (**File... Quit**).

RBVI

Displaying, Defining and Calculating Attributes

Conrad Huang



Overview

- What are attributes?
- Depicting attributes graphically
- Selecting atoms, residues and molecules using attribute values
- Using Chimera tools to add new attributes
- Defining your own attributes

What Are Attributes?

- Attributes are values associated with atoms, residues and molecules
- Chimera knows a lot about some of them
  - Atomic coordinates for graphical display
  - Atom specifiers
- Chimera knows little about others
  - Only name and value
  - For example, PDB files include temperature factor and occupancy for atoms
  - Tools for manipulating these attributes can:
    - depicting attributes graphically (e.g., by color)
    - select atoms with chosen range of attribute values

3

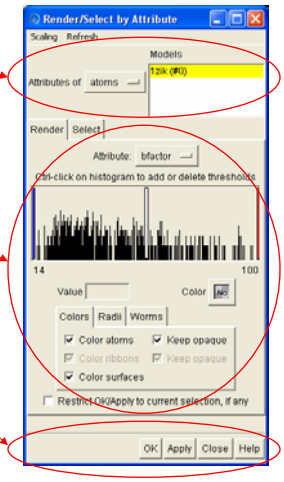
Using Attributes

- Graphical interface
  - **Tools → Structure Analysis → Render by Attribute**
- Command line interface
  - Atom specifier
    - color blue @/bfactor > 50
    - select @ca/bfactor < 50
  - Command
    - rangecolor bfactor 0 blue 50 yellow 75 red
  - Both
    - rangecolor bfactor 0 blue 50 yellow 75 red @ca

4

Render by Attribute

- Top section selects which attributes to use
- Middle section sets action type (changing graphical rendering or selection) and parameters
- Bottom buttons apply the action and/or closes the panel

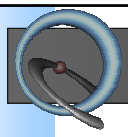


5

Changing Graphical Rendering

- Change colors
  - Select attribute to map
  - Use histogram to select thresholds and associated colors
    - Control-click to add or remove thresholds
  - Choose which colors (atoms, ribbons and/or surfaces) to change
    - "Keep opaque" discards transparencies in colors specified in histogram
    - If some atoms have no values for the selected attribute, a, you can choose the default color for these atoms
  - Click "Apply" to update display

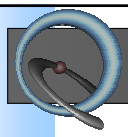
6



Changing Graphical Rendering

- Changing atomic radii
  - Select attribute to map
  - Use histogram to select thresholds and associated radius
    - Control-click to add or remove thresholds
  - Choose atom rendering style
    - If some atoms have no values for the selected attribute, a, you can choose whether radii of these atoms should change, and (if yes) the default radius
  - Click “Apply” to update display

7



Changing Graphical Rendering

- “Worms”
  - Displaying ribbons whose size is a function of attribute values
    - Only works with residue attributes
  - Use histogram to select thresholds and associated radius
    - Control-click to add or remove thresholds
  - Choose ribbon rendering style
    - Choose “non-worm” to go back to default ribbons
  - Click “Apply” to update display

8

Changing Selection

- Click the “Select” tab
- Use histogram to set a minimum and a maximum value
- Choose whether values between or outside the extrema should be selected
- Click “Apply” to update selection

9

Adding Attributes

- Some attributes (e.g., temperature factor) are read in as part of data files
- Chimera has tools that add attributes to open models:
  - MAV adds “mavPercentConserved” attribute
  - “Tools → Surface/Binding Analysis → Surface Area/Volume” adds surface area and volume attributes using the NCBI StrucTools server
- Once created, these attributes can be manipulated the same way as read-in attributes

10

Adding Your Attributes

- Attributes can be added using a text file with information on attribute name and what objects (atoms, residues or models) are affected
- Atom specifiers are used to assign values to matching objects

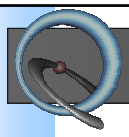
```
# Assign atomic weights to atoms
attribute: aw
match mode: any
recipient: atoms
        @/element="H"    1.00794
        @/element="C"    12.0107
        @/element="N"    14.0067
        @/element="O"    15.9994
        @/element="P"    30.973761
        @/element="S"    32.06
```

11

Adding Your Attributes

- Graphical interface
  - **Tools → Structure Analysis → Define Attributes**
- Command line interface
  - defattr *filename*
  - defattr *filename* spec *atom_specifier*

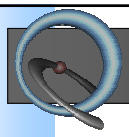
12



Calculating Attributes

- Attributes can be created by combining other attributes using **Tools → Structure Analysis → Attribute Calculator**
- Currently, only arithmetic operators, sum and average are supported

13



Summary

- Chimera has tools for manipulating "generic" attributes
  - Tools are in category **Structure Analysis**
  - **Render by Attribute** may be used to change graphical rendering and to select atoms, residues and models
  - **Define Attributes** and **Attribute Calculator** may be used to add new attributes

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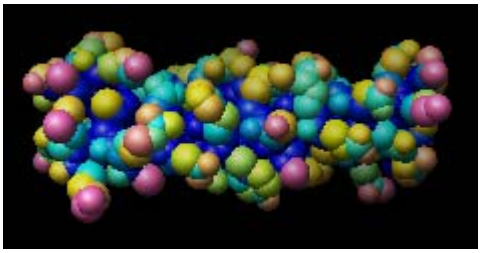
Attributes Tutorial

This tutorial demonstrates many uses of attributes, or properties of atoms, residues, and molecule models. Attributes can be numerical (such as atomic number), boolean (*e.g.*, whether a residue is an alpha-helix), or string-valued (such as atom type). Attribute values can be rendered visually and used in selection and command-line atom specification.

Part 1 uses a leucine zipper structure, and Part 2 uses the structure of a GTP-binding protein.

Attributes, Part 1 - Leucine Zipper

1zik colored by accessibleSurface



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

```
unix: chimera
```

A basic Chimera window should appear after a few seconds. Open the **Command Line** (choosing **Tools... General Controls... Command Line** is one way) and, if desired, the **Side View** for clipping and scaling.

If you have internet connectivity, structures can be obtained directly from the Protein Data Bank. Choose **File... Fetch by ID** from the Chimera menu. In the resulting dialog, check the **PDB ID** option (if it is not already checked) and fetch the PDB structure **1zik**. If you do not have internet connectivity, download the file 1zik.pdb included with this tutorial and use **File... Open** to open it.

The structure is a leucine zipper formed by two peptides. Undisplay water, change to a stick representation, and color by element:

```
Command: ~disp solvent
Command: repr stick
Command: color byelement
```

Move and scale the structure as desired throughout the tutorial.

Open the **Render by Attribute** tool (**Tools... Structure Analysis... Render by Attribute**). It is initially set to show the attributes of **atoms**. Look in the **Attribute** list to see the attributes available: **bfactor** and **occupancy**, which were read from the input PDB file. Choose **bfactor**; a histogram of the values will appear, with blue, white and red markers (or thresholds). Click **Apply** to color the atoms blue to white to red in order of increasing B-factor. You can define your own color mapping by adding and deleting thresholds (Ctrl-clicking an existing one deletes it; Ctrl-clicking elsewhere on the histogram adds one), moving them along the histogram, and/or changing their colors. The **Value** and **Color** are shown for the most recently clicked or moved threshold. The **Value** changes when the threshold is moved, or the position can be changed by entering a value and pressing return. The **Color** can be changed by clicking the adjacent color well. If you wish, try applying different color mappings. As expected, the atoms with higher B-factors are on the outside of the structure. Note that the histogram includes the B-factor values of the waters even though they are not displayed. Display waters with B-factors less than 75:

```
Command: disp solvent & @/bfactor<75
```

Next, change to the attributes of **residues** in the **Render by Attribute** dialog. The automatically available attributes are **kdHydrophobicity** and average **bfactor** and **occupancy**. The latter two are residue averages over the atomic values. Choose **kdHydrophobicity**, the Kyte-Doolittle hydrophobicity values of amino acid residues: negative values correspond to more polar residues and positive correspond to more hydrophobic residues. Undisplay atoms and show a ribbon:

```
Command: ~disp
Command: ribbon
```

Apply any coloring scheme you like to show **kdHydrophobicity**. We will also show this property with "worms." In the **Render by Attribute** dialog, change from **Colors** to **Worms**. The values are still shown in a histogram, but now the thresholds have a **Worm radius** instead of a color. The thresholds can be added, deleted, and moved like before, and the **Worm radius** can be changed. Change the mapping as desired and then click **Apply**. The worm "fatness" (along with the previously applied coloring) shows that the most hydrophobic residues tend to face the interior of the structure. To return to a normal ribbon instead of the worm, change **Worm style** to **non-worm** and click **OK** (which is equivalent to **Apply** plus **Close**).

Other hydrophobicity scales (besides Kyte-Doolittle) are available as attribute assignment files.

Next, use **Surface Area/Volume*** to calculate surface area; the area per atom will be loaded automatically as an attribute. In this case, we will focus on numerical results instead of changing the display. Choose **Tools... Surface/Binding Analysis... Surface Area/Volume** from the menu. In the resulting dialog, click **Apply** to compute the **Accessible Surface (Gerstein)**. Chimera will send the coordinates of the structure to the **StrucTools** server at http://molbio.info.nih.gov/structbio/basic.html and then load the results as an atom attribute named **accessibleSurface** (by default; a different name could have been specified in the **Surface Area/Volume** dialog). The new attribute is shown in the **Render by Attribute** dialog (which can be closed), and the total solvent-accessible surface area is reported in the status line and **Reply Log**.

* **Surface Area/Volume** requires internet connectivity. If you are not connected, instead use **Define Attribute** (**Tools... Structure Analysis... Define Attribute**) to open the file SurfVolResults1.txt (a local file linked to this tutorial), then continue on from here. The total accessibleSurface from this step is 4952.3 Å^2.

Open the **Attribute Calculator** (**Tools... Structure Analysis... Attribute Calculator**) to calculate totals over sets of atoms. Calculate a new attribute for **models** with any name you want (name is unimportant as we are only interested in the result of the calculation, not the new attribute). Enter the **Formula**

sum(atom.accessibleSurface)

Check the options to **Restrict formula domain to current selection, if any** and **Show calculation results in Reply Log**; uncheck the others. Next, select peptide chain A:

```
Command: sel :.a
```

Click **Apply** to compute the sum; open the **Reply Log** (**Tools... Utilities... Reply Log**) to see the result. Similarly, select chain B and repeat the calculation. The totals for chain A and B do not add up

to the overall total. This is because the total also includes the water molecules. Delete the waters:

Command: **delete solvent**

Go back to the **Surface Area/Volume** dialog and repeat the calculation[*] (this time clicking **OK** to also dismiss the dialog).

> [*] **Surface Area/Volume** requires internet connectivity. If you are not connected, instead use **Define Attribute** (**Tools... Structure Analysis... Define Attribute**) to open the file SurfVolResults2.txt (a local file linked to this tutorial), then continue on from here. The total accessibleSurface from this step is 4557.05 Å^2.

With the **Attribute Calculator**, again obtain totals for chains A and B (select the chain, **Apply** the calculation) to verify that they add up to the overall total. Close the **Attribute Calculator** and **Reply Log**. It is important to realize that the total for a chain only reflects the contribution of that chain to the surface enclosing both chains A and B. To obtain the area of the surface that completely encloses only one chain, only that chain must be included in the coordinates that are sent to the server. This can be accomplished by using the **Chains** tab in the **Surface Area/Volume** dialog, or by deleting the rest of the molecule before initiating the **Surface Area/Volume** calculation. If the rest of the molecule is deleted, the original structure must be opened again to perform calculations on the whole structure or the other chain.

New attributes can be used in the command line just like built-in attributes. Select atoms with solvent-accessible areas greater than 40 Å^2, promote the selection to residues, and then display the selection:

```
Command: sel @/accessibleSurface>40
Command: sel up
Command: disp sel
Command: ~sel
```

Finally, display all atoms as spheres and color them by their **accessibleSurface** values:

```
Command: ~ribbon
Command: disp
Command: repr sphere

Command: rangecol accessibleSurface 0 blue 5 cyan 20 yellow 40 hot pink
```

Rangecolor is the command alternative to **Render by Attribute** for coloring. The result should resemble the figure.

Close the model:

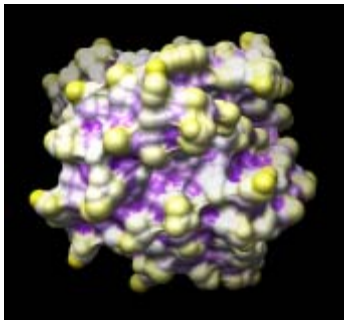
```
Command: close 0
```

Go on to **Part 2** below, **OR** terminate the Chimera session with the following command:

```
Command: stop
```

Attributes, Part 2 - GTP-Binding Protein

121p colored by convexity



Begin with Chimera started and the **Command Line** (and optionally the **Side View**) opened as described at the beginning of **Part 1**.

If you have internet connectivity, use a command to fetch the PDB structure **121p**:

```
Command: open 121p
```

If you do not have internet connectivity, download the file 121p.pdb included with this tutorial and use **File... Open** to open it.

The structure is H-ras, a small GTP-binding protein, along with a bound GTP analog, a Mg^{++} ion, and some water. Delete the water and change to a ribbon display of the protein:

```
Command: delete solvent
Command: ~disp
Command: ribbon
Command: ribrepr sharp
```

Move and scale the structure as desired throughout the tutorial. Show all residues within 4 angstroms of any ions, use the stick representation of atoms and bonds, color by element, label the residues, and color the labels red:

```
Command: display ions z<4
Command: repr stick
Command: col byelement
Command: rlabel ions z<4
Command: color red,l
```

(The latter command contains a lowercase letter l, not the number 1.) The active site Mg^{++} ion is coordinated by serine-17, threonine-35, and phosphonate oxygens in the GTP analog, which is named GTO.

In HOMSTRAD, this protein is classified in the GTP-binding protein family. Download the alignment file homstrad-gtp.pir (originally from HOMSTRAD, now included with this tutorial) and open it with **File... Open**. The file type is **Aligned NBRF/PIR**. The alignment will be shown with **Multalign Viewer**. The structure will automatically associate with the sequence named **5p21**, as indicated by the white rectangle under this sequence name.

When a structure is associated with a sequence alignment open in **Multalign Viewer**, its residues are assigned a **mavPercentConserved** attribute. From the **Multalign Viewer** menu, choose **Structure... Render by Conservation**. This opens the same **Render by Attribute** tool used in **Part 1**, except that now it shows the attribute of **residues** named **mavPercentConserved**. Render the values with **Colors**; use any coloring scheme you like to show this attribute, then close the **Render by Attribute** dialog. It is evident that many of the most conserved residues are in or near the binding site. Undisplay the labels and select residues within 6 angstroms of the ligand, GTO:

```
Command: ~rlabel
Command: select ligand z<6
```

The selection is shown in the **Multalign Viewer** sequence window as green boxes around the corresponding residues. Like other attributes, **mavPercentConserved** can be used as a command-line criterion:

> *Command*: **select ligand z<6 & :/mavPercentConserved>80**

This selects a smaller set of residues than before, only those both within 6 angstroms of the ligand and associated with positions with >80% conservation in the sequence alignment. Clear the selection (**Select... Clear Selection** is one way) and **Quit** from **Multalign Viewer**.

Finally, we will use **Surface Area/Volume** to obtain molecular and solvent-accessible surface areas for the protein atoms and then use the **Attribute Calculator** to create a new attribute from these areas. To get surface areas for the protein only (not enclosing any solvent or other bound molecules) it is necessary to first delete the other parts of the structure:

> *Command*: **delete ions | ligand**

(solvent was deleted earlier). Choose **Tools... Surface/Binding Analysis... Surface Area/Volume** from the menu.* Compute the **Surface Area (MSMS)**; click **OK** to perform the calculation and dismiss the dialog. Chimera will send the coordinates of the structure to the **StrucTools** server at http://molbio.info.nih.gov/structbio/basic.html and then load the results as atom attributes named **msmsArea_MS** and **msmsArea_SAS** (by default; different names could have been specified). The new attributes are listed in the **Render by Attribute** dialog. A warning may appear stating that not all atoms were present in the output from the server. Close the warning dialog; this is a fairly common occurrence that usually does not interfere with further calculations.

> * **Surface Area/Volume** requires internet connectivity. If you are not connected, instead use **Define Attribute** (**Tools... Structure Analysis... Define Attribute**) to open the file SurfVolResults3.txt (a local file linked to this tutorial), then continue on from here.

Open the **Attribute Calculator** (**Tools... Structure Analysis... Attribute Calculator**). Calculate another new attribute named **convexity** for **atoms** using the **Formula**

> atom.msmsArea_SAS/atom.msmsArea_MS

Check the options to **Open Render/Select by Attribute** and **Save calculation results to file**; uncheck the others. Click **OK** to perform the calculation and assignment. A warning message will appear because some atoms have a molecular surface area (**msmsArea_MS**) of zero, resulting in a divide-by-zero error. However, just close the warning dialog; the attribute **convexity** has been assigned correctly for the atoms with nonzero areas. Name the output file **convexity.txt**. In a later Chimera session with the same structure, **convexity.txt** could be opened with **Define Attribute** to assign atomic **convexity** values directly (without any recomputation). However, in this case we will render the values with color. Undisplay the ribbon and surface the protein:

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

In the **Render by Attribute** dialog, make sure that the histogram is showing the new attribute of **atoms** named **convexity**. Render the values with **Colors**. Change the lowest-value (leftmost) threshold to **purple** and the highest-value threshold to **yellow** (these names can be entered directly in the **Color name** field of the **Color Editor**). Use **white** for the middle threshold and set its **Value** to 1

(values > 1 represent convex areas, while values < 1 represent concave areas). Click **Apply**.

Small areas of other, previously used colors may peek through; this is because the atomic radii in Chimera differ slightly from the radii used by the **StrucTools** server. The colors that peek through are for atoms that are not exposed at all according to the **StrucTools** calculations. Set these areas to **purple** too, using the color well marked **No-value color** in the **Render by Attribute** dialog. Click **Apply** again; the result should resemble the figure.

If you wish, try applying different color mappings (changing colors, threshold positions, and/or number of thresholds). When finished, end the Chimera session:

```
Command: stop
```

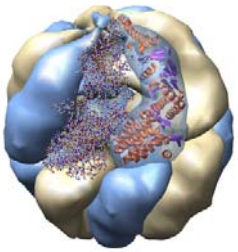
RBVI

Large Molecular Assemblies

Tom Goddard

Large Molecular Assemblies

This segment is about how to work with large molecular assemblies such as virus capsids, ribosomes, microtubules, and crystal unit cells.

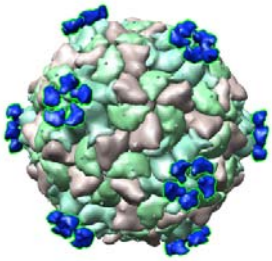


We'll use the Chimera Multiscale tool which enables:

- making multimeric structures from the asymmetric unit
- manipulating PDB chains as low resolution surfaces

Demonstration

- Thermosome protein folding machine of archaebacteria.



Hands-on Tutorial

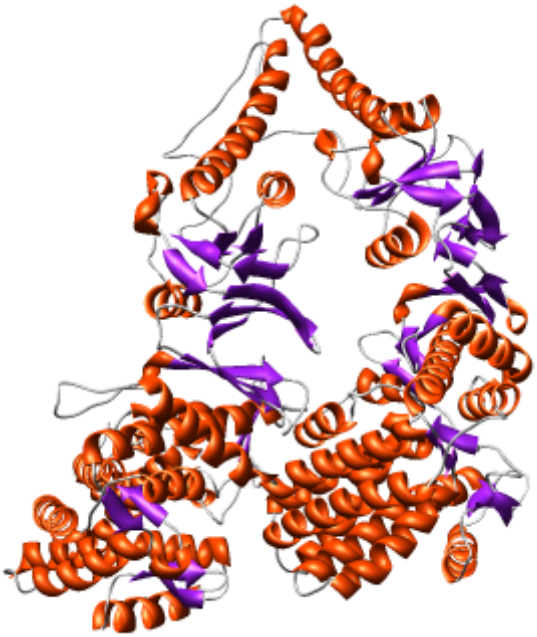
- Human Rhinovirus 2 and a fragment of its cellular receptor.

Viewing Large Molecular Complexes: Thermosome

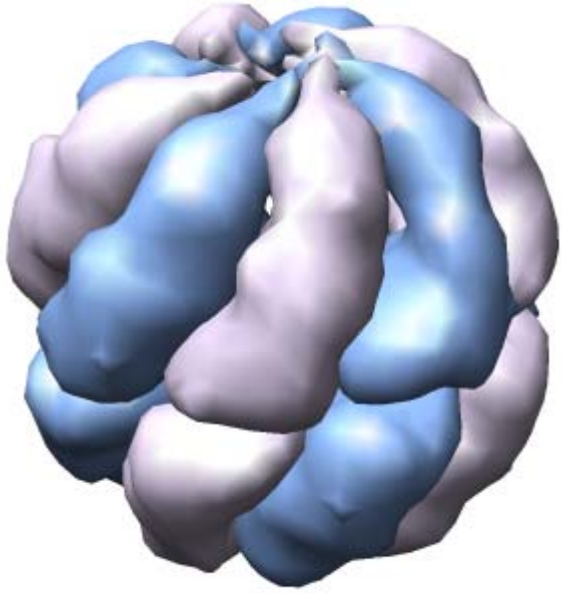
Chimera Workshop
November 17-18, 2005

Demonstration of Chimera multiscale tool for:

- making multimeric structures from the asymmetric unit
- manipulating PDB chains as low resolution surfaces



Thermosome model 1A6D has asymmetric unit consisting of 2 proteins with 61% sequence identity.

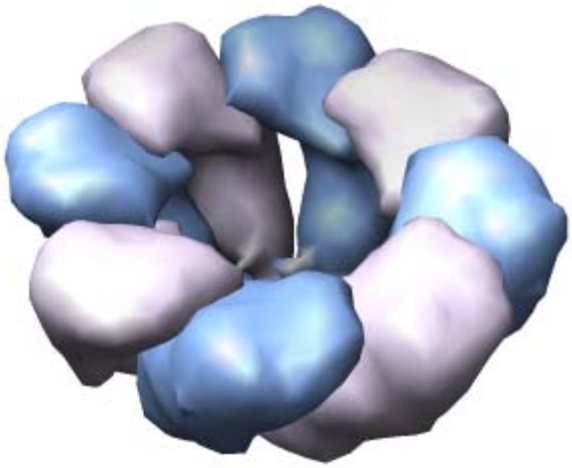


Biological unit made with Multiscale tool is 8 copies of asymmetric unit.

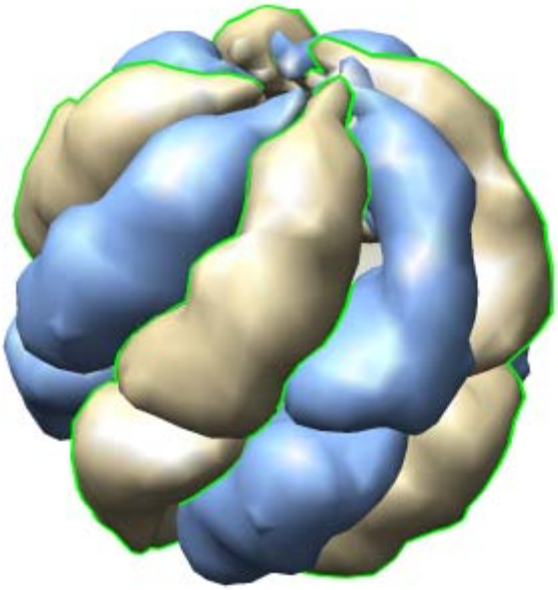
The 1A6D PDB file contains 8 matrices in REMARK 350 that define the biological unit and were read by Chimera.

```
REMARK 350 GENERATING THE BIOMOLECULE
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW.  BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, B
REMARK 350   BIOMT1   1  1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT2   1  0.000000  1.000000  0.000000        0.00000
REMARK 350   BIOMT3   1  0.000000  0.000000  1.000000        0.00000
REMARK 350   BIOMT1   2 -1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT2   2  0.000000 -1.000000  0.000000        0.00000
REMARK 350   BIOMT3   2  0.000000  0.000000  1.000000        0.00000
REMARK 350   BIOMT1   3  0.000000 -1.000000  0.000000        0.00000
```

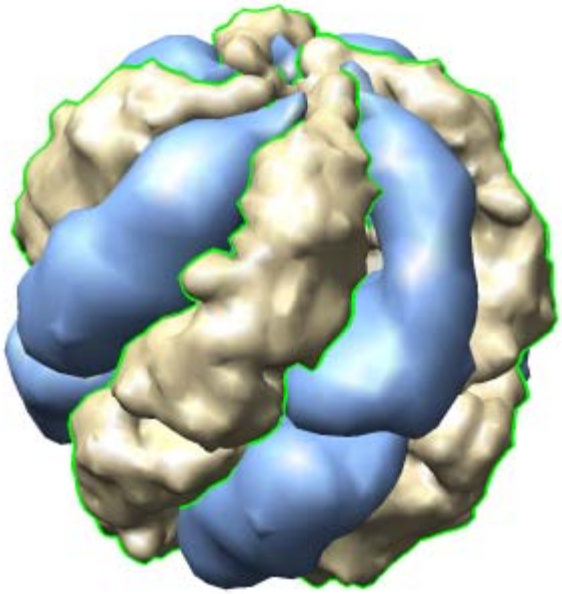
```
REMARK 350   BIOMT2   3  1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT3   3  0.000000  0.000000  1.000000        0.00000
REMARK 350   BIOMT1   4  0.000000  1.000000  0.000000        0.00000
REMARK 350   BIOMT2   4 -1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT3   4  0.000000  0.000000  1.000000        0.00000
REMARK 350   BIOMT1   5 -1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT2   5  0.000000  1.000000  0.000000        0.00000
REMARK 350   BIOMT3   5  0.000000  0.000000 -1.000000        0.00000
REMARK 350   BIOMT1   6  1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT2   6  0.000000 -1.000000  0.000000        0.00000
REMARK 350   BIOMT3   6  0.000000  0.000000 -1.000000        0.00000
REMARK 350   BIOMT1   7  0.000000  1.000000  0.000000        0.00000
REMARK 350   BIOMT2   7  1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT3   7  0.000000  0.000000 -1.000000        0.00000
REMARK 350   BIOMT1   8  0.000000 -1.000000  0.000000        0.00000
REMARK 350   BIOMT2   8 -1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT3   8  0.000000  0.000000 -1.000000        0.00000
```

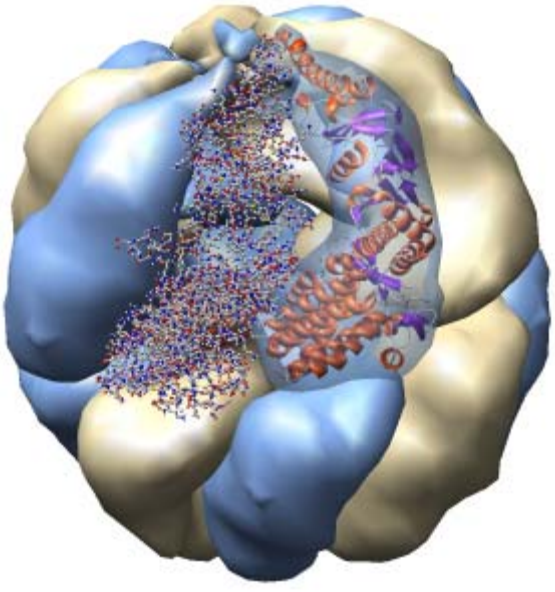


Half of shell hidden.

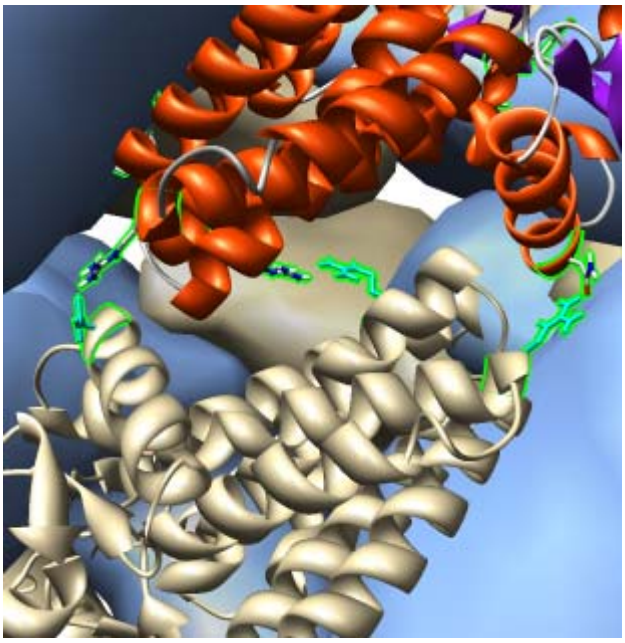


Select copies of one protein and recolor.





Change resolution of surfaces 8A -> 4A.



Show contacts within 2A of chain A with "load atoms" switch on. Show when extra copies are created in Model Panel. Promote contact atoms to residues, show as stick, and identify contact residues by hovering mouse over them.

Show ribbon and ball and stick. Add transparent surface.

Viewing Large Molecular Complexes: Rhinovirus

Chimera Workshop
November 17-18, 2005

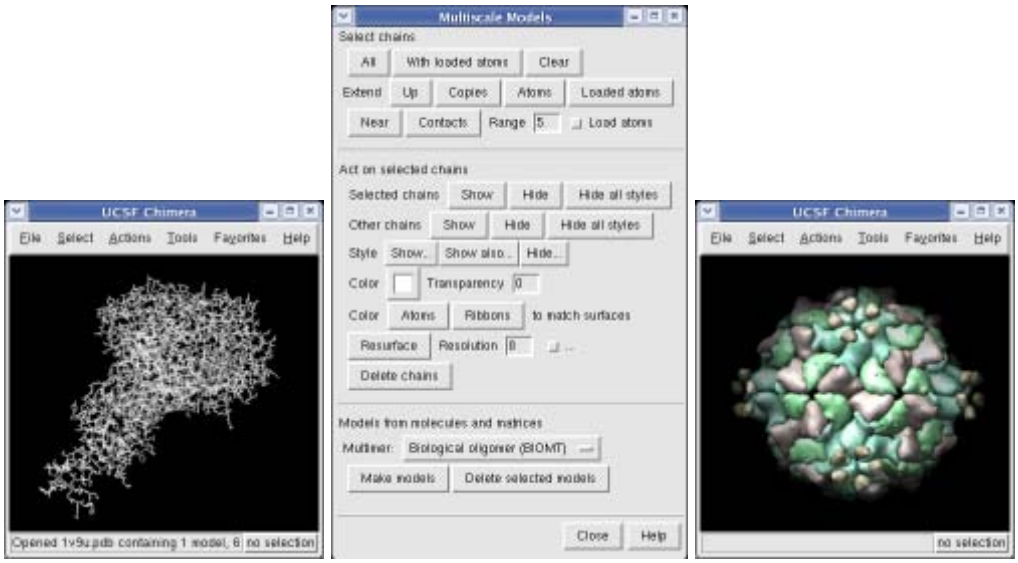
We'll look at one of the viruses that cause the common cold, Human Rhinovirus 2.

Display the Virus Capsid Atomic Model

Open the PDB model 1v9u and then create 60 copies of this asymmetric unit to show a full virus capsid.

- File -> Open, choose file **1v9u.pdb**.
- Tools -> Higher-Order Structure -> Multiscale Models
- Press the **Make models** button near the bottom of the Multiscale dialog.

Each of the 180 capsid proteins and 60 receptor fragments is shown as a separate low resolution surface.

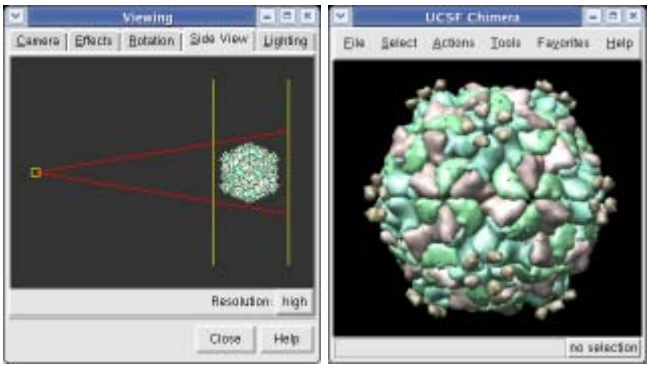


Adjust Clip Planes

The far portion of the capsid is invisible because Chimera's near and far clip planes were positioned for the 1v9u asymmetric unit, not the full capsid. Adjust the clip planes.

- Favorites -> Side View
- Drag the right vertical yellow line in the Side View dialog further to the right.

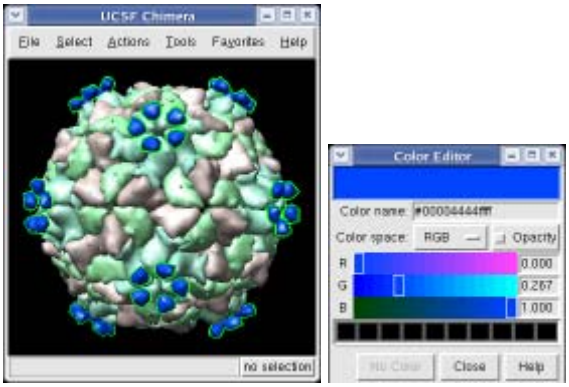
The two yellow lines in the Side View dialog are near and far clipping planes and the yellow square represents your eye position in this view from the side. Everything in front of the near clip plane or behind the far clip plane is invisible in the main Chimera window.



Color the Viral Receptor Fragment

This structure shows part of the receptor found on the surface of cells in your nose that the virus recognizes. These are the chains that appear in rings of 5 near the 5-fold symmetry axes. We'll color the receptor so it stands out.

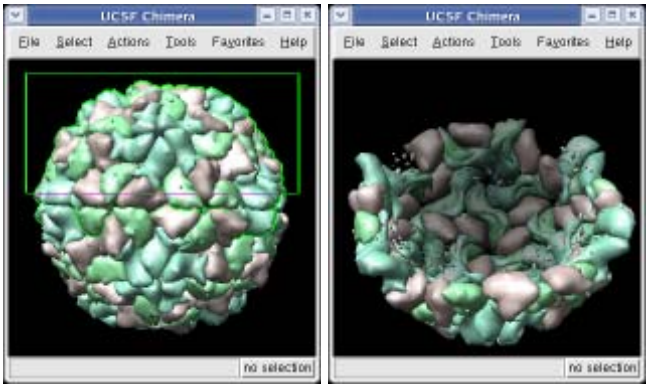
- Hold the **ctrl** key and click the **left mouse button** on one of the receptor surfaces to select it.
- Press the **Copies** button on the second line of the Multiscale dialog.
- Press the **Color** button in the middle of the dialog. It has a raised border with the color shown in the middle.
- Change the color using the color dialog.



Show the Inside of the Capsid

We'll hide the receptor fragment, and then hide half of the virus capsid to see the inside of the capsid.

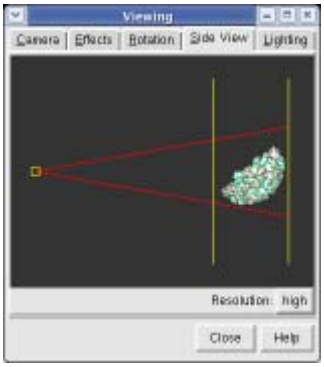
- Press the **Hide** button in the Multiscale dialog on the line that says **Selected chains** to hide the receptors you just colored.
- Select half of the capsid by dragging a rectangle using **ctrl left mouse button**.
- Press the **Hide** selected chains button again.



Depth cueing

Chimera makes objects that are further from view dimmer. Adjusting the clip planes by moving the vertical yellow lines in the **Side View** dialog changes the distance at which the dimming effect starts and ends.

- Favorites -> Side View
- Move vertical yellow lines and observe brightness changes in Chimera main window.

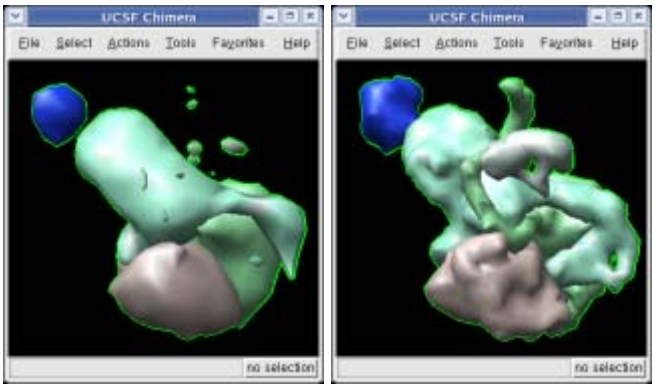


Adjust Surface Resolution

The surfaces representing each protein can be adjusted to show more detail. We will look at a single copy of the asymmetric unit, 1/60th of the icosahedral capsid.

- Press the **With loaded atoms** button at the top of the Multiscale dialog.
- Press the **Show** button on the line titled **Selected chains**.
- Press the **Hide** button on the line titled **Other chains**.
- Change the **Resolution** field value from 8 angstroms to 4.
- Press the **Resurface** button.

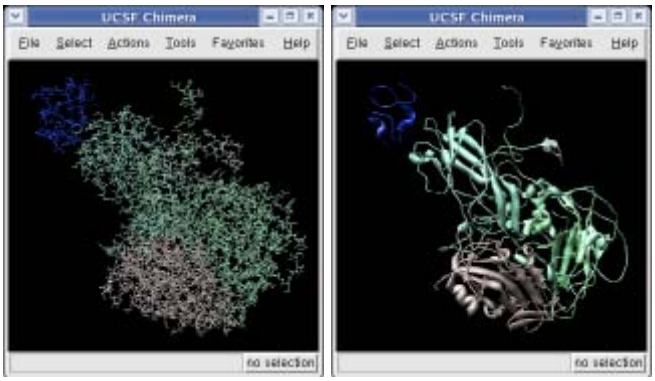
Atomic coordinates have only been loaded for one copy of the asymmetric unit. The first 3 steps show just that copy. Some of the small blobs visible at the original surface resolution are parts of larger proteins. At the 4 angstrom resolution you can see that the green protein (VP3) has two arms that wrap around the light blue protein (VP1).



Show Atoms and Ribbons

Selected proteins can be shown using atom level or residue level representations instead of surfaces.

- Press the **Show...** button on the **Style** line of the dialog and select **Ball and Stick** from the drop down menu.
- Press the **Color Atoms** button to make the atoms colors match the surface depiction colors.
- Press the **Show...** button on the **Style** line and select **Ribbon** from the drop down menu.
- Press the **Color Ribbons** button to make the ribbon colors match the surface depiction colors.



Show Contacts between Receptor and Virus

Well look specifically at the residues of the virus capsid that contact one copy of the cellular receptor fragment.

- **Ctrl left click** on the blue receptor ribbon to select one residue.
- Press the **up arrow** key on the keyboard to promote the selection to the whole receptor fragment.
- Change the **Range** value near the top of the Multiscale dialog from 5 angstroms to 3,
- Turn on the **load atoms** switch
- Press the **Contacts** button.

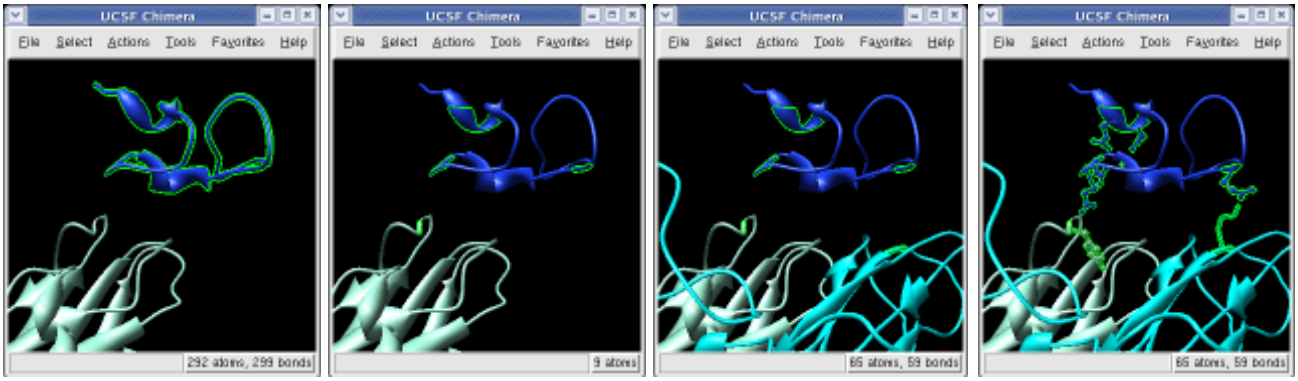
These steps find all residues within 3 angstroms of the receptor. Some contacts are with an unshown protein. To show those:

- Press **Show...** on the **Style** line and choose **Ribbon**.
- On the main window use menu entry **Actions -> Atoms/Bonds -> show**

Only the atoms within 3 angstroms of the receptor are selected. To show the full residues that contain those atoms:

- Press the **up arrow key** on the keyboard to extend the selection to the containing residues.
- Use main window use menu entry **Actions -> Atoms/Bonds -> show**

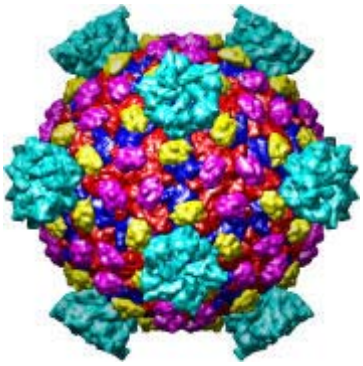
Note that 3 of the selected receptor residues are not really near the capsid, but instead surround a calcium ion. We should have selected both the receptor fragment and this ion in the initial contacts calculation to avoid picking up these residues.



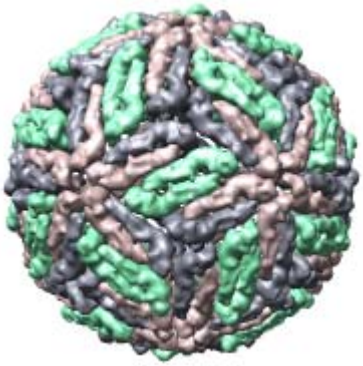
More Viruses

There are about 200 virus capsid structures known at atomic resolution (ca. 2005). Below are some of the Protein Data Bank identifiers. The Virus Particle Explorer web site contains information about these virus structures.

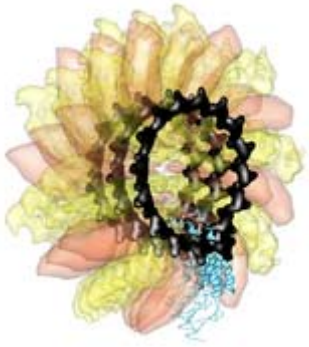
1a34 1a6c 1al0 1al2 1aq3 1aq4 1ar6 1ar7 1ar8 1ar9 1asj 1auy 1aym 1ayn 1b35 1bbt 1bev 1bms 1bmv 1c8d 1c8e 1c8f 1c8g 1c8h 1c8m 1c8n 1cd3 1cov 1cwp 1d3e 1d3i 1d4m 1ddl 1dgi 1dnv 1dwn 1dyl 1dzl 1dzs 1e57 1e6t 1e7x 1eah 1ej6 1ev1 1f15 1f2n 1f8v 1fmd 1fod 1fpn 1fpv 1fr5 1frs 1gav 1gff 1gkv 1gkw 1gw7 1gw8 1h8j 1h8t 1hb5 1hb7 1hb9 1hdw 1he0 1he6 1hri 1hrv 1hxs 1if0 1ihm 1ijs 1jew 1js9 1k3v 1k4r 1k5m 1kuo 1kvp 1laj 1ld4 1lp3 1m06 1m0f 1m11 1m1c 1m4x 1mec 1mqt 1mst 1mva 1mvb 1mvm 1n6g 1na1 1na4 1ncq 1ncr 1nd2 1nd3 1ng0 1nn8 1nov 1ny7 1ohf 1ohg 1oop 1opo 1p58 1p5w 1p5y 1pgl 1pgw 1piv 1po1 1po2 1pov 1pvc 1qbe 1qgc 1qgt 1qju 1qjx 1qjy 1qjz 1qqp 1r08 1r09 1r1a 1rb8 1rhi 1rmu 1ruc 1rud 1rue 1ruf 1rug 1ruh 1rui 1ruj 1rvf 1s58 1sid 1sie 1smv 1stm 1sva 1tge 1thd 1tme 1tmf 1tnv 1u1y 1uf2 1upn 1v9u 1vak 1vb2 1vb4 1vba 1vbb 1vbc 1vbd 1vbe 1vrh 1w39 1wcd 1wce 1x9p 1x9t 1yc6 1zdh 1zdi 1zdj 1zdk 2bbv 2bpa 2btv 2cas 2hwb 2hwc 2hwd 2hwe 2hwf 2mev 2ms2 2plv 2r04 2r06 2r07 2rm2 2rmu 2rr1 2rs1 2rs3 2rs5 2stv 2tbv 4dpv 4rhv 4sbv 5msf 6msf 7msf



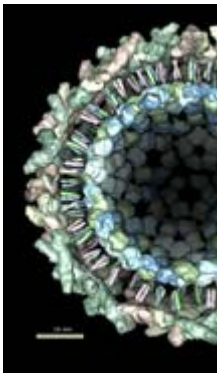
Reovirus core, 1ej6



Dengue virus, 1k4r



Ribgrass mosaic virus (helical), 1rmv



Sindbis virus, 1l

Virus structures without biological unit matrices

About half of the virus models from the Protein Data Bank (primarily older ones) do not contain the symmetry matrices needed to generate the capsid. When you press the Make models button you just get surfaces for the asymmetric unit. For these viruses you can download alternate coordinates from the Virus Particle Explorer web site instead of from the Protein Data Bank. Then set the **Multimer** type to **Icosahedral symmetry, ViPER Z(2)35X(2)**, before pressing Make models.

More Information on the Web

Chimera

- User manual documentation for the Multiscale Models tool.
- Poster about Chimera virus display
- Viruses in the Chimera Image Gallery.
- More Chimera created virus images and a table of virus shapes.

Other Sites

- Virus Particle Explorer web site.
- Protein Data Bank

RBVI

Volume Data

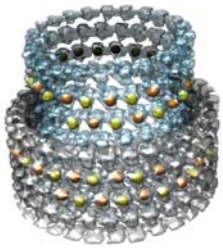
Tom Goddard

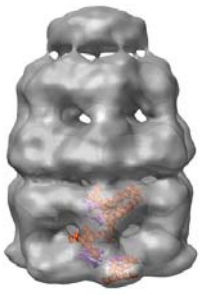
Volume Data

This segment introduces how to work with volume data. Volume data means a 3-dimensional grid of data values.

We'll look at three kinds of volume data:

- electrostatic potential
- x-ray crystallography density map
- electron microscopy density map





Demonstration

__Microtubules composed of alpha and beta-tubulin proteins.

Hands-on Tutorial

__Chaperonin protein folding machine.

Volume Data Demonstration: Tubulin

Chimera Workshop
November 17-18, 2005

EMD 1130 is GDP bound bovine microtubule at 12 angstroms.

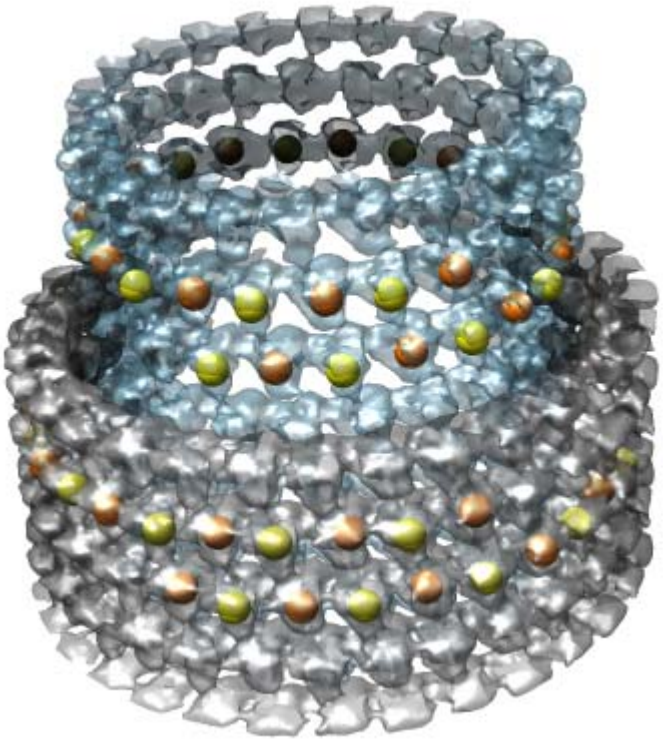


Image shows EMD 1129 (inner layer) and EMD 1130 (outer layer) of double walled microtubule. Yellow and orange balls are alpha and beta tubublin proteins.

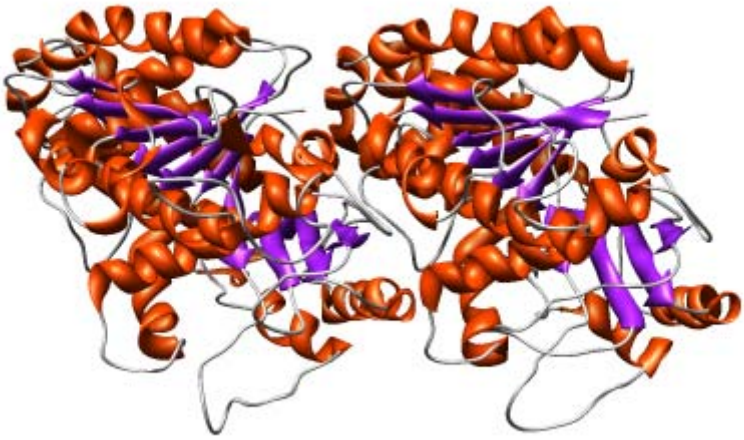
1jff is a bovine alpha/beta tubulin by electron diffraction of 2D taxol stabilized sheets, 3.5 angstroms.

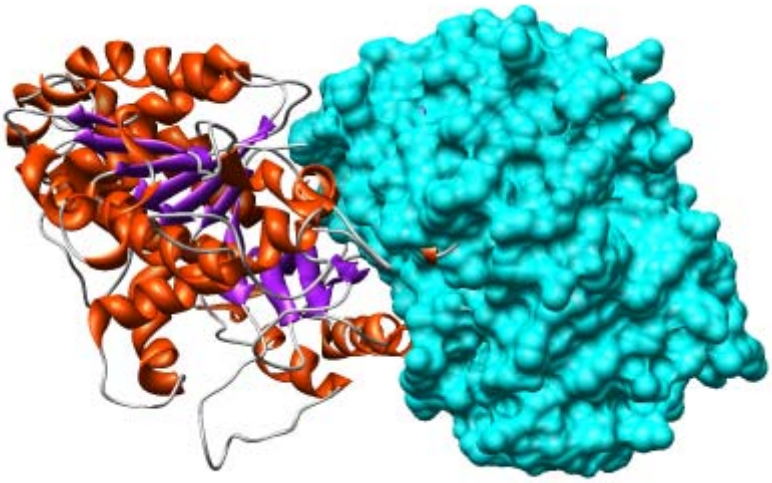
2bto is bacterial tubulin called btuba thought to be horizontally transferred from eukaryotes, found in only one bacteria, has 30-40% seq identity and RMSD 1-2 angstrom differences. Chose this one because crystallographic data (2.5 angstroms) available.

Electrostatic Potential of Alpha and Beta Tubulin

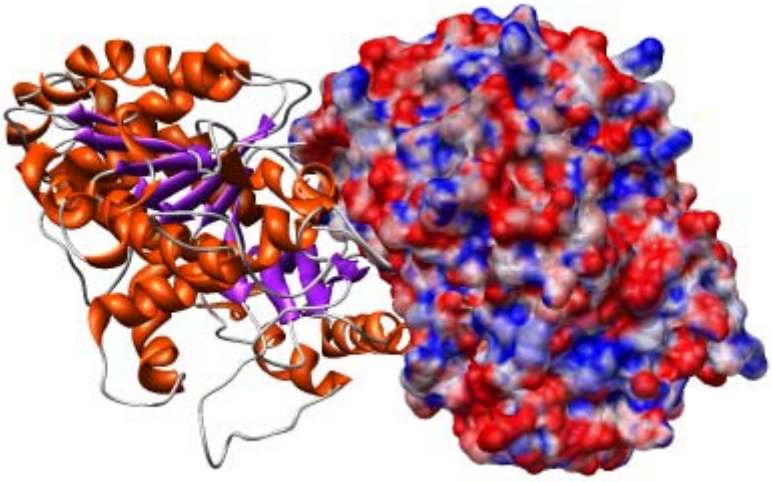
Beta tubulin is on the left, alpha tubulin on the right (1jff). Slightly different loop shapes.

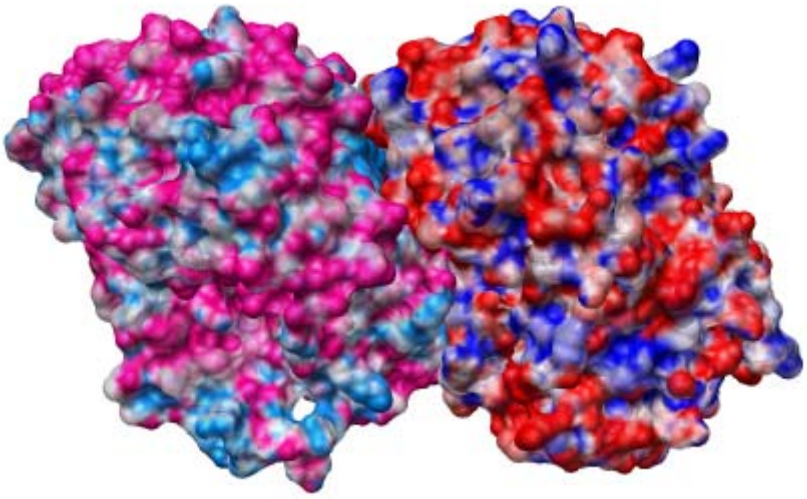
Use **surfcat A :.A** and **surf A** to surface individual chain.





Use different colors for alpha and beta electrostatics to easily see the boundary between them.



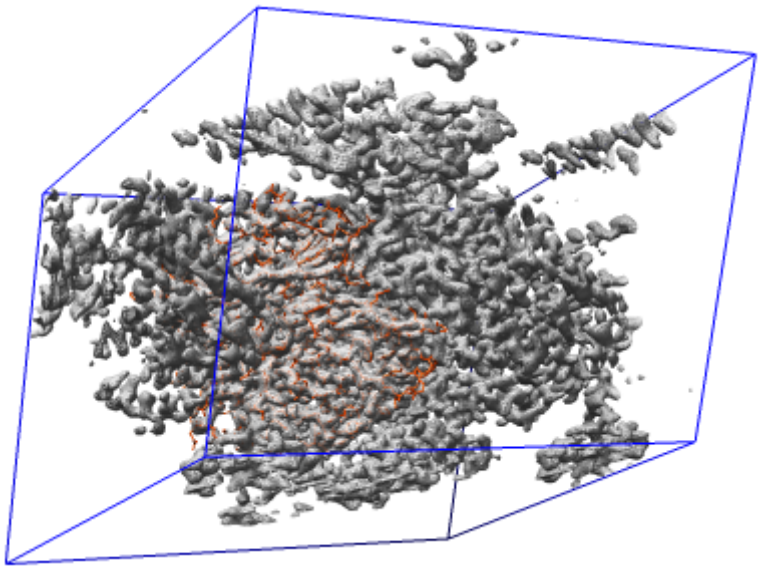


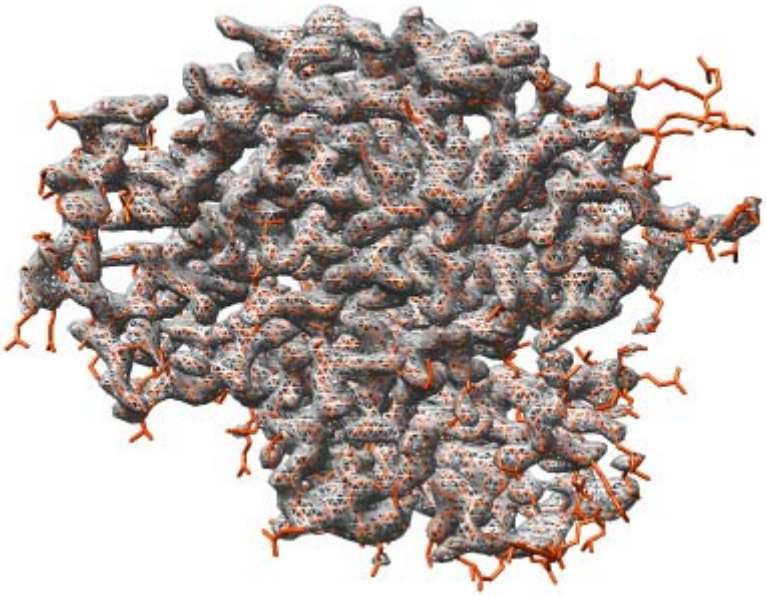
Crystallographic Density Map of Bacterial Tubulin

The previous bovine tubulin structure was determined by electron diffraction of a 2-D crystal, for which I don't have a density map. Look at bacterial tubulin (2bto) with density map from EDS.

Color model orange-red for contrast with white density.

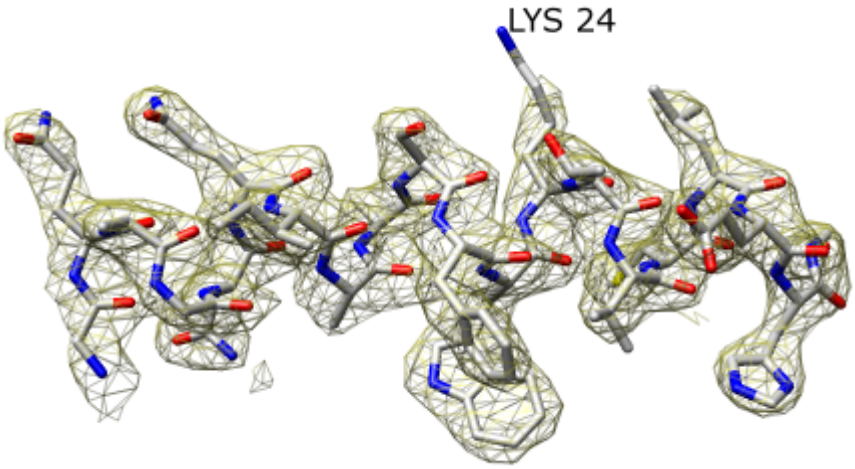
Restrict density map display with surface zone to chain A. Use invert selection and hide atoms to restrict model display.





Use Sequence dialog (Tools -> Structure Analysis -> Sequence) to select first alpha helix. Restrict map and model to it. Make mesh transparent and yellow.

Show lysine sticking out. Hover mouse to identify residue.



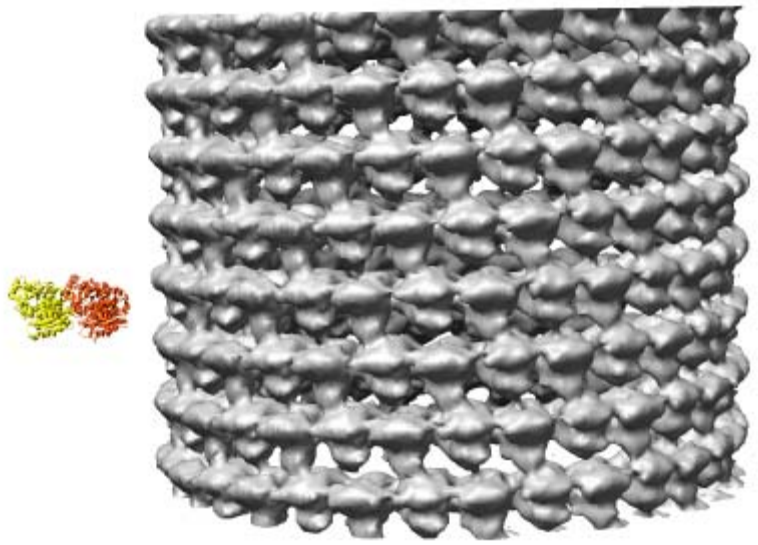
Fit Alpha/Beta Tubulin Dimer into Electron Microscopy Density Map

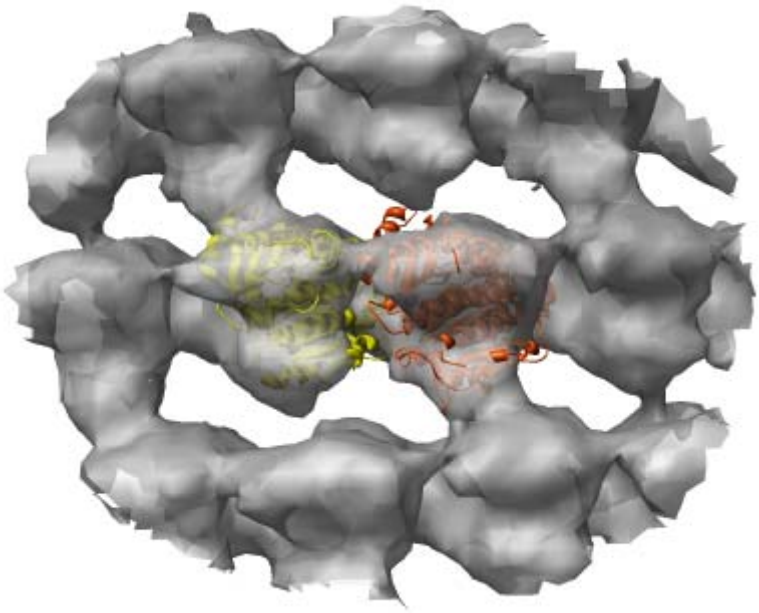
Show alpha and beta monomers as ribbons and color yellow and orange.

Move into density map, select all atoms, zone at 50 A radius (for faster rotation), make map transparent, and optimize fit. Clear selection before inspecting fit (for faster rotation and clearer view).

Can try fit shifted right by 1 monomer. Slightly different fit. Would be interesting to try fitting each monomer separately.

The EMD 1130 map appears to have incorrect handedness compared to the Nogales paper images.





Working with Volume Data: Chaperonin

Chimera Workshop
November 17-18, 2005

This tutorial shows how to work with volume data in Chimera. Volume data means a 3-dimensional grid of data values.

We'll look at three kinds of volume data:

- electrostatic potential
- x-ray crystallography density map
- electron microscopy density map

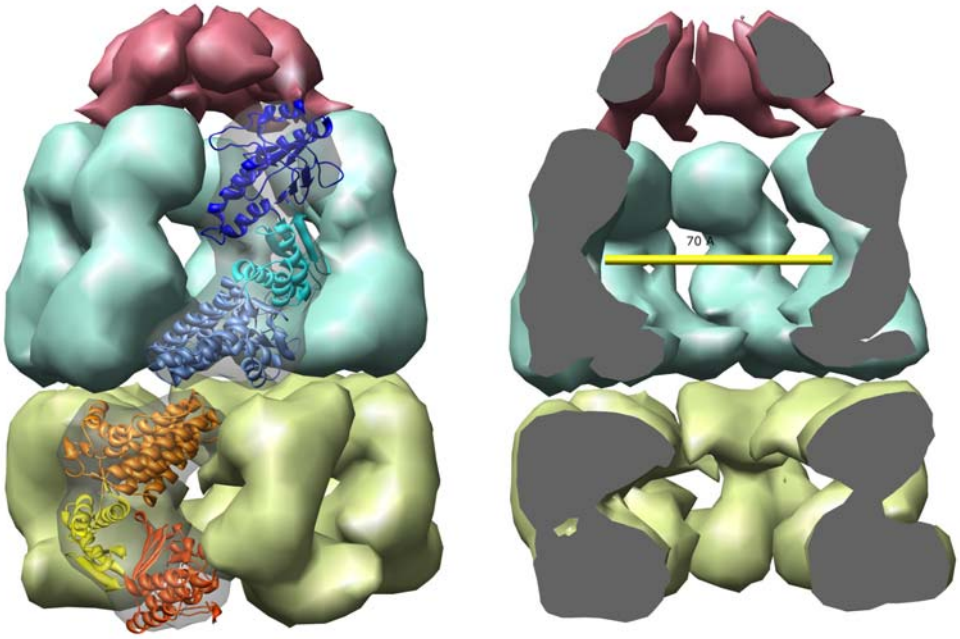


Figure 1: E coli chaperonin shown using the Chimera MultiScale tool. The top red cap is GroES, the blue and yellow rings are GroEL. Protein Data Bank model 1AON.

The examples will all involve a 21 protein molecular complex called chaperonin. Chaperonin is a barrel inside which proteins are folded. In bacteria it consists of 3 rings each containing 7 proteins. Two rings of 14 identical proteins form a barrel called GroEL. The cap, called GroES, is formed from 7 copies of a different protein.

Electrostatic Potential of GroES

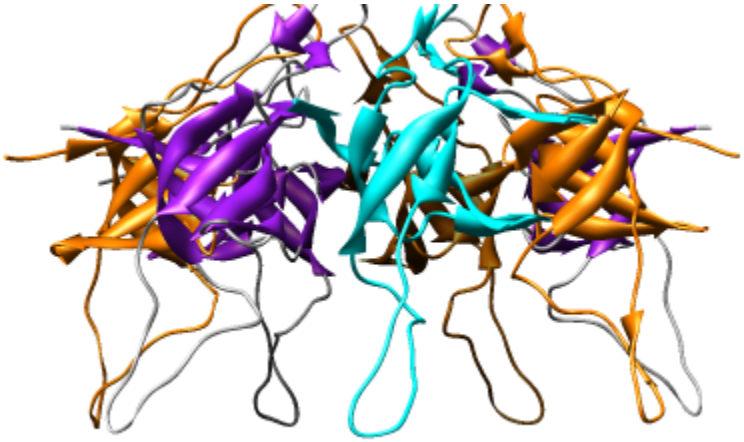
We will color a molecular surface to show electrostatic potential.

Open in Chimera the Mycobacterium tuberculosis GroES structure. The protein data bank model 1p3h contains two copies of GroES but the file you've opened contains just one copy.

- Menu entry **File -> Open**, choose **1p3h_half.pdb**

Show Ribbons

Change from an all-atom view to a round ribbon display. You can use menu entries:



- Actions -> Ribbon -> show
- Actions -> Atoms/Bonds -> hide
- Actions -> Ribbon -> round

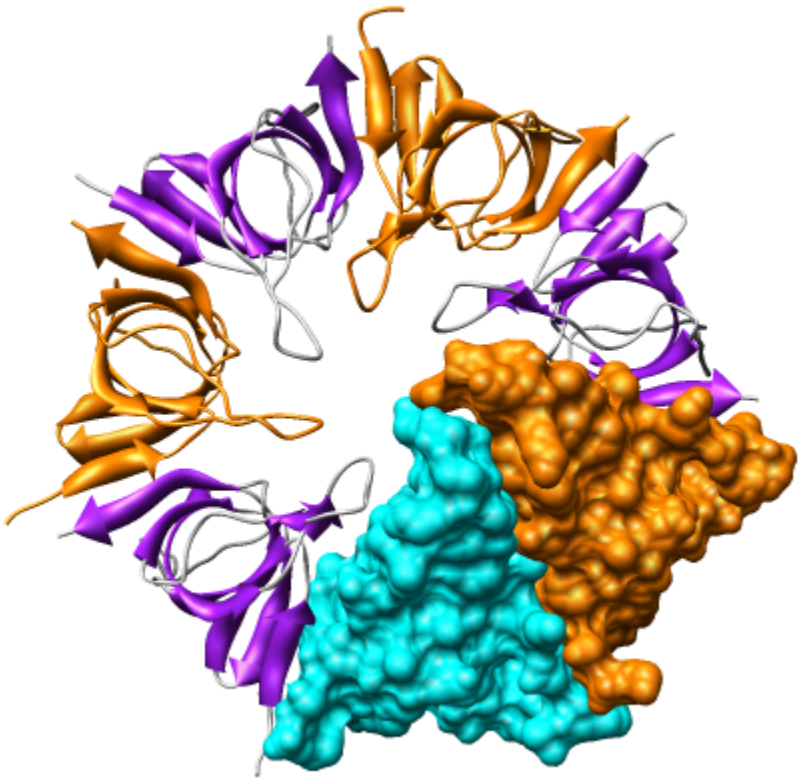
Color Ribbons

The 7 proteins can be given different colors.

- Hold **ctrl** and click the **left mouse button** on one ribbon residue to select it.
- Press the **up arrow key** to extend the selection to the whole chain.
- Use menu entry **Actions -> Color -> orange** to color the chain.

Show Molecular Surface

Create a molecular surface for chain A. The Actions menu allows you to make a single surface covering all 7 chains, but to surface just one requires using Chimera commands:



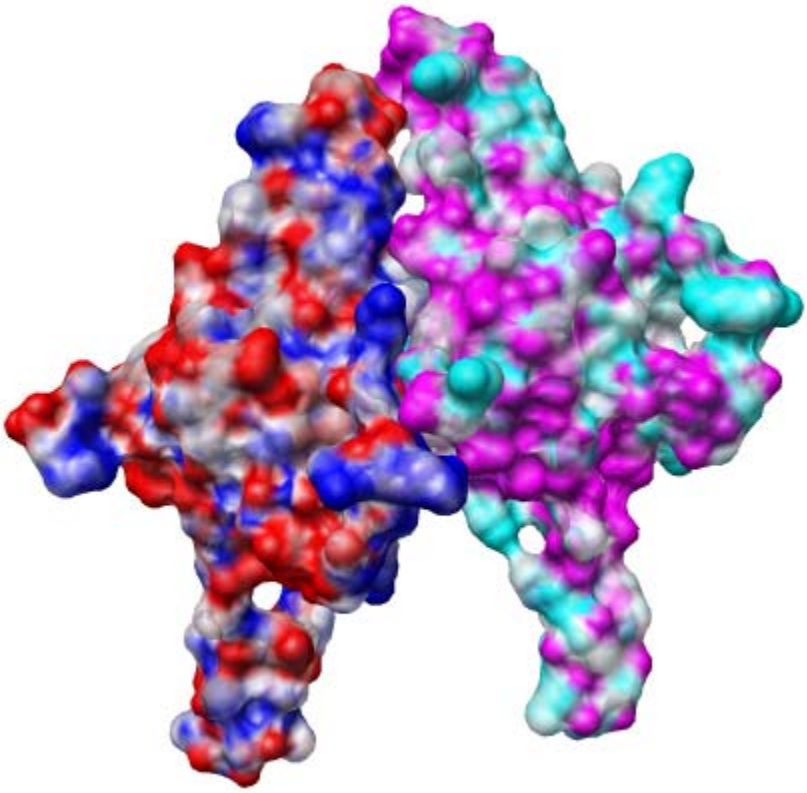
- **Favorites -> Command Line** shows the command line at the bottom of the Chimera window.
- Command **surfcat a :.A** defines a surface category called "a" that consists of chain A.
- Command **surf a**

Color Molecular Surface

To color the molecular surface according to electrostatic potential.

- Tools -> Surface/Binding Analysis -> Electrostatic Surface Coloring.
- Press the **Browse...** button on the third line of the Surface Color dialog and select file **1p3h_chain_A.nc**.
- Press the **Color** button at the bottom of the Surface Color dialog.

The file **1p3h_chain_A.nc** is electrostatic potential volume data calculated by the Adaptive Poisson Boltzmann Solver (APBS) for chain A outside of Chimera. Chimera is not able to calculate the potential itself. Running APBS is not part of this tutorial.



The colors represent potential values, blue at potential 10 kT/e, red at -10 kT/e, and white at 0 kT/e, with linear interpolation of colors at intermediate potential values.

Electrostatics of a Second Monomer

Repeat the surface display and electrostatics coloring steps for chain B to see the electrostatic potential on the neighboring monomer. In the Surface Color dialog you will need to choose to color **MSMS b surface** and use the potential file **1p3h_chain_B.nc** that was calculated for chain B.

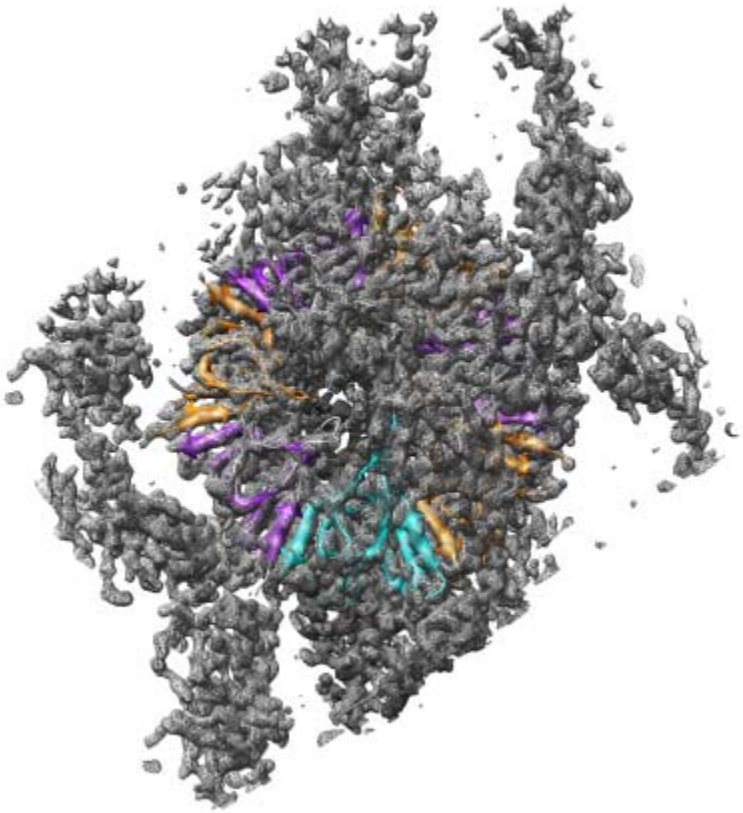
Pressing the red and blue color buttons on the Surface Color dialog you can change the surface colors. Then press the **Color** button at the bottom of the Surface Color dialog to apply these new colors. That will help visually distinguish the surfaces for chains A and B.

Are the potential values for chains A and B at their interface complementary, that is, positive on one side and negative on the other?

X-ray Density Map of GroES

The GroES model above was determined by x-ray crystallography. We'll now look at the agreement between the atomic model and the x-ray density map.

Clean Up



First clean up from the previous electrostatics example.

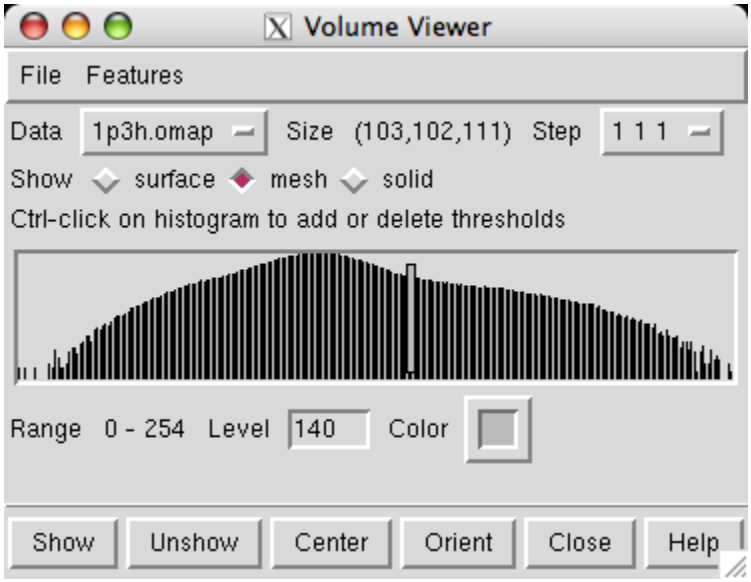
- Favorites -> Model Panel
- Click on each molecular (MSMS) surface listed in the Model Panel dialog and press the **Close** button in the right column of buttons.
- Close the Surface Color dialog.

Open Density Map

Open the 2.8 angstrom resolution crystallographic density map 1p3h.omap which came from the Uppsala Electron Density Server web site.

- File -> Open, choose density map **1p3h.omap**

Adjust Density Map Display



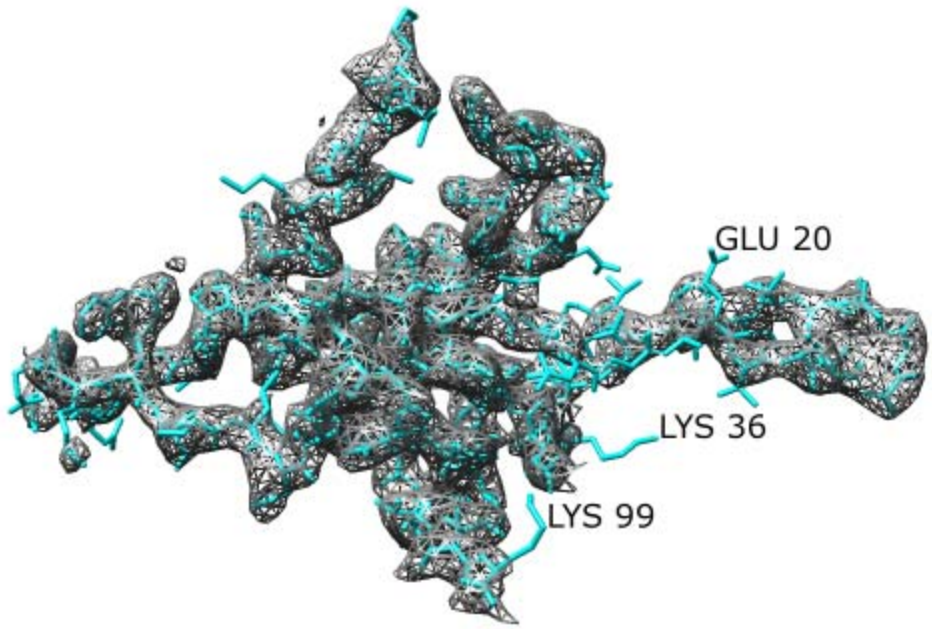
Opening the density map causes the **Volume Viewer** dialog to be displayed. It shows that the map grid is of size 103 by 102 by 111 and a histogram of the density values is shown. The vertical bar on the histogram indicates the currently displayed surface contour level. The bar can be moved with the mouse to change the contour level. The initial **step** setting is 2 2 2 indicating that every other plane of the data is being displayed.

Adjust some density map display settings.

- Click the **mesh** option in the volume dialog.
- Adjust the contour **level** to around 140.
- Change the **step** to 1 1 1 to show all the data.

Limiting Density Display

To compare the density map and model it is necessary to look at a small piece. We'll look at the density near chain A.



- Menu entry **Select -> Chain -> A**
- Volume dialog menu entry **Features -> Zone**
- Press the volume dialog **Zone** button.

Show Chain A Atoms

Show chain A atoms and hide all other chains.

- Actions -> Atoms/Bonds -> show
- Actions -> Atoms/Bonds -> stick
- Actions -> Ribbon -> hide
- Select -> Invert (all models)
- Actions -> Ribbon -> hide

Residues Sticking Out of Density

See what types of residues are sticking out of the density map.

- Place the mouse over a residue. Text will pop up identifying the residue.

Long side chains like lysines, arginines and glutamic acid on the surface probably assume variable positions in the crystal. Their exact positions in the model should not be trusted.

Electron Microscopy Density Map of Chaperonin

Now we will try fitting a protein into a density map of E coli chaperonin determined by electron microscopy.

Clean Up

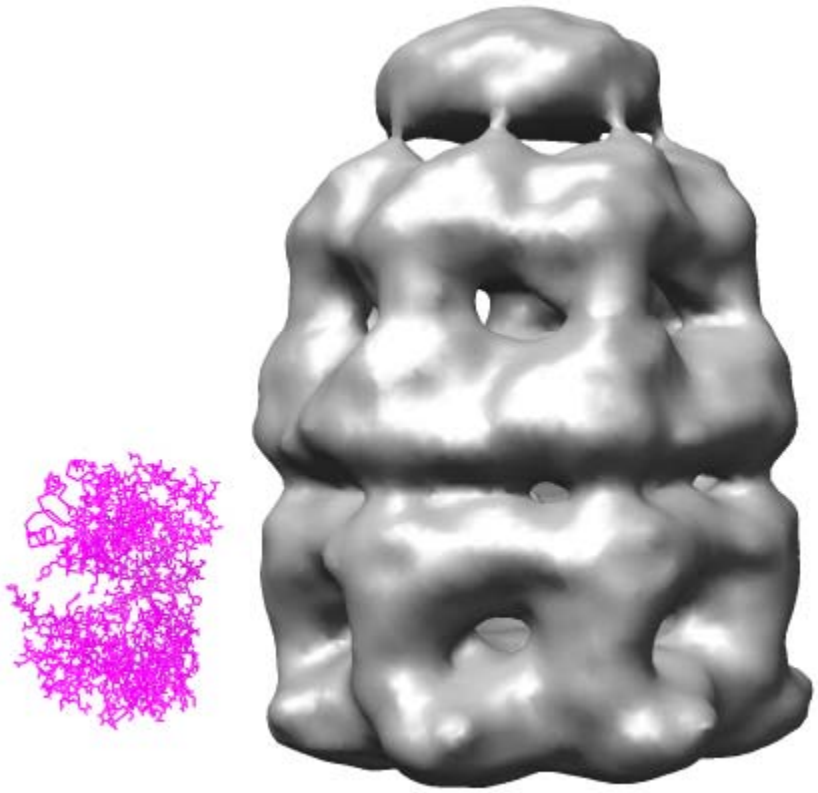
Clean up from the previous x-ray density map example.

- File -> Close Session

Open Density Map and Protein Model

Open the 23.5 angstrom chaperonin density map which was determined by single particle reconstruction using 2-D electron micrographs of 1448 particles, and the 2.8 angstrom GroEL protein crystal structure.

- File -> Open, choose density map **emd_1046.map**
- File -> Open, choose pdb model **1grl_near.pdb**



Adjust Map Appearance

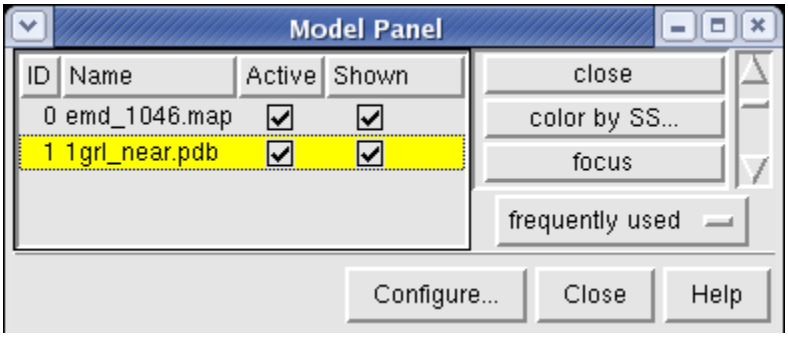
Adjust the map contour level and step size and display style in the volume dialog.

- Adjust map **level** to around 0.09.
- Set map **step** to 1 1 1.
- Click the **mesh** checkbutton.

Adjust Molecule Appearance

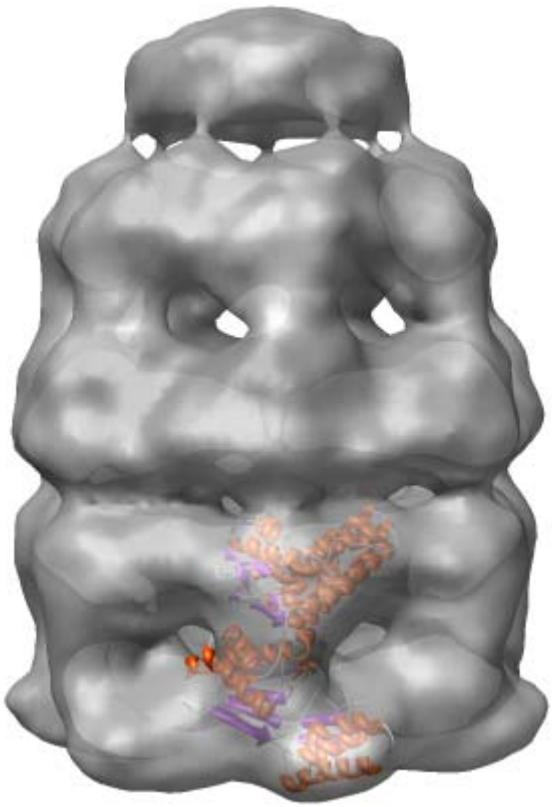
Show the molecule as a ribbon colored according to secondary structure (alpha helices orange, sheets purple).

- Actions -> Ribbon -> show
- Actions -> Ribbon -> round
- Actions -> Atoms/Bonds -> hide
- Favorites -> Model Panel



- Select 1grl_near.pdb in Model Panel list.
- Press on **color by SS...** button in Model Panel
- Press **OK** in Color Secondary Structure dialog

Hand Align Molecule in Map

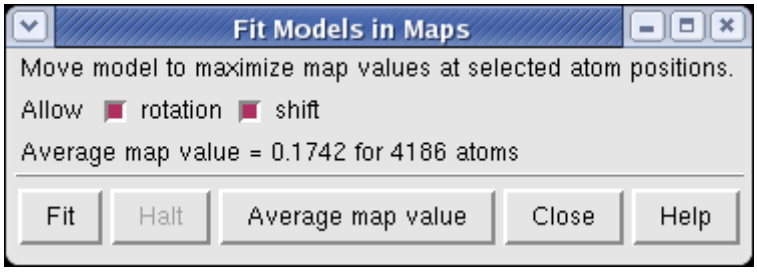


Lock the position of the density map and move the molecule into the map using the mouse.

- Turn off the **Active checkbutton** next to emd_1046.map in Model Panel. This prevents the map from being moved with the mouse.
- Move the molecule into the map using the mouse. To move the molecule into and out of the screen holding the ctrl key while using the middle mouse button.
- Turn on the **Active checkbutton** as needed to rotate both map and model to view from different angles.

Optimize Fit of Molecule in Map

The molecule can be automatically moved to the nearby position that maximizes the density values at atom positions.



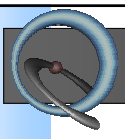
- Menu entry **Select -> Select all**.
- Menu entry **Tools -> Volume Data -> Fit Models in Maps**, press **Fit** button

Fitting the molecule upside down gives an average density value at atom positions of 0.167, while the correct orientation gives 0.174.

RBVI

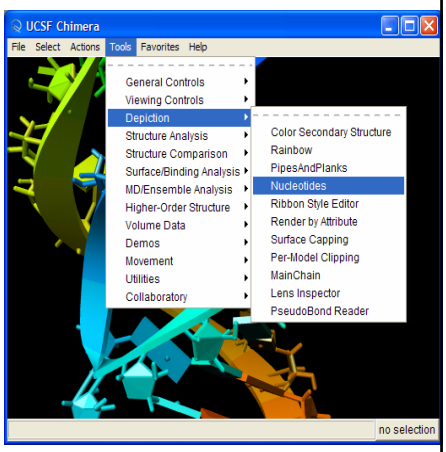
Producing Images and Movies

An introduction to several useful tools for creating publication-quality images and movies



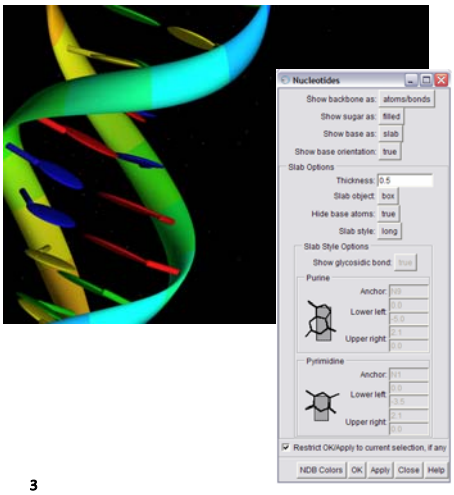
Depiction Tools

In addition to the Actions menu and the Selection Inspector, there are many other tools for tweaking the visualization



Nucleotides

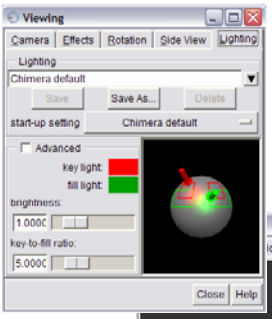
The **Nucleotides** tool can be used to obtain highly stylized renditions of nucleotide structures

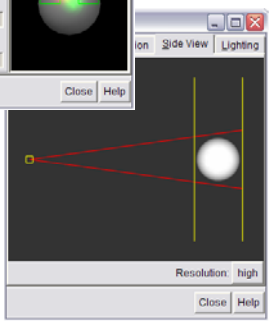


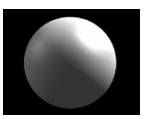
3

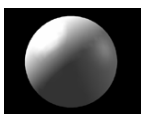
Visual Effects

Several tools enable you to control the visual components of the scene





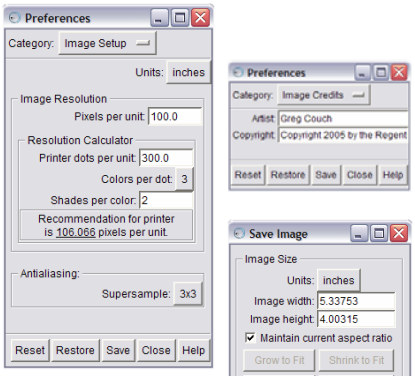


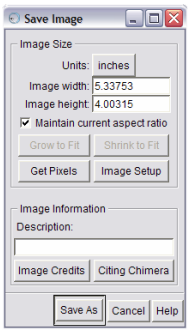


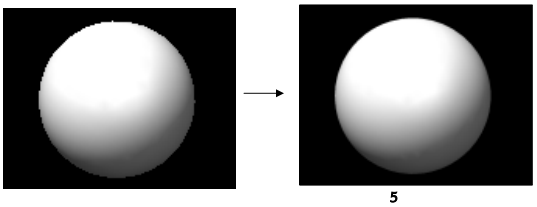
4

Publication-Quality Images

Support for multiple image formats, antialiasing, high-resolution images





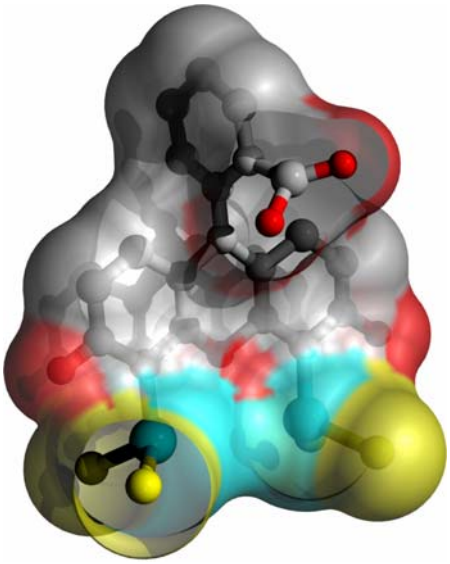


5

Alternate Renderers

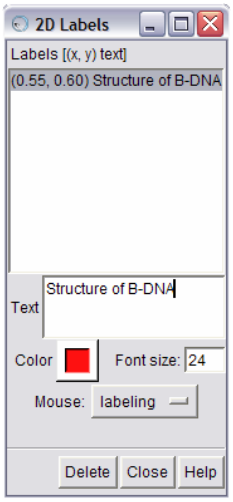
Chimera can export the current scene in X3D, Pov-ray, and RenderMan formats. Browser plugins exist for X3D. Pov-ray is a raytracing format. RenderMan is used for commercial video.

Image generated by free RenderMan renderer from www.3delight.com



6

Image Annotation

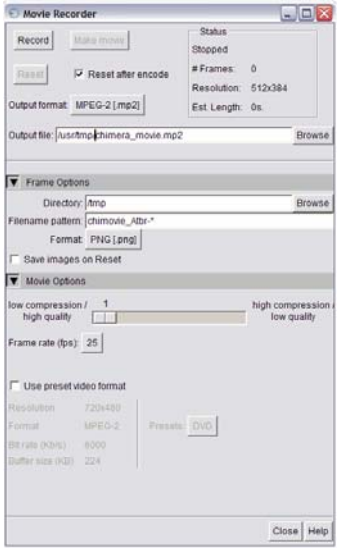


Add annotations in the graphics window using the **2D Labels** tool; label color and size are configurable

7

Capture Movies

The **Movie Recorder** tool enables you to make a movie from the contents of the graphics window; supports encoding in popular video formats

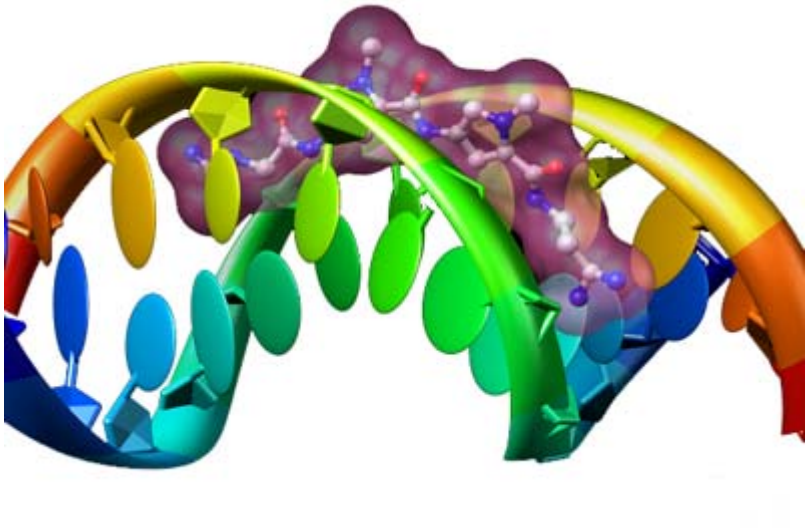


8

Producing Images and Movies in Chimera

Introduction

In addition to its utility as an in-depth analysis tool, Chimera also has many helpful facilities for creating presentation-quality media in the form of still images or movies. This tutorial will cover the usage of several of these tools. It is organized as follows:

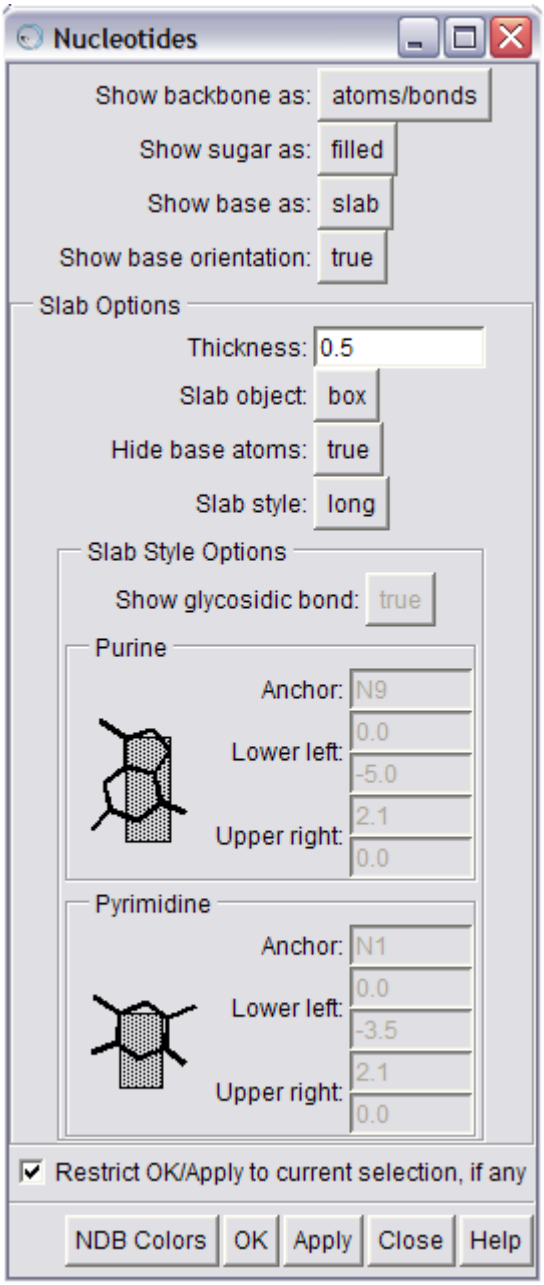


Netropsin bound to double-stranded DNA (PDB entry 6bna). Taken from the Chimera Image Gallery.

Setting the scene

The system that will be used throughout this tutorial is is the PDB model `1BNA` (structure of B-DNA dodecamer). Open the file 1BNA.pdb by choosing **File→Open** from the Chimera menu and browsing to the file.

Using the Nucleotides tool



The Nucleotides tool can be used to create abstract representations of nucleic acid models.

Chimera's **Nucleotides** tool can be used to obtain highly stylized renditions of nucleotide structures, including VRML (*Virtual Reality Modeling Language*) representations of the base and sugar moieties.

Start Chimera's **Nucleotides** tool (**Tools→Depiction→Nucleotides**).

You can click the **NDB Colors** button at the bottom of the panel to use the standard Nucleic Acid Database coloring scheme. Try changing other parameters on the **Nucleotides** dialog to alter the characteristics of the abstract rendering. For example, one configuration could be:

Show backbone as:	**ribbon**
Show sugar as:	**tube**
Show base as:	**slab**
Show base orientation:	**false**
Thickness:	**0.5**
Slab object:	**ellipsoid**
Hide base atoms:	**true**
Slab style:	**big**

When you have set the desired parameters, press the **Apply** button to see the changes applied to the model in the graphics window. When you are satisfied with the nucleotide representation, dismiss the **Nucleotides** dialog by clicking on the **Close** button.

The little dots that look like a starfield surrounding the model are water molecules. They can be undisplayed in one of several ways. You can select one water molecule by **Ctrl**-left-clicking on it, then press the ↑ (up-arrow) key to promote the selection to include all the molecules in the water chain. Alternatively, you can select the water chain by choosing **Select→Chain →water** from the Chimera menu. Then undisplay the selection by using the command `~disp sel` in the Command Line.

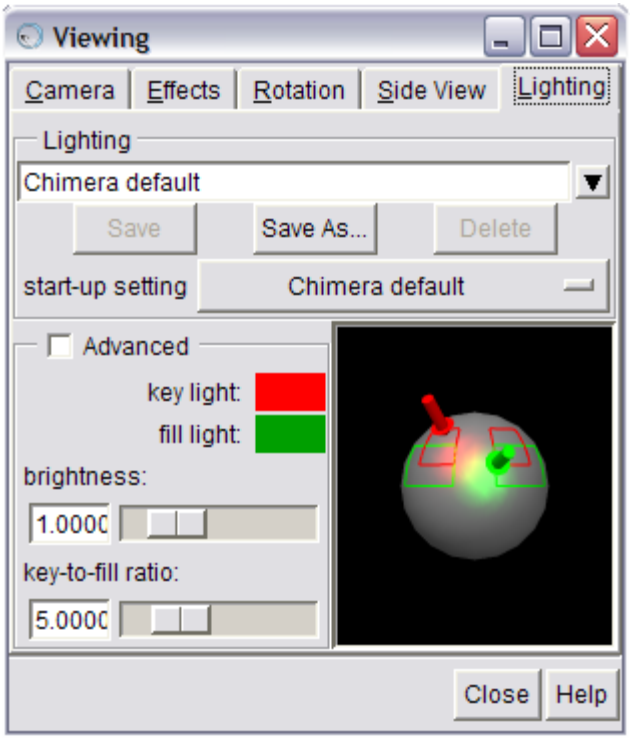
One more refinement to try is changing the representation style of the ribbon by either issuing the

command `ribrepr smooth`, or choosing **Actions→Ribbon→round** from the menu. Other available ribbon representations are `flat` and `edged`.

Viewing Controls

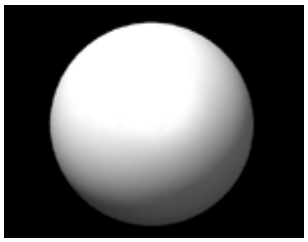
The next set of tools enables you to manipulate visual settings in Chimera. They are accessible as tabs on the **Viewing** tool, or directly from the **Viewing Controls** menu (**Tools→Viewing Controls**).

Lighting

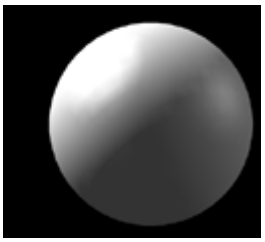


The Lighting tool lets you change the position of Chimera's two lights.

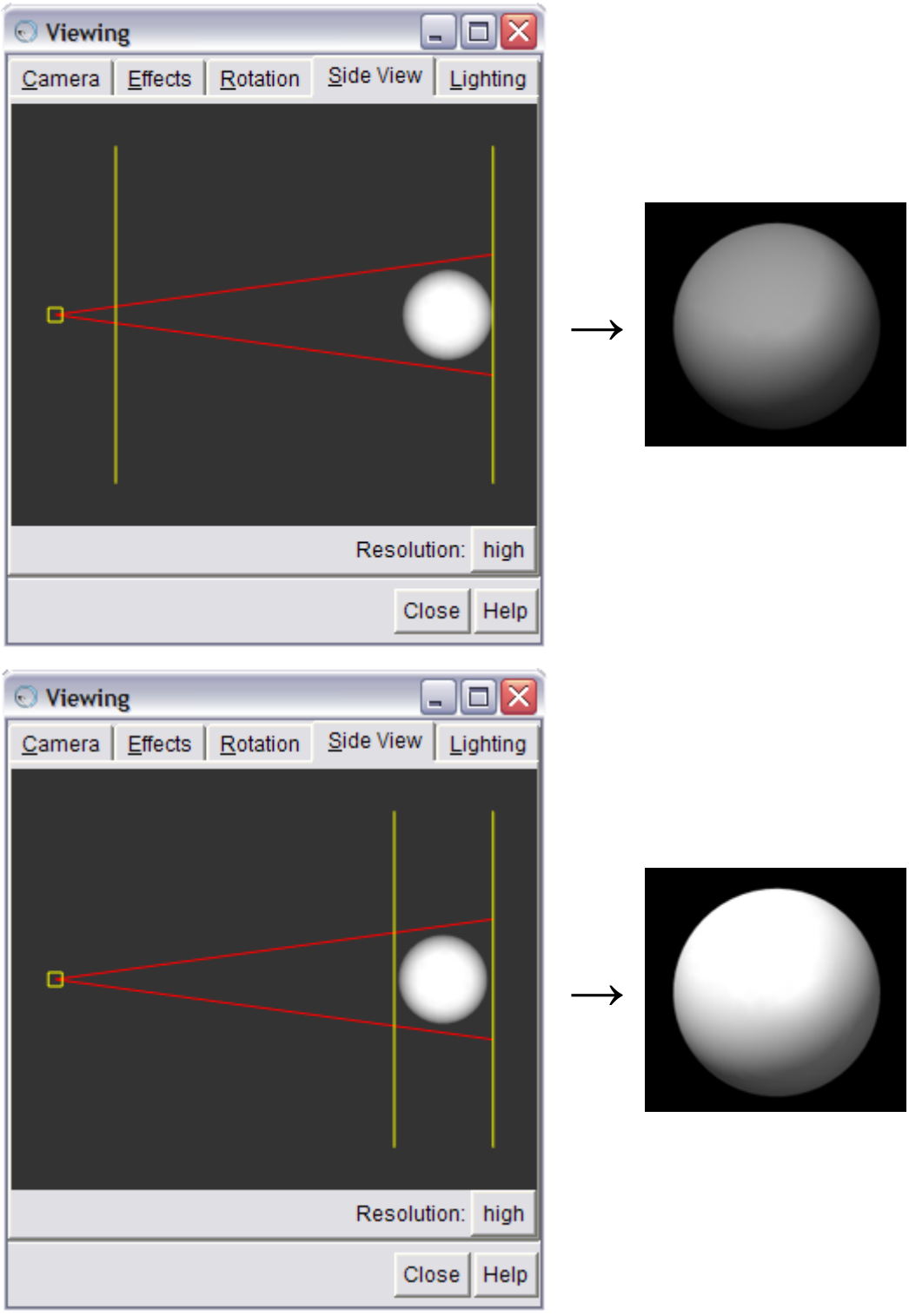
The scene starts out a little too dark for view
of light to light the scene. The orientation the
tool (**Tools→Viewing Controls→Lighting**). This
configurations, then save them into your pref
main illumination of your models while the **f**
green outlines on the sphere (for the **key light**
typically give favorable results. Try dragging
scene in the graphics window. See the discus
lighting in Chimera.



Chimera default lighting configuration



key light upper left, fil light middle right



An object that is far from the front clip plane (*top*), will appear dark, while an object that is close to the front clip plane (*bottom*) appears brighter.

Depth cueing

Chimera dims parts of the scene that are further from you to give a sense of depth (called **depth cueing**). This feature can be turned off by unchecking the **depth cueing** checkbox in the **Effects** dialog (**Tools→Viewing**

Controls→Effects). This dialog also lets you change other characteristics of depth cueing, such as color; different color backgrounds may look better with a corresponding depth cueing color.

Side View

The dimming of the scene occurs between the near and far clip planes. The clip planes can be adjusted

in the **Side View** tab of the **Viewing** tool (also accessible directly from the menu — **Tools→Viewing Controls→Side View**). The **Side View** window displays the open models as seen from the side. Two vertical yellow lines indicate the front and back clip planes. The left line is the front clip plane. If you drag the front clip plane (yellow vertical line) towards the models with the mouse you will see the brightness in the main graphics window increase (provided depth cueing is turned on). If you move the front clip plane so it intersects the models, you will see the surface cut in the main graphics window.

The small yellow box at the left in the **Side View** is your eye position. You can drag this right or left to zoom in and out.

Rendering quality

The **Effects** dialog also allows you to control rendering quality. The smoothness of curved surfaces in the stick, ball-and-stick, sphere, and ribbon molecular representations can be increased by raising the **subdivision quality**. Higher values increase smoothness but may slow performance. When saving images, the quaility is temporarily increased to 5 if it is lower. The maximum quality is 20.0. The default quality of 1 is designed for interactive use.

Similarly, the smoothness of molecular surfaces (not included in this example) can be increased by increasing the **vertex density** in the surface attributes panel (opened by choosing a surface model in the left side of the **Model Panel** [**Tools→General Controls→Model Panel**] and then clicking **attributes...** on the right).

Shininess

You can control how shiny the models appear using menu entry **Tools→Viewing Controls→Shininess Control**. The shininess parameter effects the size of **specular highlights**. Specular highlights are the lighting spots on the model. The **brightness** parameter just effects the brightness of the highlights, not the whole surface.

Background color

The background can be any color, but white is often good for publication. The background color can be changed by issuing the `set bg_color` command (e.g., `set bg_color white`), using **Actions→Color** in the menu, or setting **Background color** in the **Background** preference category (**Favorites→Preferences**). Further, if system hardware permits, starting Chimera with the **--bgopacity** option enables background transparency. Images saved with a transparent background are easier to composite with different backgrounds in image-editing applications.

Saving an image

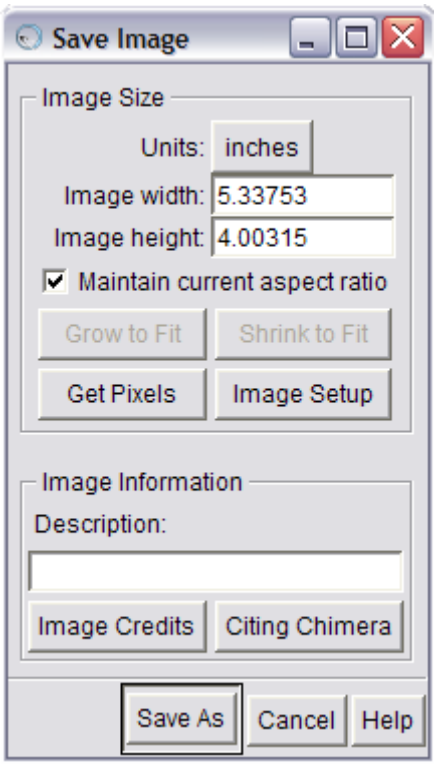
Two tools control all the options for saving images in Chimera — the **Save Image** panel and the **Image Setup** preferences category.

Save Image panel

Use the menu entry **File→Save Image** to open the **Save Image** panel. This panel lets you specify the target dimensions for your image. The dimensions can be specified directly in pixels, or in units of length. If units of length, the number of pixels per unit can be controlled in the **Image Setup** preferences category.

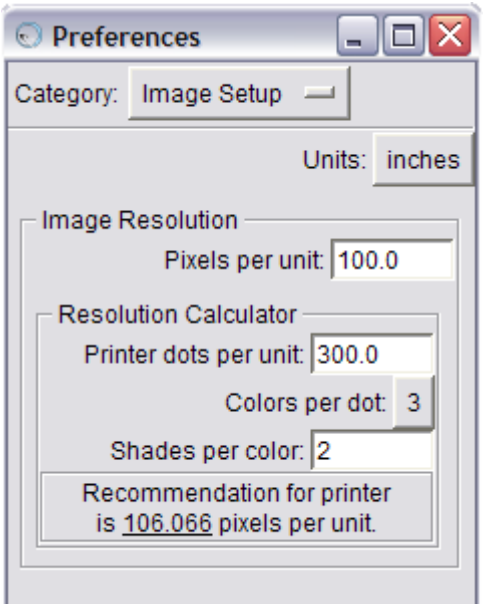
If you want an image with exactly the same number of pixels as the Chimera window on the screen, press the **Get Pixels** button. This fills in **Image width** and **Image height** with the exact size in pixels of the Chimera graphics window.

It is important that the aspect ratio of the graphics window match the aspect ratio of the desired image size. When the **Maintain current aspect ratio** checkbutton is on, editing the value for one dimension (**Image width** or **Image height**) and then clicking in the field for the other dimension adjusts the latter automatically. When the **Maintain current aspect ratio** checkbutton is off, you must either use **Grow to Fit** (make one dimension larger) or **Shrink to Fit** (make one dimension smaller) to make the aspect ratio of the graphics window match the aspect ratio dictated by **Image width** and **Image height**.



The Save Image dialog can be used to specify the target size of the image to be saved.

Image Setup preferences

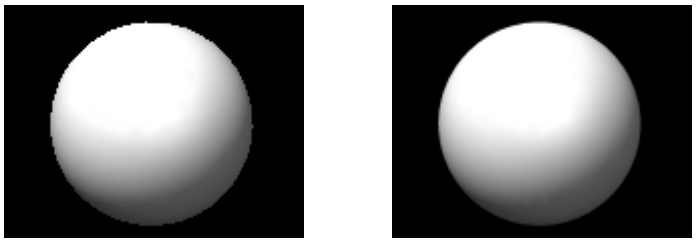


The **Image Setup** preferences category sets specifications for images saved to files using the **Save Image** panel.

For example, if a journal requirement calls for an image to be 85 mm (3.346 in) with a resolution of at least 300 dpi, you could use the **Save Image** panel to set **Units** to inches and **Image width** to at least 3.346, then use the **Image Setup** preferences to set **Pixels per unit** to 300.

Supersampling

The Image Setup preference category The **Image Setup** preferences can also be used to set the level of supersampling. Sometimes straight edges in the graphics window may appear as tiny zigzags, especially against a white background. Supersampling gets rid of such jagged edges within saved images by making an initial image larger than that requested and then sampling it down to the final size. The default value of **3x3** is generally sufficient for publication.



The image without supersampling (*left*) has jagged edges around the perimeter of the sphere, while the supersampled image (*right*, supersampling set to 6x6) has smoother edges.

Stereo pairs

To generate stereo images, change the **camera mode** setting in the **Camera** tool (**Tools→Viewing Controls→Camera**) before saving an image file. Due to current problems with the **cross-eye stereo** and **wall-eye stereo** options, the best approach is to save separate images using the **stereo left eye** and **stereo right eye** options and assemble them in the desired order to give a cross-eye or wall-eye stereo image.

Writing to a file

Once all the desired options have been set, press the **Save As** button on the **Save Image** panel to save to a file.

Clicking **Save As** causes the image to be redrawn in an appropriate size for saving. Because this is generally a different resolution than that shown on the screen, different portions of the image will "flash" within the graphics window.

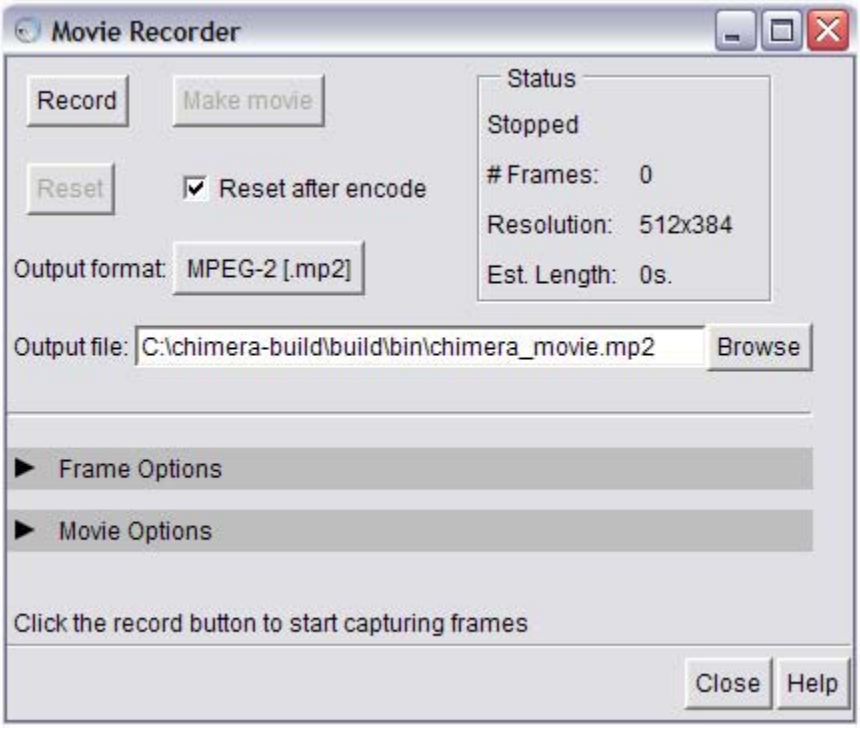
Note: It is important that you don't move any windows on top of the Chimera graphics window while saving an image and that the Chimera graphics window be completely on-screen. Because of current limitations in the way Chimera saves images, any window that is placed over the graphics window (or clipping due to being partially off-screen) while Chimera is capturing its contents will make an unwanted appearance in the saved image.

When the image computation is finished, a file name and file type (format) can be specified, or the save can be canceled.

Using the Movie Recorder tool

Chimera's **Movie Recorder** tool enables you to make movies from the contents of the graphics window. The movie recording process can be split into two steps:

1. capturing a series of frames
2. encoding captured frames into a movie



The Movie Recorder tool lets you make a movie from the contents of the graphics window.

Open the **Movie Recorder** dialog by selecting **Tools→Utilities→Movie Recorder** from the Chimera menu. Buttons that control frame recording and movie encoding are at the top of the dialog. The **Status** section keeps track of information such as the number of frames that have been captured and the current size of the Chimera graphics window. Advanced options can be found in the **Frame options** and **Movie options** sections, which are hidden by default. These sections can be expanded by clicking on the right arrow next to their respective label (these options are described at the end of this section).

Step 1 - Capturing Frames

Moving images are composed of a series of single frames, shown in rapid succession. Film in a movie theatre is played back at 24 frames per second, video on Digital Video Disc (DVD) is shown at 30 frames per second, etc. Thus, the first step to making a movie is capturing a series of frames.

Download `dna-movie.cmd` (a Chimera command file) to an easily accessible location on your computer. It contains a series of commands that will change the orientation of the open `1BNA` model over the course of many frames.

Choose **File→Open** from the menu to bring up the **Open File** dialog. Browse to the location where you saved `dna-movie.cmd` but don't open it just yet — you'll want to start recording before executing this file. Keep the **Open File** dialog open; you'll be needing it again shortly.

A note on frame resolution

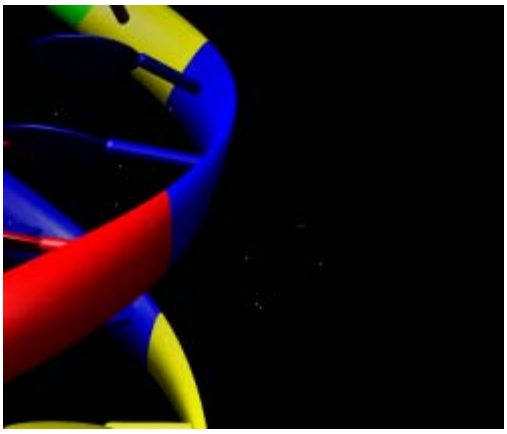
The **Status** section displays the current size of the Chimera graphics window. When the size of the graphics window changes (e.g., you resize the window), this will automatically be reflected in the **Status** section of the **Movie Recorder** dialog.

The resolution of the graphics window directly affects the resolution of the frames that are captured,

and the subsequent resolution of the movie that is encoded: if the graphics window is 512 pixels wide by 384 pixels high (512x384), all captured frames will be 512x384, and by default, the resulting movie will have a resolution of 512x384. It is not advisable to change the size of the Chimera window when you already have some frames recorded, as encoding a movie from different-sized frames will most likely cause the encoder to crash.

Action!

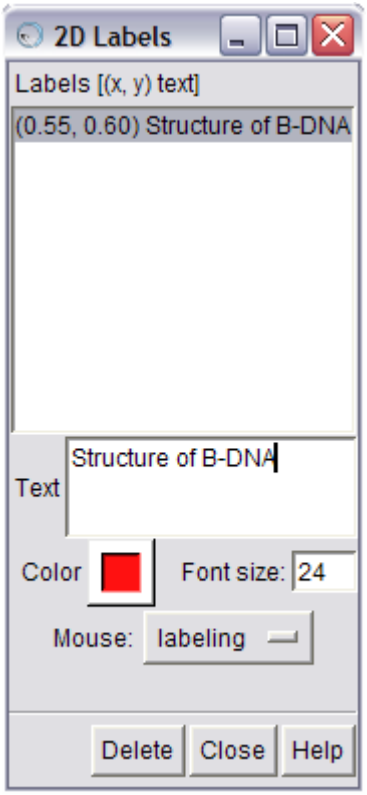
This next part calls for some planning. The goal is to start recording frames, then quickly open the command file (`dna-movie.cmd`) that was downloaded earlier. One way to do this is to have both the **Movie Recorder** dialog and the **Open File** dialog open, with the **Open File** dialog already browsed to the file. Take a deep breath, click **Record** (on the **Movie Recorder** dialog), then click **Open** (on the **Open File** dialog), then sit back and watch... the script runs for about three minutes and should consume about 2500 frames, depending on the speed of your machine.



This is what the graphics window will look like when the `dna-movie.cmd` script has finished running. Press the Stop button!

The **Status** section keeps track of the number of frames that have been recorded. You may notice that Chimera appears to slow down while frames are being captured; this is normal, and happens because Chimera is working hard trying to save a picture of the graphics window many times per second. When Chimera has finished running the script, all motion will stop, and the DNA model will be positioned vertically, half-off the left-hand side of the window. Click the **Stop** button (which was formerly labeled **Record**) to stop capturing frames. Now it's time to add some annotations to the scene.

Annotation with 2D Labels



The 2D Labels tool lets you place two-dimensional labels in the graphics window.

Chimera's **2D Labels** tool can be used to place labels of arbitrary text, font size, and color within the Chimera graphics window. These labels are saved in Chimera session files, and they can be saved in images.

Note: The frames that are saved by **Movie Recorder** are not supersampled.

Adding a new label

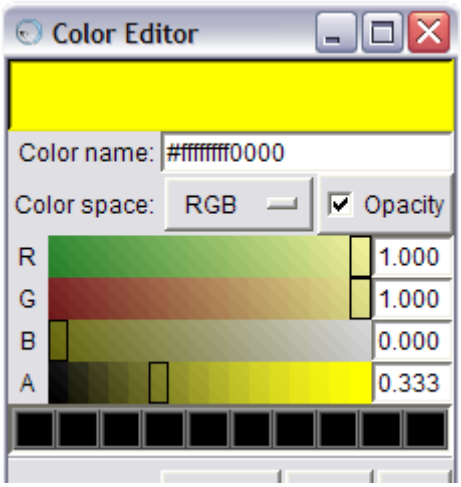
Start the **2D Label** tool by selecting **Tools→Utilities→2D Labels** from the Chimera menu. To make a new label, click into the Chimera graphics window and just start typing. You will see your text appear as a label in the graphics window, as well as in the box labeled **Text** in the **2D Labels** dialog. Click and drag on a label in the Chimera graphics window to move it to a new location. You can change the size of the label by entering a new **Font size** and pressing **Return**, or the color by clicking on the color well (box with a raised border) labeled **Color** and selecting a new color. To delete a label, select it from the **Labels** list and click the **Delete** button at the bottom of the dialog.

2D Label mouse modes

When the **2D Labels** dialog is displayed, left-mouse clicks in the Chimera graphics window (which are normally interpreted as model rotation) are assumed to be label-related, i.e., intended to create a new label or move an existing one. The **Mouse** drop-down menu in the **2D Labels** dialog reflects this state; it is by default set to **labeling**. So if you are trying to rotate a model in the graphics window and it does not appear to be responding, it could be that you forgot to **Close** the **2D Labels** dialog, and you just unknowingly added a new label. You can restore the normal mouse behavior (e.g., model rotation) while the **2D Labels** dialog is displayed by selecting the **normal** setting from the **Mouse** drop-down menu. Additionally, **Close**ing the **2D Labels** dialog will return left-mouse click behavior to normal.

Using color opacity to fade labels

One neat trick is to use the opacity of label colors to give the effect of fading in or out over a series of frames. Add a label to the Chimera graphics window as described above.



→

A lower opacity value on the 'A' slider (*top*) makes a color more transparent (less opaque), while a higher opacity (*bottom*) makes it less transparent (more opaque).

In the **2D Labels** dialog, select a label, then click on the color well. Click the checkbox called **Opacity**. This adds another slider, labeled **A** to the existing **R**, **G**, and **B** slider bars. Moving the **A** slider bar to the left (lower values) results in a color with lower opacity, or more transparency, while moving it to the right (higher values) achieves the opposite affect. Thus, labels can be essentially hidden by setting their opacity to zero. Try starting with zero opacity, and slowly moving the slider to the right for a fade-in effect.

Restart the capturing of frames, which will now include the annotations added with **2D Label**, by clicking the **Record** button in the **Movie Recorder** dialog. This will append frames to the existing series already captured. Click **Stop** when you are finished adding labels.

Step 2 - Encoding frames into a movie

Now that you have some frames saved up (as evidenced by the **# Frames** field in the **Status** box), you can make a movie. You can specify where you would like the movie to be saved by typing in or browsing for a filename in the **Output file** field. The default movie format is MPEG-2 (.mp2), but you can select a different format from the **Output format** drop-down box. Now click the **Make movie** button to encode a movie file from saved frames. Status information will appear at the bottom of the **Movie Recorder** window.

Once the movie has finished encoding, the **Status** will change to reflect the result of the encoding process (*Successfully encoded* if everything went smoothly, *Encoding error* if an error occured during encoding, or *Canceled* if encoding was canceled by clicking on the **Cancel movie** button). The path describing where the movie was saved (or any errors, if something went wrong) will be printed to the **Reply Log**.

A note on movie resolution

Note that while it is possible to encode a movie at a different resolution than the size of the frames that comprise it (by choosing a **preset video format**, as described below in the **Advanced movie encoding options** section), encoding a movie at the same resolution as its source frames will result in better quality.

Resetting the Movie Recorder

Movie Recorder can be reset in one of two ways:

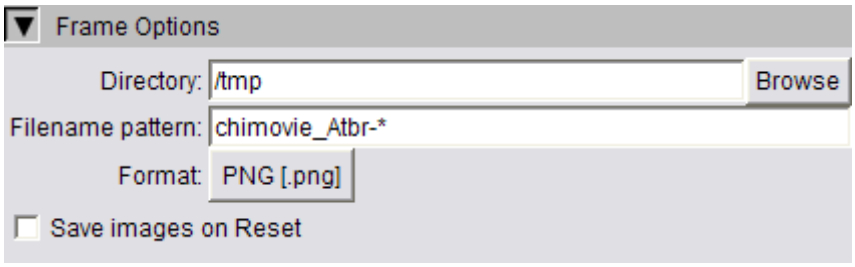
- automatically, upon successfully encoding a movie, or
- manually, by pressing the **Reset** button at any time

If the movie is encoded successfully, the default behavior is for the **Movie Recorder** to reset, setting the frame count back to zero and enabling you to start another movie. This "automatic reset" behavior can be controlled by toggling the **Reset after encode** checkbutton at the top of the **Movie Recorder** dialog.

Where are all the captured frames?

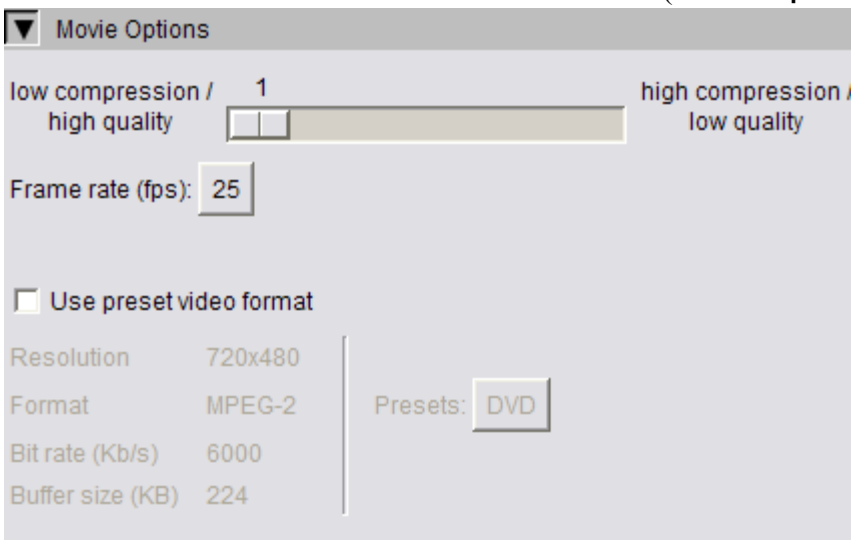
By default, when the **Movie Recorder** is reset (either as a result of a movie being successfully encoded, or as a result of manually pressing the **Reset** button), all frames that have been saved during the recording phase are deleted. However, it may be desirable to keep these frames, e.g. to use in another video editing application. Enabling the **Save images on Reset** checkbutton, located in the **Frame Options** section, will ensure that captured frames are saved. The location and names of the saved frames are dictated by the **Directory** and **Filename pattern** options.

Advanced options



The Frame Options section

The settings in the **Frame Options** section control several aspects of how frames are saved. You can specify the directory into which frames will be stored (**Directory**), the pattern by which sequential frames will be named (**Filename pattern**), the image format of saved frames (**Format**), and whether the captured frames should be saved when the Recorder is reset (**Save images on Reset**).



The settings in the **Movie Options** section control several parameters of the movie encoding process. The slider bar lets you specify the tradeoff between movie quality and compression, and the

Frame rate option lets you choose the target frame rate of the movie in frames per second. Clicking on the **Use preset video format** option enables you to choose one of several standardized video formats, each with associated encoding parameters such as **Format** and **Resolution**. Choosing the **Custom** preset lets you customize the parameters for a given video preset. Note that if **Use preset video format** is selected, it overrides the format specified by the **Output format** option at the top of the **Movie Recorder** dialog.

Command-line interface

The functionality of **Movie Recorder** is accessible from the command line with the `movie` command. While using the **Movie Recorder** graphical interface may be easier for interactive use, the `movie` command can be very useful in a scripting context. For example, if you have a script that opens a model, changes the representation, then executes some commands to change the orientation, you can add a few `movie` commands to automatically start capturing frames once the model is set up, then encode a movie once all orientation changes have occurred. For example:

```
open 1gcn
color cornflower blue
surf
# start capturing frames, in .png format
movie record fformat png
roll y 1 180; wait
roll z 1 90; wait
roll y 1 180; wait
close #0
# stop recording frames
movie stop
# write status information to reply log
movie status
# encode a movie in mp4 format from recorded frames
movie encode mformat mp4 output C:\\tmp\\path-to-movie.mp4
```

The documentation page for the movie command has more information about its usage.

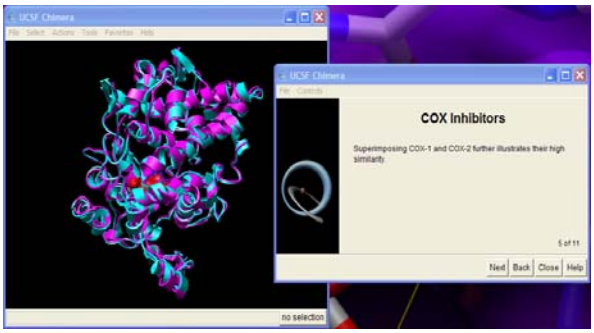
More information

Here are links to more information about the topics covered in this tutorial:

- Chimera User's Guide
- The Nucleotides manual page
- Images for Publication Tutorial
- Image Setup Preferences manual page
- Save Image panel manual page
- The Viewing Tool manual page (includes Lighting, Side View, Depth Cueing)
- The 2D Labels manual page
- The Movie Recorder manual page
- List of useful commands for scripting animations

Chimera Scripts and Demos

An introduction to scripting chimera and creating presentations



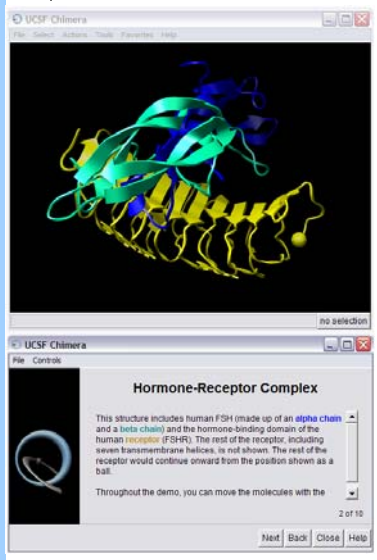
1

Scripting

- Chimera has 3 interactive interfaces
  - The graphical user interface (GUI)
  - The Command Line tool
  - Python code via the IDLE tool
- Scripts are a file-based interface to replay commands and/or code

2

Demos



- Demos are presentations within chimera
- A demo can include several panels consisting of
  - A set of operations
  - Explanatory text
- Demo Editor prepares demo source files

3

Chimera Scripts and Demos

Prerequisites

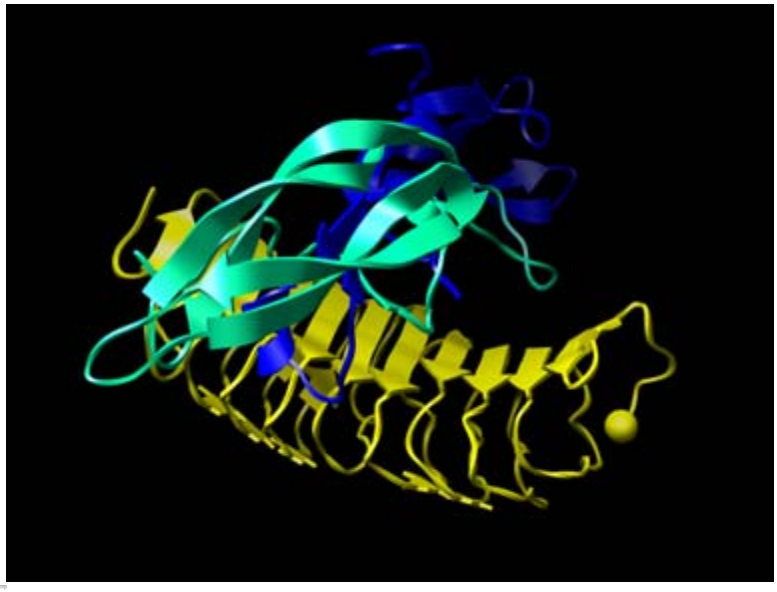
In this tutorial, it is assumed that you have used chimera before, that you have used the chimera command line, and you'd like to learn how to create a presentation.

Introduction

Chimera has three interactive methods for manipulating data: the graphical user interface (GUI), the command line (**Tools / General Controls / Command Line**), and Python code (**Tools / General Controls / IDLE**). Except for the GUI, the typed-in commands can can be scripted, *i.e.*, replayed from a file. Chimera also provides a Demo tool to organize scripts with a simple GUI that steps through the script and provides explanatory text.

Scripts are an excellent way to create content for animations.

This tutorial will cover developing scripts from commands, from Python code, and organizing them with the Demo Editor tool. It is organized as follows:



Follicle-stimulating Hormone (FSH) — Receptor Complex

Command Line Scripts

Frame-based commands

Most chimera commands take effect immediately. For example, when you color a molecule, all of the atom colors are immediately changed. Some commands, given below, can be spread out over time. Those commands have an extra parameter which is the number of frames to spread the effect over. Chimera keeps track of time by the number of frames that have passed, by default a frame is roughly 1/30 of a second.

line

```
1  #
2  # Chimera command script showing green fluorescent protein (PDB 1gfl)
3  #
4  2dlabels create lab1 text 'Green Fluorescent Protein' color light sea green size 2
5  open 1gfl; del ~ :.a; window; linewidth 3; scale 1.6; rainbow; wait
6  sleep 3
7  chain @n,ca,c,o; wait 1
8  sleep 3
9  ~disp; ribbon
10 2dlabels change lab1 visibility hide frames 90; wait
11 2dlabels delete lab1
12 roll y 1 180; wait
13 ribrepr edged
14 roll y 1 180; wait
15 ribrepr smooth
16 roll y 1 180; wait
17 ribbackbone; repr sphere :1.a,230.a@ca; color white,a :1.a,230.a@ca; disp :1.a,230
18 roll y 1 90; wait
19 scale 1.015 20; wait
20 disp :65-67.a; color byatom :65-67.a; repr cpk :65-67.a; wait 1
21 clip hither -1 20; wait
22 sleep 5
23 clip hither 1 20; wait
24 scale 0.98 10; wait
25 disp :99.a,153.a,163.a,167.a,202.a,203.a,222.a;repr bs :99.a,153.a,163.a,167.a,202
26 sleep 2
27 roll y 1 180
28 echo script finished
```

1gfl.com command file

Take this time to review the frame-based commands, examine the example command file 1gfl.com — duplicated above in a table with reference line numbers, and run it.

There are many chimera idioms in that script:

On line 5:

`del ~ :.a` — permanently deletes all atoms except for those in chain a. The atom specification syntax is very powerful.

`window; scale 1.6` — The `window` command causes the view to be centered around the

molecule such that it can be rotated in any direction and still be completely visible. Usually, that leaves some extra space around the molecule. So the view is `scale`d up.

`linewidth 3` — makes the lines more visible. This is useful when using an overhead projector. An alternative would be to use `sticks` for the atoms and bonds.

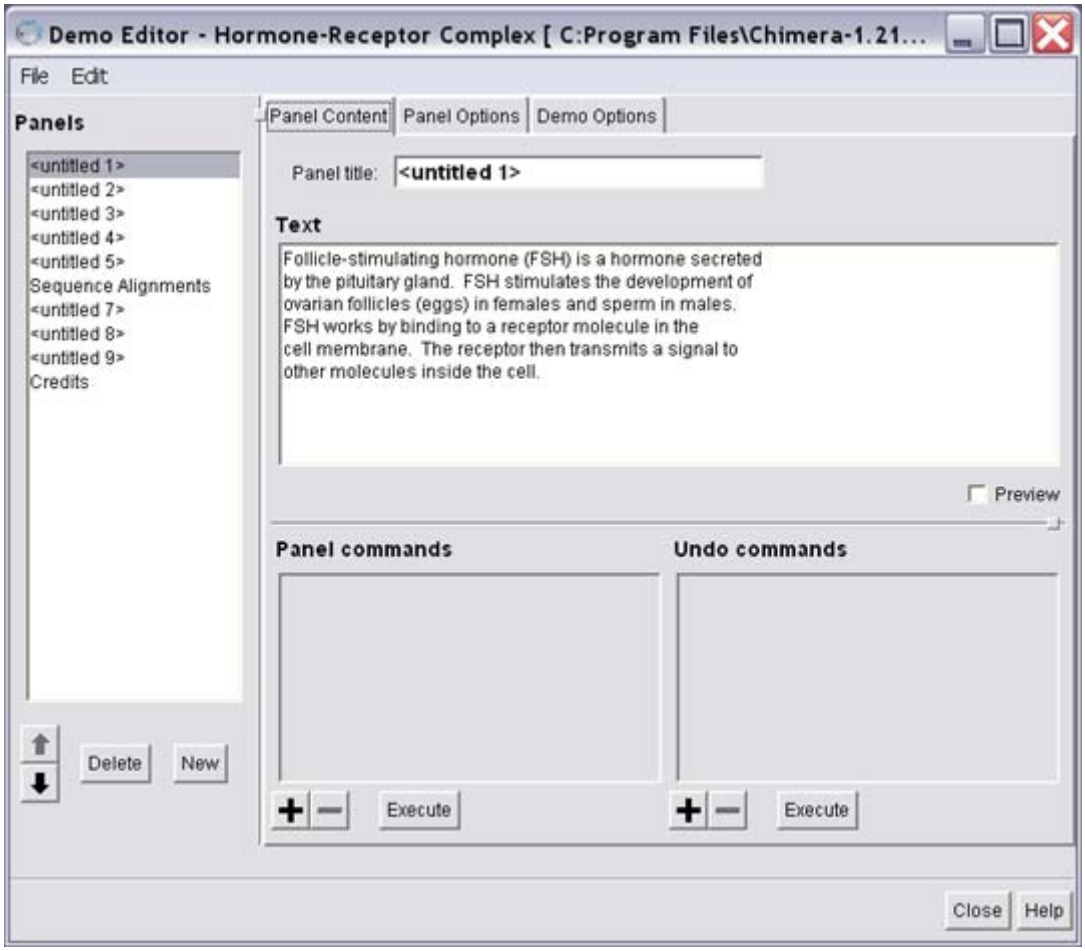
`wait` — a historical artifact from when `scale` commands without a frame count were delayed as if the count were one.

On line 7:

`wait 1` — changes in representation only become visible when the next frame is drawn. This insures that the next frame is drawn before the script continues. And `wait` by itself wouldn't do anything because there are no queued actions.

If the script opened a session file, then much more can prepared in advance. The `savepos` and `reset` commands can save and restore positions. Selections can be saved for simpler manipulation, using **Name Selections...**.

Demo Editor



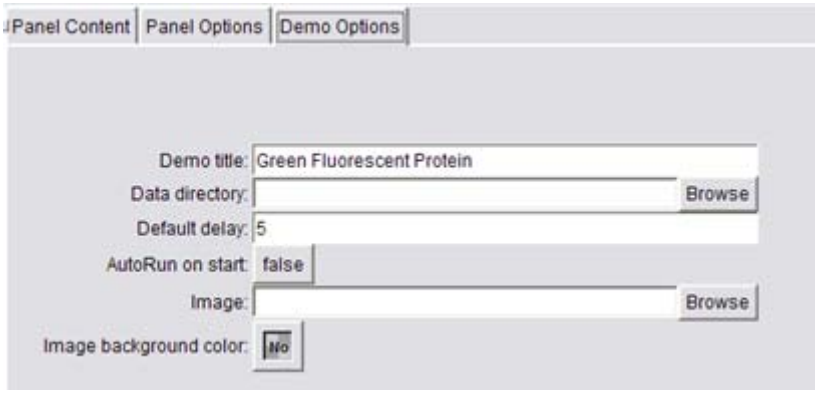
The Demo Editor tool

The goal of this section is to take the command script from the previous section and convert it into a demo using the Demo Editor.

If you haven't done so already, save the 1gfl.com file (as a text file) so you can copy & paste lines from it (the realistic scenario). Or you can scroll back to the previous section and copy & paste from there.

Next, run a demo to see what they're like. Either the **Tools / Demos / COX Inhibitors Demo** or the **Tools / Demos / Hormone-Receptors Complex Demo.** You will see a sequence of panels with explanations about what is happening in the main graphics window.

Now, bring up the Demo Editor dialog, **Tools / Demos / Demo Editor**. The Demo Editor has two parts, the list of demo panels and a tabbed control to select between **Panel Content**, **Panel Options**, and **Demo Options**. Start with **Demo Options** and set the title of your demo. You can also change the image from the default chimera logo. Switch back to **Panel Content** when you're done.



Demo Options

Deciding what should be in a

demo and in what order is beyond the scope of this tutorial. Instead, you are going to break up the contents of the 1gfl.com script into panels by using the natural breaks given by the `sleep` commands, so each panel will be the code in between. Each panel is created by clicking the **New** button under the **Panels** section. You will need five panels for this exercise.

Filling in Demo Content

1gfl.com starts with displaying a 2D label with the name of the protein. Since the demo provides a separate panel for text, that should be moved over to the **Text** portion of the **Panel Content**. It would also be nice to credit the paper that originally presented the solved protein structure — if you **File / Fetch** 1gfl, you can get the PDB headers with that information by bringing up the **Favorites / Model Panel**, clicking **attributes...**, and then clicking **PDB Headers...**. To copy & paste, use the mouse to select text and the normal keyboard shortcuts for your platform.

Next, create an empty **Panel Command** by clicking the **+** button. And copy line 5 of 1gfl.com, starting with `open 1gfl`. You are now done with the first panel.

Next fill in the rest of the panels by copy & pasting the command in 1gfl.com into the appropriate **Panel Command**s. The hardest part might be deciding what the test for each panel should be.

Finally, show your demo to someone else.

Python scripts

While the command line can be used for many things, the ultimate control of chimera is through Python scripts. Assuming you already know Python (if not, google for "Python tutorial" and be prepared to spend some time), the Chimera Programmer's Guide has many valuable examples. If you need more information, please send email to the chimera developers mailing list. In the past, additional examples have been the result of questions.

For this tutorial and in general, experiment with Python code in chimera by using the **Tools / General Controls / IDLE** tool. Another method is to create Python code using your favorite text editor, and running chimera from a terminal shell (on Windows, the Command Prompt) with that file as an argument. If you give the `--nogui` option to chimera, you can use chimera to do batch molecular computations. Python scripts can executed in chimera by opening the file, either through **File / Open** or with the **open** command.

Before continuing, go to the Chimera Programmer's Guide and go through the first two examples: **Chimera's Object Model** and **Molecular Editing Using Python**.

Saving commands as Python code

When the command line is present, **Favorites / Command Line**, you can save a Python equivalent to the commands you've typed in. The drop down arrow button on the right side of the command line brings up a list of recent commands you've typed in that you can re-edit by clicking on one. The last entry entry, **Command History...**, is special and brings up the list of all of the commands you've typed in, and the **Record...** button will save the commands to file as commands or as equivalent Python code.

The Python code is naive:

```
import chimera
from chimera import runCommand
runCommand('open 1gfl')
```

Using the Midas module

If you know Python, it is more flexible to use the functions in the **Midas** module that implements the basic commands. (chimera's predecessor was called midas and most of the commands carried over.) The previous example becomes:

```
import Midas
modellist = Midas.open('1gfl')
```

And then you can interate through the *modellist* and manipulate the models programmatically.

To find out all of the functions using IDLE, type:

```
import Midas
help(Midas)
```

And you'll see all of the functions provided by the Midas module. In general, there is a one-to-one correspondence to the commands listed in the User's Guide. Python's help function works everywhere.

If you are looking for coding examples beyond what is provided in the Programmer's Guide, looking at the source to the Midas module is very instructive, particularly CHIMERA/share/Midas/__init__.py, where CHIMERA is where chimera is installed.

More information

Here are links to more information about the topics covered in this tutorial:

General Information
- Chimera User's Guide

Command line
- The Getting Started Tutorial — Command Version
- Index of commands
- frame-based commands for scripting animations

Demos
- The Demo Tool manual page (includes Demo Editor)

Python Coding
- Python documentation
- Python tutorial
- Chimera Programmer's Guide

Workshop Evaluation

Thank you for participating in the UCSF Chimera Workshop. We really appreciate your time and attention! In order to help us continue to improve the quality and utility of the workshops, please take a few moments to provide us some feedback on your experience.

The Chimera Team

	Clarity & Style					Quality of Materials				
Introduction to UCSF Chimera	Not clear	Sometimes Not clear	About right	Very good	Excellent	Insufficient	Needs help	About right	Very good	Excellent
Eric Pettersen	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Hands-on tutorial	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Comments: _____

_____

	Clarity & Style					Quality of Materials				
Exploring sequence-structure relationships	Not clear	Sometimes Not clear	About right	Very good	Excellent	Insufficient	Needs help	About right	Very good	Excellent
Elaine Meng	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Hands-on tutorial	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Comments: _____

_____

	Clarity & Style					Quality of Materials				
Screening docked ligands	Not clear	Sometimes Not clear	About right	Very good	Excellent	Insufficient	Needs help	About right	Very good	Excellent
Elaine Meng	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Hands-on tutorial	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Comments: _____

_____

	Clarity & Style					Quality of Materials				
MD trajectories	Not clear	Sometimes Not clear	About right	Very good	Excellent	Insufficient	Needs help	About right	Very good	Excellent
Eric Pettersen	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Hands-on tutorial	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Comments: _____

_____

(over)

	Clarity & Style					Quality of Materials				
Attributes	Not clear	Sometimes Not clear	About right	Very good	Excellent	Insufficient	Needs help	About right	Very good	Excellent
Conrad Huang	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Hands-on tutorial	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Comments: _____

_____

	Clarity & Style					Quality of Materials				
Large molecular asemblies	Not clear	Sometimes Not clear	About right	Very good	Excellent	Insufficient	Needs help	About right	Very good	Excellent
Tom Goddard	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Hands-on tutorial	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Comments: _____

_____

	Clarity & Style					Quality of Materials				
Volume data	Not clear	Sometimes Not clear	About right	Very good	Excellent	Insufficient	Needs help	About right	Very good	Excellent
Tom Goddard	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Hands-on tutorial	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Comments: _____

_____

	Clarity & Style					Quality of Materials				
Images and movies	Not clear	Sometimes Not clear	About right	Very good	Excellent	Insufficient	Needs help	About right	Very good	Excellent
Greg Couch	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Hands-on tutorial	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Comments: _____

_____

	Clarity & Style					Quality of Materials				
Scripts and demos	Not clear	Sometimes Not clear	About right	Very good	Excellent	Insufficient	Needs help	About right	Very good	Excellent
Greg Couch	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
Hands-on tutorial	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Comments: _____

_____

	Value				
Overall Assessment	**Not worth the time**	**Could be better**	**About right**	**Well worth it!**	**Extremely Valuable**
Presentations	☐	☐	☐	☐	☐
Hands-on tutorials	☐	☐	☐	☐	☐

Comments: _____

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_____

Anything we should have done, but didn't?

_____

_____

_____

Anything we did that we shouldn't have?

_____

_____

_____

UCSF Chimera
QUICK REFERENCE GUIDE
September 2005

Commands

*reverse function ~**command** available

2dlabels	create arbitrary text labels and place them in 2D
ac	enable accelerators (keyboard shortcuts)
addaa	add an amino acid to a peptide C-terminus
addh	add hydrogens
*alias**	create an alias or list aliases
align	align two atoms along the line of sight
angle	measure a bond angle or torsion angle
*bond**	add/delete bonds
*bondcolor**	color bonds independently from atoms
bonddisplay	control how bond display depends on atom display
bondrepr	control the representation of bonds (wire, stick)
brotation	make a bond rotatable
cd	change the working directory
center	center the view on specified atoms
chain	chain specified atoms, undisplay the others
chirality	report the R/S configuration of a chiral center
*clip**	move clipping planes
close	close a model
*cofr**	report or change the center of rotation
*color**	color atoms/bonds, ribbons, labels, and surfaces
colordef	define a new color
conic	create a shadowed space-filling image (static; UNIX only)
copy	save or print the displayed image
defattr	assign attribute values to atoms, residues, or models
delete	delete atoms and bonds
*display**	display specified atoms
*distance**	measure the distance between two atoms
echo	send text to the Reply Log
focus	adjust the view and center of rotation to the specified atoms
freeze	stop all motion
getcrd	report untransformed coordinates
*hbonds**	(*findhbond*) identify possible hydrogen bonds
help	display the manual page for a command
ksdssp	determine secondary structure from protein coordinates
*label**	display atom labels
labelopt	control the information in atom labels
linewidth	control the width of lines in the wireframe representation
load	restore a saved Chimera session
longbond	find and remove excessively long bonds
match	superimpose two models
matrixcopy	apply the transformation matrix of one model to another
matrixget	write the current transformation matrices to a file
matrixset	read and apply transformation matrices from a file
mmaker	(*matchmaker*) align models in sequence and then superimpose them accordingly
modelcolor	set color at the model level
*modeldisplay**	set display at the model level
move	translate along the X, Y, or Z axis
movie	capture image frames and assemble them into a movie
neon	create a shadowed solid stick image (static; UNIX only)
*objdisplay**	display graphical objects
*open**	open structures or data for display or execute a command file
pdbrun	send an annotated PDB file of the current display to the system shell (UNIX only)
push,pop	push or pop images on the picture stack
rainbow	color residues, chains, models over a range (default blue to red)
rangecolor	color over a range according to attribute values
read	execute a command file, updating the display at the end
represent	control the representation of atoms and bonds (wire, stick, bs or b+s, sphere or cpk)
reset	restore default or saved orientations
*ribbackbone**	allow residue ribbon and backbone atoms to be displayed simultaneously
*ribbon**	display a secondary structure ribbon
ribbonjr	create a ribbon image (static; UNIX only)
*ribcolor**	set ribbon color
ribrepr	control the ribbon representation (flat, edged, round)
*rlabel**	display residue labels
rmsd	evaluate the RMSD between specified sets of atoms
rock	rock about the X, Y or Z axis
roll	roll about the X, Y, or Z axis
rotation	make a bond rotatable
save	save the current Chimera session
*savepos**	save the current orientations
*scale**	scale the view
section	move the clipping planes in parallel
*select**	activate models for motion or select atoms for further operations
*set**	set options (see **Set/Unset Options**)
*show**	display specified atoms, undisplay the others
sleep	suspend command processing for a specified length of time
source	execute a command file, updating the display continually
stereo	switch amongst stereo options and mono viewing
stop	exit from Chimera
*surface**	calculate and display molecular surface
surfcat	(*msms cat*) group atoms for subsequent surface calculations
surfcolor	set whether surface color is determined at the atom or model level
surfrepr	(*msms repr*) control surface representation (solid, mesh, dot)
swapaa	mutate amino acid residues
swapna	mutate nucleic acid residues
system	send a command to the system shell
tcolor	color using texture map colors
texture	define texture maps and associated colors
thickness	move the clipping planes in opposite directions
turn	rotate about the X, Y, or Z axis
*vdw**	display van der Waals (VDW) surface
vdwdefine	set VDW radii
vdwdensity	set VDW surface dot density
version	show copyright information and which version of Chimera is being used
wait	suspend command processing until motion has stopped
window	adjust the view to contain the specified atoms
write	save a molecule model as a PDB file
writesel	write a parsable text file containing specifications of the currently selected (or unselected) items
x3dsave	save the graphical scene as an X3D file

Set/Unset Toggle Options

autocolor	make each newly opened model a unique color
independent	make each model rotate about its own center of mass instead of the combined center of mass

Set/Unset Value Options

bg_color	set background color; *value* can be any color name
dc_color	set depth cue color; *value* can be any color name

Miscellaneous Operations (Default Settings)

Action	Procedure
picking from the screen	Ctrl-left mouse button
adding to a selection	Shift-Ctrl-left mouse button
XY-rotation	left mouse button when inside the "spaceball"
Z-rotation	left mouse button when outside the "spaceball"
XY-translation	middle mouse button
Z-translation	Ctrl-middle mouse button
scaling	right mouse button or the Side View (below)
Side View	Tools...Viewing Controls...Side View
Command Line	Tools...General Controls...Command Line
Reply Log	Tools...Utilities...Reply Log
Preferences	Favorites...Preferences
listing of tools/extensions	Tools category of Preferences (above); also specify which tools start when Chimera starts, which appear in the Favorites menu, and which icons appear in the tool bar

Atom Specification Symbols

Symbol	Function	Usage
#	model number	# *model* (integer)
#.	submodel number	**#.** *submodel* (integer)
:	residue	**:** *residue* (name or number)
::	residue name	**::** *residue*
:.	chain ID	**:.** *chain*
@	atom name	**@***atom*
@.	alternate location ID	**@.** *alt_loc*
–	range	specifies a range of models, submodels, or residues
,	name separator	separates models or residues, ranges of models or residues, or names of atoms
*	whole wildcard	matches whole atom or residue names, *e.g.*,**:*@CA** specifies the alpha carbons of all residues
=	partial wildcard	matches partial atom or residue names, *e.g.*, **@C=** specifies all atoms with names beginning with C
?	single-char wildcard	used for atom and residue names only, *e.g.*, **:G??** selects all residues with three-letter names beginning with G
;	command separator	separates multiple commands on a single line
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)

Atom Attributes

Usage	Description
@/altLoc=*altloc*	*altloc* is the alternate location ID
@/bfactor=*bfactor*	*bfactor* is the B-factor
@/color=*color*	*color* is the color assigned on a per-atom basis
@/drawMode=*mode*	*mode* can be 0 (dot, as in wireframe), 1 (sphere, as in CPK), 2 (endcap, as in stick), or 3 (ball, as in ball-and-stick)
@/defaultRadius=*rad*	*rad* is the default VDW radius
@/display	whether display is enabled at the atom level
@/element=*atno*	*atno* is the atomic number
@/idatmType=*type*	*type* is the atom type
@/label	whether the atom is labeled
@/label=*label*	*label* is the text of the atom label
@/labelColor=*labcolor*	*labcolor* is the color of the atom label
@/name=*name*	*name* is the atom name
@/occupancy=*occupancy*	*occupancy* is the occupancy
@/radius=*radius*	*radius* is the current radius (may have been changed from the default VDW radius)
@/serialNumber=*n*	*n* is the atom serial number in the input file
@/surfaceCategory=*catname*	*catname* is the category the atom belongs to for surface calculation purposes (main, ligand, *etc.*)
@/surfaceColor=*surfcolor*	*surfcolor* is the color of the atom's molecular surface
@/surfaceDisplay	whether molecular surface display is turned on for the atom
@/vdw	whether VDW surface display is turned on for the atom

Residue Attributes

Usage	Description
:/isHelix	whether the residue is in an alpha helix
:/isHet	whether the residue is in HETATM records in the input PDB file
:/isStrand *or* **:/isSheet**	whether the residue is in a beta strand
:/isTurn	whether the residue is in a turn according to PDB TURN records
:/kdHydrophobicity=*value*	*value* is the Kyte-Doolittle hydrophobicity
:/ribbonColor=*ribcolor*	*ribcolor* is the color of the residue's ribbon segment
:/ribbonDisplay	whether ribbon display is turned on for the residue (can be true for residues such as water that cannot be shown with ribbon)
:/type=*resname*	*resname* is the residue name

Molecule Model Attributes

Usage	Description
#/color=*color*	*color* is the color assigned on a per-model basis
#/display	whether display is enabled at the model level
#/explicitHydrogens	whether the model has hydrogen atoms
#/lineWidth=*width*	*width* is the wireframe linewidth
#/pointSize=*size*	*size* is the font size of labels
#/vdwDensity=*density*	*density* is the dot density used for VDW surfaces

Atom Specification Examples

#0
- all atoms in model 0

#3:45-83,90-98
- residues 45 through 83 and 90 through 98 in model 3

:lys,arg
- lysine and arginine residues

:12,14@ca
- alpha carbons in residue 12 and residue 14

:12:14@ca
- all atoms in residue 12 and the alpha carbon in residue 14

:.A@ca,c,n,o
- peptide backbone atoms in chain A

:50.B,.D
- residue 50 in chain B and all residues in chain D

:12-15,16-18.a,15.b@ca
- CA atoms within the following residues: 12 through 15 (with no chain ID), 16 through 18 in chain A, and 15 in chain B

#0.1-3,5
- submodels 1-3 of model 0 and all of model 5

#0.1-3,.5
- submodels 1-3 of model 0 and submodel 5 of all models

ligand
- any/all residues automatically classified as ligand

element.S
- all sulfur atoms

@ca/!label and color!=green and color!=red
- atoms named CA which are not labeled, and are not green or red

@/color=yellow or color=blue and label
- atoms that are yellow and atoms that are both blue and labeled

:asn/isHelix
- asparagine residues in alpha helices

#1:asp,glu & #0 z<10
- aspartate and glutamate residues in model 1 within 10 angstroms of model 0

solvent & Ng+ z<3 | solvent & N3+ z<3
- solvent residues within 3 angstroms of guanidinium nitrogens or *sp*3-hybridized, formally positive nitrogens

@/bfactor>50 & ~ solvent & ~ ions
- atoms with B-factor values over 50, excluding solvent and ions