

Molecular Visualization with UCSF Chimera: Electron Microscope Density Map Analysis

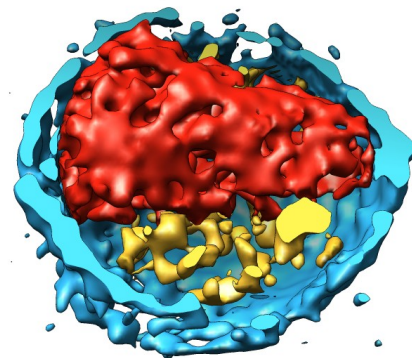
- Presentation and follow-along tutorial
-

Chimera Tutorial: Visualizing Electron Tomography

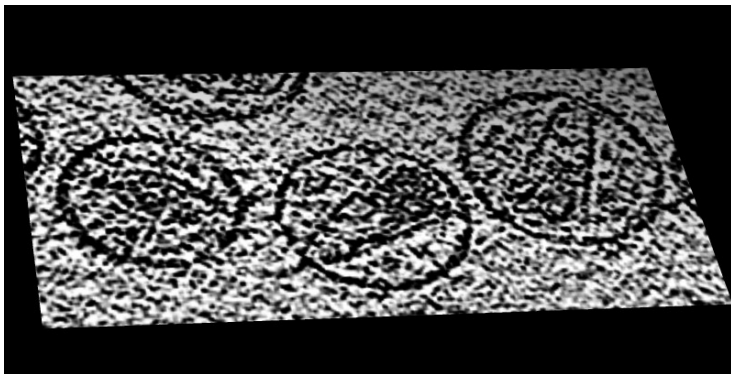
Tom Goddard
October 3, 2012

This tutorial covers basic techniques for viewing, filtering, and segmenting noisy electron tomography maps using [Chimera 1.7](#).

We will look at a map of HIV virus particles from the Fuller lab, EM Databank [1155](#).

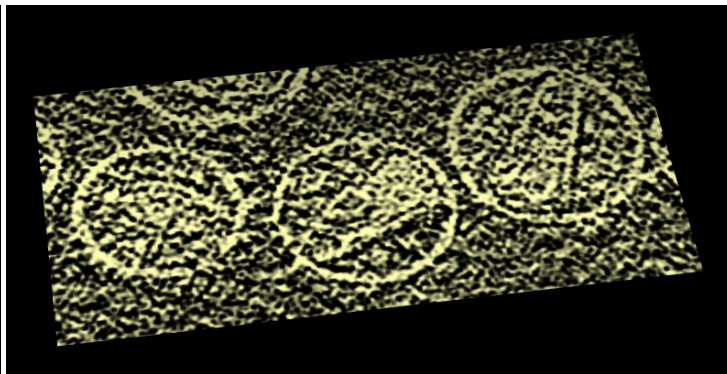


Displaying XY Planes



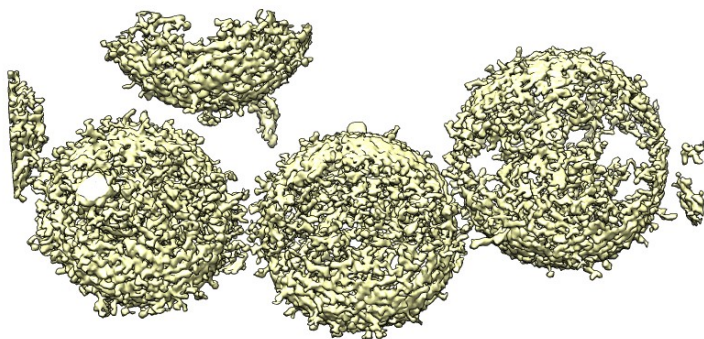
1. Open map emd_1155.map.
2. Volume dialog, Features / Planes, press One button.
3. Drag markers on histogram brightness yellow curve.
4. Move Plane slider to flip through planes.
5. Change plane axis to z and flip through planes.
6. Show all planes.

Inverting Intensity Values



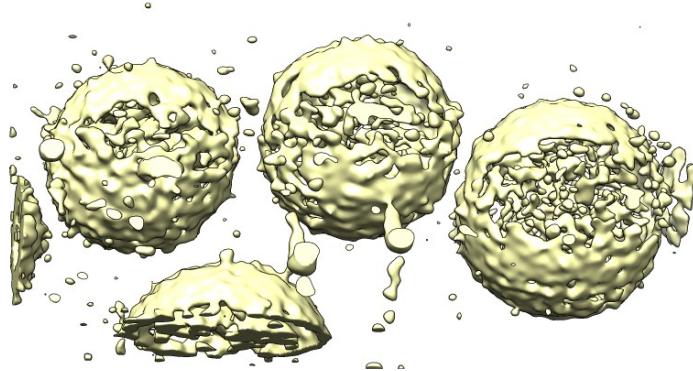
7. Note small map values are high density. Want large map values for high density.
8. Volume dialog, Tools / Volume Filter, type Scale, scale -1, options turn off displayed subregion only, press Filter.
9. Hide original map by clicking "eye" icon above histogram.
10. Switch from surface style to solid, One plane.

Hide Dust



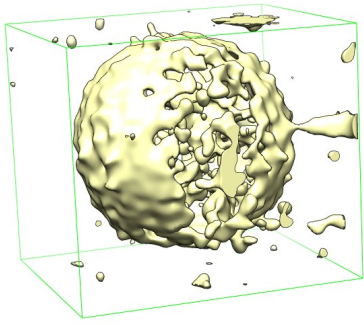
11. Hide small surface blobs to reduce noise.
12. Volume style surface, All planes.
13. Volume dialog, Tools / Hide Dust, Surface emd_1155.map scaled, press Hide.
14. Drag vertical bar on volume dialog histogram to lower contour level.
15. Move size slider in hide dust dialog.
16. Press Unhide.

Gaussian Filtering



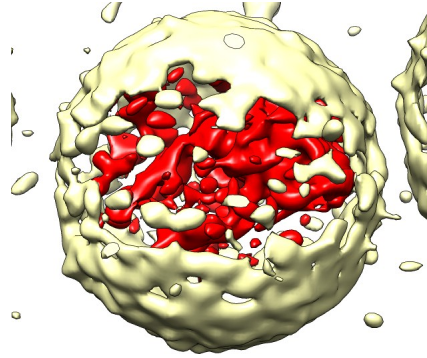
17. Smooth map to reveal large-scale features.
18. Volume dialog, Tools / Volume Filter, type Gaussian, width 30 Angstroms, value type float32, select scaled map in volume dialog, press Filter.
19. Planes One, depth 10, move plane slider.

Extract One Virus



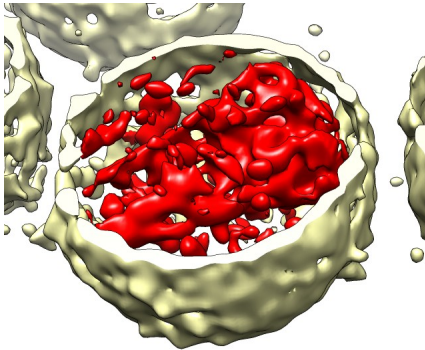
20. Volume dialog, Features / Subregion Selection, enable "Select subregions", drag box around middle virus particle, press Crop.
21. Click on green outline box face (not edge) and drag. Press Crop.
22. Uncheck "Select subregions" to move map using mouse.
23. Can save map to new file with volume dialog, File / Save Map As....

Mask Virus Membrane



24. Show command line using Favorites / Command Line
25. Enter command "shape sphere radius 550".
26. Click off "Active" sphere model #3 below command-line to stop mouse from moving sphere.
27. Move map to be centered on sphere. Ctrl-middle-mouse moves in z direction.
28. Mesh display style can help see sphere inside map.
29. Create map for inside of sphere, command "mask #2 #3"
30. Hide sphere, Favorites / Model Panel, uncheck shown button for sphere.
31. Create map outside sphere, command "mask #2 #3 invert true".
32. Color inside map red, command "volume #4 color red".

Clip Virus Membrane



33. Cut virus membrane in half to see inside.
34. Tools / Depiction / Per-Model Clipping, Model #5, check "Enable clipping".
35. Check "Adjust clipping with mouse", move clip plane by dragging with middle mouse button in graphics window.

Chimera Tutorial:

Fitting Molecular Models in Single-Particle EM Maps

Tom Goddard
October 3, 2012

Topics

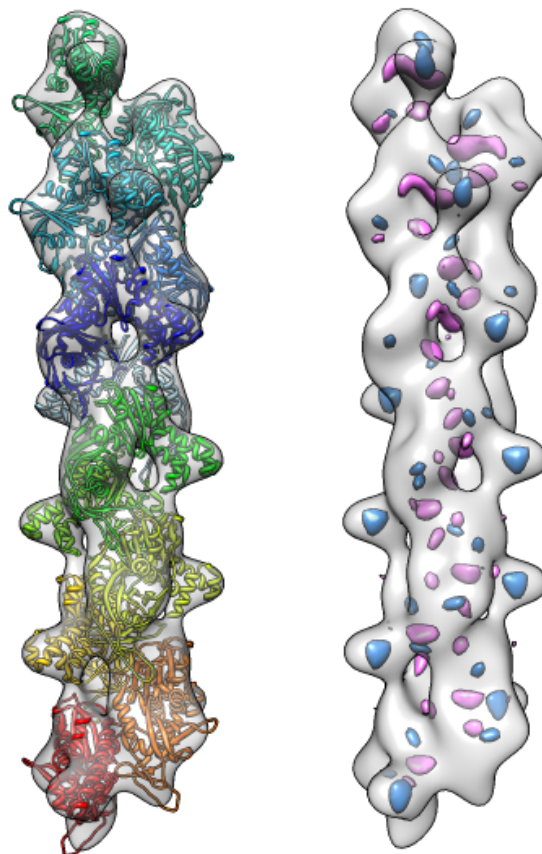
- Fitting molecules in maps with global search.
- Calculating map symmetry and creating symmetric molecule copies.
- Symmetric fitting to avoid molecular clashes.
- Calculating and displaying difference maps.

What does ParM do?

- The ParM protein forms filaments that segregates DNA plasmids prior to cell division.
- To partition low copy number DNA plasmids in E coli evenly during cell division between the two daughter cells, a plasmid is attached to each end of a growing ParM filament that pushes them to opposite sides of the mother cell.
- ParM filaments look similar to actin filaments.
- Filament growth is driven by ATP and filaments have dynamic instability like microtubules.

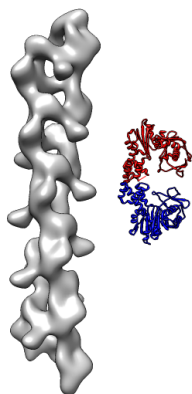
Modeling a ParM Filament

- ParM monomers bind ATP and can have the binding cleft open or closed.
- We'll build a model of the open state filament with the ATP binding site empty using x-ray structure [1mwk](#) and cryoEM map EMDB [5129](#) (19 Angstroms).
- Closed state data is also available: x-ray model [1mwm](#) and map EMDB [5128](#) (17 Angstroms). Won't have time to look at those.

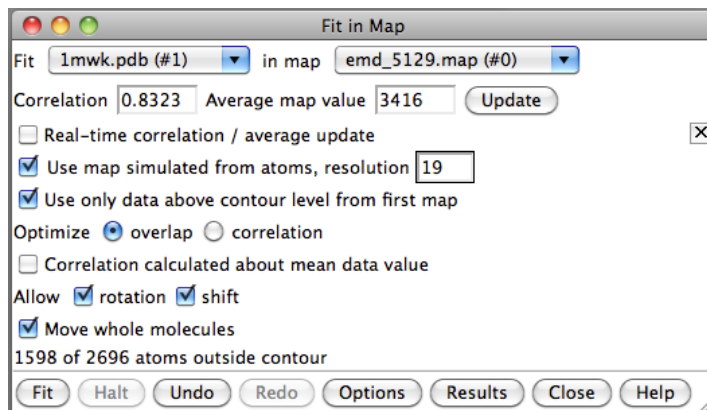
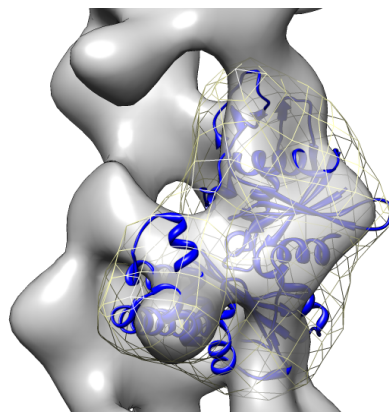


Analysis Steps

Show Molecule and Map



Fit Molecule in Map



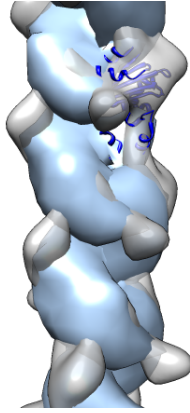
1. Open PDB 1mwk, EMD 5129.
2. Show Command Line (Favorites menu).
3. Deactivate map (model 0) below command-line to move 1mwk away from map.
4. Command "rainbow chain" to color two ParM monomers.
5. Delete chain B. Use menu Select / Chains / B, then menu Actions / Atoms / Delete.
6. Fit 1mwk in map.
7. Move 1mwk into map.
8. Press Fit button in Fit in Map dialog (volume dialog Tools menu).
9. Fit using correlation: Fit dialog Options button, enable "Use map simulated from atoms..." resolution 19. Press Fit.
10. Show simulated map (Volume dialog eye icon) as mesh.
11. Correlation depends on domain of calculation. Change simulated map threshold and press Update in Fit dialog.
12. Spend a few minutes trying alternative fit positions.

Global Fit Search



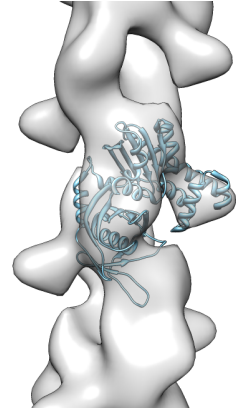
13. Search for best fit using 30 tries with command "fit #1 #0 search 30"
14. Fits appear all along filament, many are equivalent due to symmetry of the filament.

Calculate Map Symmetry



15. Determine map symmetry to eliminate equivalent fits.
16. Command "measure symmetry #0 helix 20,180,opt minimumCorrelation 0.95".
17. The "helix" option gives Chimera a hint about helical parameters.
18. The "minimumCorrelation" option accounts for this unusual map where the helix does not extend to the edges of the volume box.
19. View symmetry copies of molecule with command "sym #1 group #0 surf true".
20. Remove symmetry copies with "~sym #1" (note leading tilde character which means "undo" in Chimera commands).

Fit Asymmetric Unit



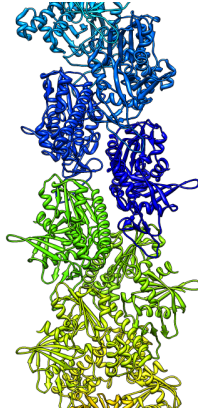
21. Clear fit list.
22. Rerun previous fitting command "fit #1 #0 search 50".
23. Clear fit list.
24. Use correlation optimization "fit #1 #0 search 50 res 19".

Make Filament Model



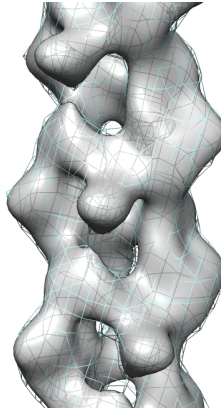
25. Show symmetric molecule copies for best fit. Command "sym #1 group #0 update true".
26. Color molecules distinctly. Command "rainbow model".

Reduce Molecular Clashes



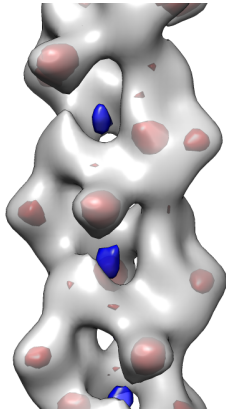
27. Inspect clashes between adjacent ParM molecules.
28. Fit asymmetric unit including all overlapped symmetric molecules. Command "fit #1 #0 sym true res 19"
29. Note increased space between molecules.

Calculate Predicted Map



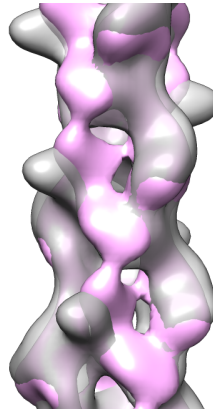
30. Compute difference map between experimental map and predicted map for molecular model.
31. First delete extra ParM molecules outside experimental map. Ctrl-drag mouse to select outside molecules. Press up-arrow key to extend selection to full molecules. Menu Actions / Atoms / Delete to delete.
32. Calculate predicted map. Command "molmap #1,2, 19"

Difference Map



33. Subtract two maps, scaling the second to minimize difference.
Command "vop subtract #0 #3 minRMS true"
34. Adjust difference map contour level. Add negative contour with ctrl-click on histogram. Adjust contour colors.
35. Hide molecular models with Model Panel (menu Favorites).

Compare "Open" and "Closed" Filaments.

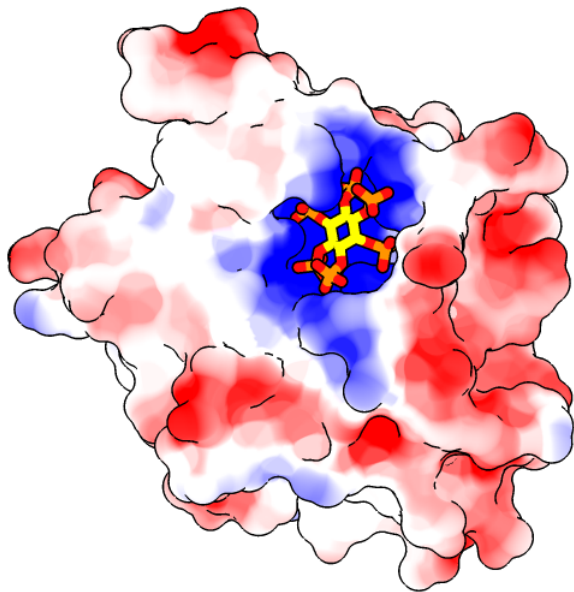


36. Load "closed" filament (GDP bound), EMDB 5128,
menu File / Open...
37. Flip closed map 180 degrees and fit to open map.
38. Compute closed map on same grid as open map.
Command "vop resample #5 onGrid #0"
39. Use Morph Map (Tools menu of volume dialog) to
morph between maps. [Movie](#).

Molecular Visualization with UCSF Chimera: Making Images

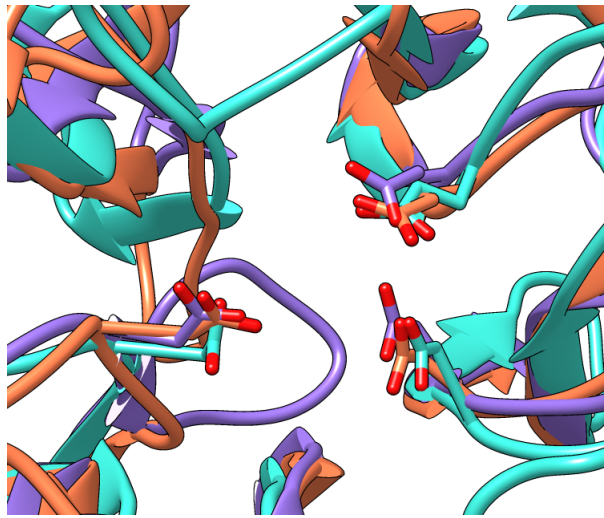
- Presentation (~15 mins):
 - tips and tricks for making images

Surface Properties (~15 minutes)



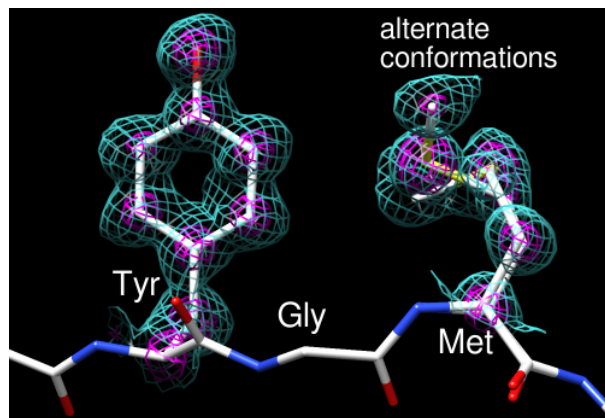
Protein surface colored to show hydrophobicity and electrostatic potential.

Hydrolases (~25 minutes)



Structural similarities among members of glycoside hydrolases families 32, 43, and 68.

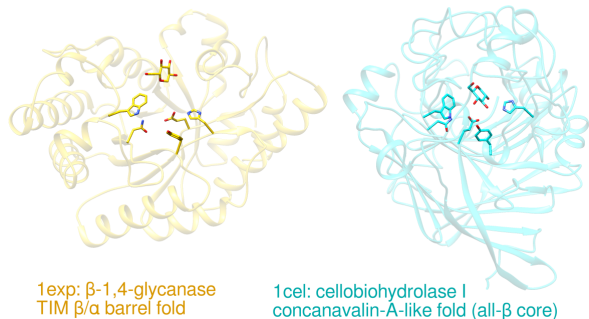
Density Display (~20 minutes)



Alzheimer's amyloid precursor protein copper-binding domain with its electron density map.

Similar Sites (~40 minutes)

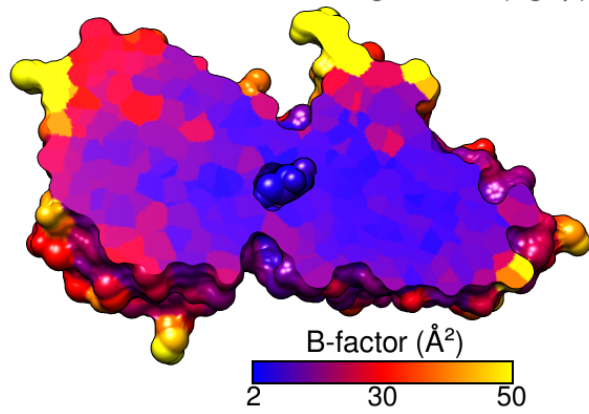
Similar binding sites in different protein folds



β-1,4-glycanase and cellobiohydrolase I have different folds but a similar pattern of amino acids near a glucose residue.

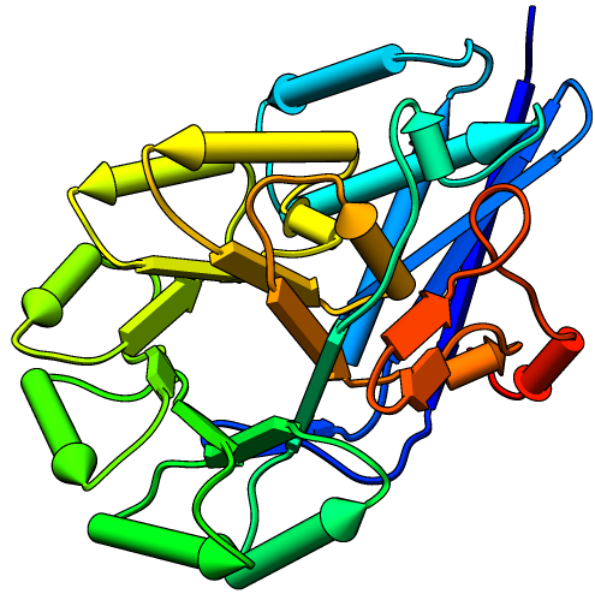
B-Factor Coloring (~25 minutes)

Galactose/Glucose-Binding Protein (2gbp)



Galactose/glucose-binding protein colored by temperature factor.

Pipes and Planks (~10 minutes)



Mandelate racemase with secondary structures shown as cylinders and boxes.

Image Tutorial: B-Factor Coloring

The recipe here is just one possibility; there are usually several ways to get the same or similar results. See also:

[presets](#), [tips on preparing images](#)

Start [Chimera](#) and show the [Command Line](#) (for example, with **Favorites... Command Line**). Fetch Protein Data Bank entry [2gbp](#):

Command: [open 2gbp](#)

Use the "all atoms" preset and delete the water:

Command: [preset apply int 2](#)

Command: [delete solvent](#)

Resize the window as desired, either by dragging its lower right corner with the mouse or by using the command [window size](#). The window dimensions define the aspect ratio (width:height) of output images, but image resolution (pixel dimensions) can be specified independently when an image is saved.

The [example image](#) was saved with pixel dimensions 573 x 443 from a window of that same size:

Command: [window size 573 443](#)

Move and scale the structure [using the mouse](#) and the [Side View](#) as you wish throughout the tutorial.

Coloring by B-Factor

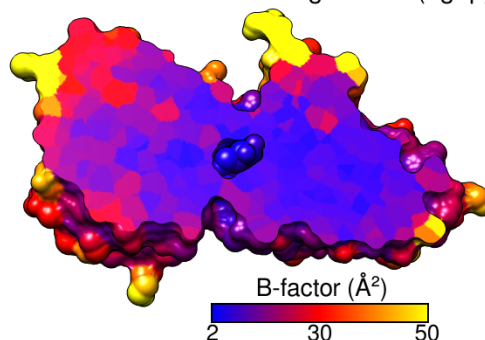
Start [Render by Attribute](#) (under **Tools... Depiction**) and make sure it is set to show the [attributes](#) of **atoms**. Look in the **Attribute** list to see what is available: **bfactor** and **occupancy**, which were read from the input PDB file. Choose **bfactor**; a histogram of the values will appear, with blue, white and red vertical bars (or [thresholds](#)).

You can control how colors will map to B-factor values by dragging the thresholds 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 square [color well](#) and using the [Color Editor](#). The slider positions in the editor can be adjusted, or a [color name](#) simply entered in the **Color name** field.

To make the [example image](#), a **blue** threshold at value 2, a **red** threshold at 30, and a **yellow** threshold at 50 were used. Clicking **Apply** shows the currently defined color scheme on the structure. Once you have the desired coloring, click **Create corresponding color key**, but then just **Close** both the [Color Key](#) and [Render by Attribute](#) dialogs. Although the color key has now been set up to match the coloring scheme, we will not draw it in the Chimera window until later.

Alternatively, instead of the graphical interface, a command could have been used to perform the coloring:

Galactose/Glucose-Binding Protein (2gbp)



Command: [rangecolor](#) bfactor key 2 blue 30 red 50 yellow

The **key** keyword sets up the [Color Key](#) dialog; as above, just close that dialog for now. While the command approach is more concise, the [Render by Attribute](#) graphical interface is friendlier in that it does not require previous knowledge of the attribute names, and it provides visual (histogram) information on the value distribution.

Clipping the Surface

Display the molecular surface:

Command: [surf](#)

Start [Per-Model Clipping](#) (under **Tools... Depiction**). In that dialog, set **Model** to the surface (not **2gbp** itself, which contains the atoms) and turn on **Enable clipping**. Now part of the surface but not the atoms should be chopped away. The planar cap is not yet colored by B-factor; that will have to be done in a separate step. Keep the clipping dialog open.

Hide all atoms except for the ligand, glucose:

Command: [show ligand](#)

Next, adjust the clipping of the surface to the desired angle and position relative to the structure. In the [Per-Model Clipping](#) dialog, turn on **Adjust clipping with mouse as below** and use the specified mouse buttons to translate and rotate the clipping plane. A transparent green disk will be shown while you are making these adjustments. The mouse button assignments can be changed if you prefer. To return the mouse buttons to their normal functions, turn off **Adjust clipping with mouse as below**. It may be necessary to turn it on and off a few times to position the clipping plane to your satisfaction. Once that has been done, either turn off **Adjust clipping with mouse as below** or just **Close** the clipping dialog to return the mouse buttons to their normal functions.

Select all atoms and use [Color Zone](#) to make the planar cap match these atoms:

Command: [select #](#)

Command: [start Color Zone](#)

This tool is also under **Tools... Depiction** in the menu. Click the **Color** button and increase the **Coloring radius** as needed to color the whole cap. A radius of $\sim 3\text{-}4$ Å should suffice. **Close** that tool and clear the selection:

Command: [~select](#)

The color patches on the planar cap look somewhat fuzzy because of coarse surface triangulation. Start [Surface Capping](#):

Command: [start Surface Capping](#)

and change the **Mesh subdivision factor** to **3** to make the triangles smaller and the color patches on the cap more distinct. **Close** that tool.

Finishing Touches, Labels, Color Key

Use a publication preset to make the background white, turn on black silhouette edges, and generate a smoother molecular surface:

Command: [preset](#) apply pub 1

This preset also turns off depth-cueing (fog).

Place and orient the structure for the final image, leaving room for the title and color key. If you want to, save the position:

Command: [savepos](#) p1

Then if you accidentally move the structure later, the position can be restored with:

Command: [reset](#) p1

If you decide a later position is better, you can save it to a new name, or the same name to overwrite the previously saved position:

Command: [savepos](#) p1

Open the [Color Key](#) dialog (under **Tools... Utilities**). In that dialog, set the **Label color** to **black** by clicking the [color well](#) and using the [Color Editor](#). The appropriate **Font size** depends on the window size; **26** was used with a 573 x 443 window.

Make sure that **Use mouse for key placement** is turned on and then click-drag in the main window to draw the key. It may take a few tries; click-drag to start over, or click on the middle of the key to drag it around. To rotate the structure instead (and/or to prevent erasing the existing color key), turn off **Use mouse for key placement**. After drawing the key to your satisfaction:

- set **Numeric label separation** to **equal** in order to space the value labels 2, 30, and 50 evenly rather than based on their values
- change **Border color** to **black**
- adjust **Border width** to **2**

To add additional text to the image, click the tab to go to the **Labels (2D Labels)** section of the same dialog. Set the **Color** to **black**, then click in the graphics window to start a label and type to enter its contents. Each label can be repositioned by dragging and its font size can be edited to a different value. What font sizes are appropriate depends on the window size; use what you think looks best. The [example image](#) was created using window size 573 x 443, font size 30 for the main title, and font size 28 for the text above the color key. The Å symbol and superscript ² can be included by using the **Insert symbol** menu. Alternatively, symbols can be copied from text displays (such as a [symbols page](#) or even the preceding sentence!) and pasted into the **Text** area of the [2D Labels](#) dialog. **Close** the dialog as soon as the labels are done, to allow rotating the structure and to avoid accidentally creating more labels.

Saving Your Work

[Saving a session](#) (see the **File** menu) right before or after saving the image is recommended if you might need to regenerate the same or a similar figure later, say at a different resolution or with modified coloring.

The [image](#) was saved at the same size as the window (573 x 443 pixels) using **File... Save Image** with default settings.

Image Tutorial: Density Display

Background

These images show part of Protein Data Bank entry [2fma](#), the Alzheimer's amyloid precursor protein (APP) copper-binding domain, along with its electron density map (2fo-fc) available from the Electron Density Server.

Image How-To

The recipe here is just an example; there are usually many routes to the same or similar results. See also: [presets](#), [tips on preparing images](#), and on the Chimera web site, the [Image Gallery](#) and [Guide to Volume Display](#)

[Start Chimera](#) and enlarge the window as desired. Show the [Command Line](#) (for example, with **Favorites... Command Line**).

Fetch **2fma** from the [Protein Data Bank](#), change its model color to white, then apply interactive preset #2 to display all atoms with heteroatom color-coding:

Command: [open](#) 2fma

Command: [modelcol](#) white

Command: [preset](#) apply int 2

Fetch the density map for this structure from the [Electron Density Server](#):

Command: [open](#) edsID:2fma

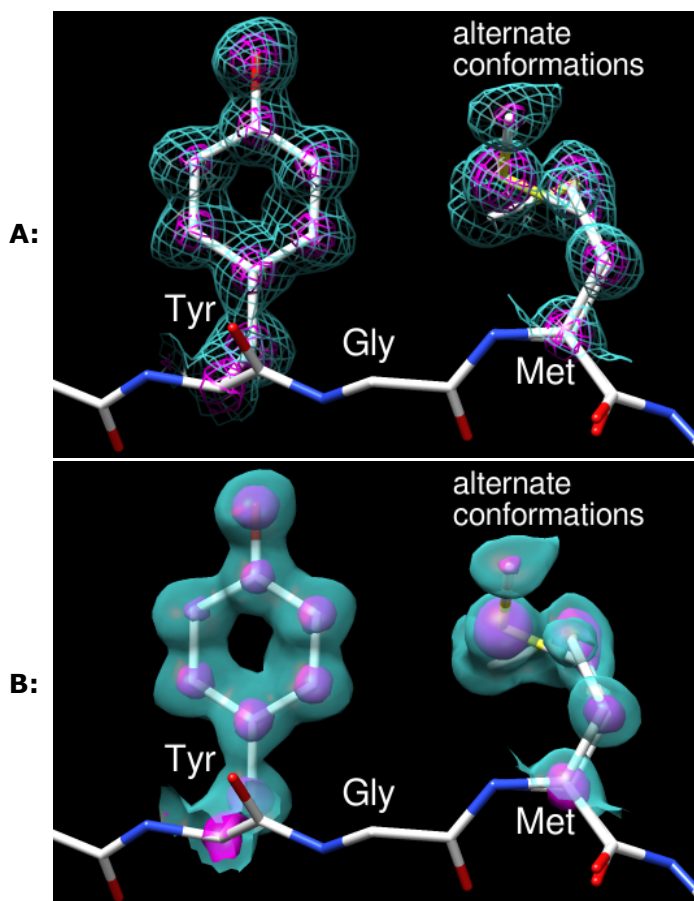
Click the little eye icon on the [Volume Viewer](#) dialog to hide the electron density for now. Move and scale [using the mouse](#) and the [Side View](#) as you wish throughout the tutorial.

Since one goal was to show an example of alternate conformations, residues with atoms in alternate conformations were identified by labeling:

Command: [rlab](#) @.a

Met-170 and Glu-183 have alternate conformations; a stretch of residues near Met-170 was chosen for the figure. Show just residues 168-170 along with the backbone of the flanking residues:

Command: [~rlab](#)



Command: [show](#) :168-170
Command: [focus](#)
Command: [disp](#) :167,171@n,ca,c,o


Change to the stick representation and make the sticks thinner:

Command: [rep](#) stick
Command: [setattrr](#) m stickScale 0.5

Select the sidechains only of Tyr-168 and Met-170; this selection will be used to limit the density display to a zone.

Command: [sel](#) :168,170 & without CA/C1'

The **without CA/C1'** part is shorthand for the menu entry **Select... Structure... side chain/base... without CA/C1'**. All terminal menu entries under **Select... Structure** can be used as [command-line specifiers](#).

If [Volume Viewer](#) has gotten buried under other windows, one way to resurrect it is by clicking the lightning-bolt icon  near the bottom of the Chimera window to show the [Rapid Access](#) interface, then clicking the **Volume Viewer** button under "Active Dialogs." In the [Volume Viewer](#) dialog,

1. click the eye icon to turn density display back on
2. choose **Features... Zone** from the menu and click the **Zone** button that appears within the dialog. This limits the density display to a zone near the selected atoms. After that, the selection can be cleared (for example, by Ctrl-clicking in empty space). The zone will continue to center on those atoms, and its **Radius** can be adjusted by moving the slider or entering a new value. A zone radius of 1.96 Å was used for the [figures](#).
3. the vertical bar (**threshold**) on the histogram represents a contour level;
 - o to change the level, drag the threshold to the left or right with the mouse or type a different value into the **Level** field below the histogram; to see more density, move the threshold to the left (use a lower level)
 - o to change the **Color**, click the square [color well](#) below the histogram and use the [Color Editor](#): check the **Opacity** option in that tool to adjust transparency (1-A) as well as color components (R red, G green, B blue); the sliders can be dragged, or values can be entered directly
 - o to add another contour level, Ctrl-click on the histogram; changes in **Level** and **Color** apply to the threshold most recently dragged or clicked
4. choose **Features... Surface and Mesh Options** from the menu to reveal additional display settings

Volume display settings (other than defaults) for [figure A](#):

- **Style** mesh
- two contour levels:
 1. **Level** 0.426, **Color** (RGBA) 0.36 1.0 1.0 0.5
 2. **Level** 2.06, **Color** (RGBA) 1.0 0.0 1.0 1.0 (**magenta**)
- turned on **Smooth mesh lines**
- **Mesh line thickness 1.5 pixels**

By default, Chimera shows only the topmost layer of transparency. This is recommended in most situations because it simplifies the view and serves to de-emphasize the transparent parts.

However, for both of these figures, single-layer transparency was turned off so that multiple transparent layers would be visible:

Command: [~set singleLayer](#)

The setting can be toggled (**set singleLayer** and then **~set** again, as above) if you want to review the difference.

For [figure B](#), the same contour levels and RGB colors are used, but different transparencies and style. Volume display settings (other than defaults):

- **Style** surface
- two contour levels:
 1. **Level** 0.426, **Color** (RGBA) 0.36 1.0 1.0 0.4
 2. **Level** 2.06, **Color** (RGBA) 1.0 0.0 1.0 0.6
- turned on **Surface smoothing iterations 2 factor 0.3**

Use [2D Labels](#) (under **Tools... Utilities**) to add label text. The labels are the same for the two [figures](#). Click in the graphics window to start a label and type to enter its contents. Each label can be repositioned by dragging. Each label's color can be adjusted by clicking the [color well](#) and using the [Color Editor](#), and its font size can be edited to a different value. What font sizes are appropriate depends on the window size; use what you think looks best. In this case, the labels are all **white**, and the residue labels are in a slightly larger font than "alternate conformations." The latter was typed with return (Enter) between the two words so that they would appear on different lines.

The [figures](#) were saved as PNG files with the same pixel dimensions as the Chimera window by using **File... Save Image** with default settings.

[Saving a session](#) (see the **File** menu) right before or after saving the image is recommended if you might need to regenerate the same or a similar figure later, say at a different resolution or with modified coloring. The session will include the [position](#) at the time of session saving, named **session-start**. This is useful when you [restore a session](#) and move things around but then want to restore its initial position:

Command: [reset session-start](#)

Image Tutorial: Glycoside Hydrolases

This tutorial describes superimposing structures, saving positions and sessions, and creating publication-quality images. The process described here is only one of many possibilities. Internet connectivity is required to fetch the structures **1uyp**, **1gyd**, and **1oyg**.

See also: [presets](#), [tips on preparing images](#), and on the Chimera web site, the [Image Gallery](#)

Background and Setup

Glycoside hydrolases (GH) are a large, heterogeneous set of enzymes that hydrolyze bonds between sugars and other groups. Based on sequence comparisons, these enzymes have been categorized into many families; see the [CAZy web site](#) for details.

This tutorial describes the creation of images to show structural similarities among members of GH families 32, 43, and 68. These enzymes were grouped into different families because their similarities were not evident from sequence comparisons.

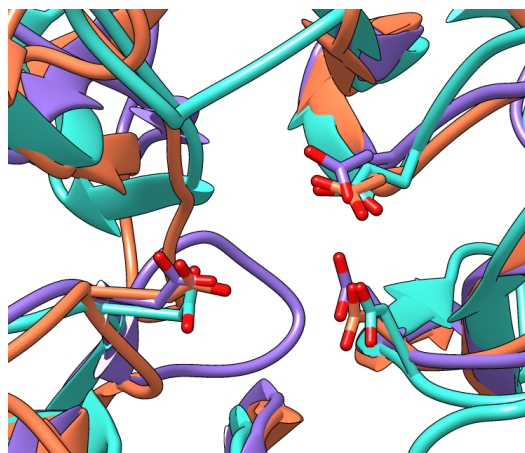
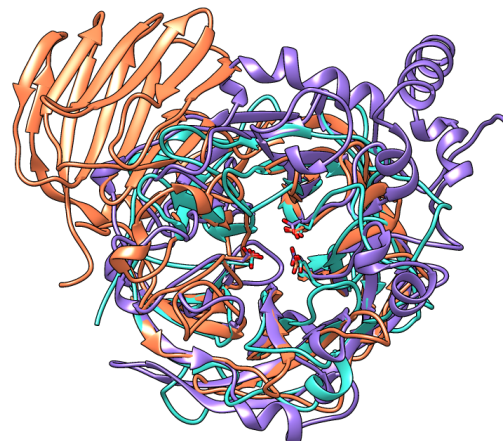
[Three acidic residues are at the active site of a beta-propeller architecture in glycoside hydrolase families 32, 43, 62, and 68.](#) Pons T, Naumoff DG, Martínez-Fleites C, Hernández L. *Proteins*. 2004 Feb 15; **54**(3):424-32.

[The three-dimensional structure of invertase \(beta-fructosidase\) from *Thermotoga maritima* reveals a bimodular arrangement and an evolutionary relationship between retaining and inverting glycosidases.](#) Alberto F, Bignon C, Sulzenbacher G, Henrissat B, Czjzek M. *J Biol Chem*. 2004 Apr 30; **279**(18):18903-10.

[Start Chimera](#) and enlarge the window as desired. Show the [Command Line](#) (for example, with **Favorites... Command Line**).

Structures can be obtained directly from the [Protein Data Bank](#). Choose **File... Fetch by ID** from the Chimera menu. In the resulting dialog, choose the **PDB** database and check the option to **Keep dialog up after Fetch**. Fetch the PDB structures **1uyp**, **1gyd**, and **1oyg**, in that order, and then **Close** the dialog.

Some salient features of these structures:



Invertase (GH 32) is coral, arabinanase A (GH 43) is turquoise, and levansucrase (GH 68) is purple. Despite significant divergence, the enzymes share similar overall folds (top) and highly conserved active site residues (bottom).

PDB ID	enzyme	family	chains	conserved residues	model # in Chimera
--------	--------	--------	--------	--------------------	--------------------

1uyp	invertase, <i>T. maritima</i>	GH32	A-F	Asp17	Asp138	Glu190	0
1gyd	arabinanase A, <i>C. japonicus</i>	GH43	B	Asp38	Asp158	Glu221	1
1oyg	levansucrase, <i>B. subtilis</i>	GH68	A	Asp86	Asp247	Glu342	2

Simplify the situation by deleting unwanted (for our purposes) portions of the structures such as extra chains and solvent:

Command: **[delete](#) #0:.b-f**

Command: **[delete](#) solvent | ligand | ions**

[Move and scale](#) the structures as desired throughout the tutorial.

Ribbons

Choose **Presets... Interactive 1 (ribbons)** from the menu; depending on your settings, this may not change the display very much. Ribbon styles include **flat**, **edged**, and as used in the preset, **rounded**.

Command: **[ribrep](#) flat**

Command: **[ribrep](#) edged**

Command: **[ribrep](#) rounded**

Ribbon scalings are secondary-structure-specific heights and widths. Try the "licorice" scaling and then go back to the default.

Command: **[ribscale](#) licorice**

Command: **[ribscale](#) "Chimera default"**

Custom ribbon [styles](#) and [scalings](#) can be created with the [Ribbon Style Editor](#) (**Tools... Depiction... Ribbon Style Editor**).

Although the [examples](#) show ribbons for the entire chains, each residue's ribbon segment can be shown or hidden. For example, the following hides ribbons for the C-terminal domain of the first structure (model 0):

Command: **[~ribbon](#) #0:296-end**

A command without residues specified affects all residues:

Command: **[ribbon](#)**

Important Residues

Alias the [conserved residues](#) to some short name for convenience:

Command: **[alias](#) myres #0:17,138,190#1:38,158,221#2:86,247,342**

Show only those atoms/bonds:

Command: [show myres](#)

Even though all atoms of the residues are “displayed,” by default the backbone atoms are hidden when ribbon is shown (this can be controlled with the command [ribbackbone](#)).

Matching the Structures

The relative positions of the structures are not meaningful and merely reflect their coordinates as deposited in the Protein Data Bank. Chimera includes a few different ways of [superimposing structures](#).

Since structurally equivalent residues are known, one way to superimpose the structures is by [specifying atoms](#) to use in a least-squares fit. The [match](#) command requires equal numbers of atoms from the two models being matched. The following specifies using the backbone atoms of the [conserved residues](#):

Command: [match](#) #1:38,158,221@n,ca,c,o #0:17,138,190@n,ca,c,o

Command: [match](#) #2:86,247,342@n,ca,c,o #0:17,138,190@n,ca,c,o

Model 0 (invertase) was used as the reference structure for both pairwise matches. The number of points used for fitting and the resulting RMSD values are reported in the [Reply Log](#). Chain identifiers did not have to be given in the commands since each model has only one chain (chains B-F were deleted from model 0). Chain identifiers are only needed to distinguish cases where the same residue number appears in more than one chain of the same model.

Reorient the structures so that you can see the conserved residues, then use the following commands to focus the view, scale up a bit, and save the matched position so that it can be compared to the result of a different matching method that will be used next. A **position** includes the scale, locations, and orientations of the structures.

Command: [focus](#)

Command: [scale](#) 2

Command: [savepos](#) pos1

Another way to superimpose the structures is with [matchmaker](#) (for which the reference structure is given first):

Command: [mm](#) #0 #1

Command: [mm](#) #0 #2

Command: [savepos](#) pos2

Matchmaker uses the protein sequences and secondary structure assignments to generate alignments, then fits the CA atoms of the aligned pairs. Again, the number of points used for fitting and the resulting RMSD values are reported in the [Reply Log](#).

Review the two superpositions to decide which is better:

Command: [reset](#) pos1 30

Command: [reset](#) pos2 30

Repeat as desired. The number at the end of the [reset](#) command is the number of frames over which to gradually restore the position. A gradual rather than abrupt transition between positions may make them easier to compare.

In this case, the light blue structure (model 1, arabinanase) is better superimposed with the others in the result from [matchmaker](#) (**pos2**).

Positions for Images

Resize the Chimera window to the desired aspect ratio and find positions suitable for the images.

A window size of 750x636 pixels and two positions were used for the [example images](#). A view of the overall structures was generated by interactive manipulation, then saved (with [savepos](#)) as a position named **overall**. Another position zoomed into the active site was generated from **overall** by scaling and translation only (to maintain a consistent view) and saved as the position **closeup**.

Saved positions are included in saved [sessions](#) and can be restored before [saving images](#).

Coloring the Structures

The current model colors could be used, but typically users will want to apply their own scheme. Several factors should be considered in [choosing colors](#), including what the colors are meant to indicate, their distinguishability, and whether viewers may have color vision deficiencies. The colors named **coral**, **turquoise**, and **medium purple** were used for models 0, 1, and 2, respectively, in the [example images](#).

Open the [Color Actions](#) dialog (**Actions... Color... all options**) and near the bottom, check **Show all colors** to expand it. Select a model:

Command: [sel](#) #0

and click the desired color in the dialog. Repeat for models 1 and 2, then close the coloring dialog. Clear the selection:

Command: [~sel](#)

To use heteroatom color-coding so that sidechain oxygens are red:

Command: [color](#) byhet

Effects and Lighting

The background can be any color, but white is often best for publication images.

Command: [background](#) solid white

Depth cueing is front-to-back shading of the scene, which looks like "fog" when the depth cueing color is pale. By default, the depth cueing color automatically matches the background. Turn off depth cueing to remove the fog effect:

Command: [~set](#) depthCue

Ribbons, sticks, and other spacefilling [display styles](#) are made up of planar facets. The coarseness of the facets is controlled by the subdivision parameter, which ranges from 1 to 20 (default 1.5). Increase smoothness by increasing the subdivision:

Command: [set](#) subdivision 5

Silhouette edges are outlines that highlight boundaries and discontinuities. Turn on silhouette edges:

Command: [set silhouette](#)

The silhouettes look rough in the Chimera window, but they will be smooth in the saved images due to [supersampling](#).

Instead of the four preceding commands, publication preset 1 could be used to achieve the same result (command [preset apply pub 1](#) or menu item **Presets... Publication 1**). Silhouette edges and increased subdivision may degrade interactive response; if so, adjust these settings last before saving [sessions](#) and [images](#).

The contrast, or darkness of shading, is another important contributor to the clarity of figures. Decrease the contrast (default 0.83):

Command: [light contrast 0.55](#)

Graphical interfaces to [Effects](#) and [Lighting](#) are available under **Tools... Viewing Controls** in the menu.

Sessions

A [session](#) file can be saved with **File... Save Session As** in the Chimera menu. It is generally prudent to save sessions for publication images, as this decreases the labor necessary if the figures have to be redone. Often minor adjustments such as changing a color or displaying a different set of side chains will be required.

Later, the session can be restarted with **File... Restore Session**, and any saved [positions](#) within that session restored with the command [reset](#).

Saving Images

Previously saved positions can be restored, for example:

Command: [reset overall](#)

Choosing **File... Save Image** brings up the [Save Image panel](#) for specifying the output file location, name, and type (**PNG** was used for the [examples](#)), and other options.

Supersampling refers to generating an initial image larger than requested and then sampling it down to the final size. This smooths edges within the image with little effect on file size. The default [Supersample](#) setting of 3x3, used for the [examples](#), is generally sufficient for publication.

The **Image Size** can be specified directly in pixels, or in units of length (when [Use print units](#) is on). If units of length, the output pixel dimensions are calculated using the specified [Print resolution](#). The graphics window can be resized manually or with the command [window size](#).

To make an image for a single-column width of 85 mm (3.346 in) with a resolution of at least 300 dpi, possible approaches include:

- with **Units** set to **pixels**, setting the **Image width** to at least 1004 pixels (3.346 x 300)
- activating [Use print units](#), and with **Units** set to **inches**, setting the **Image width** to at least 3.346 inches and the [Print resolution](#) to 300 dpi

- activating [Use print units](#), and with **Units** set to **millimeters**, setting the **Image width** to at least 85 mm and the [Print resolution](#) to 300 dpi

Clicking **Save** dismisses the dialog and initiates saving the image.

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Image Tutorial: Pipes and Planks

This tutorial describes showing protein helices as “pipes” (cylinders) and strands as “planks” (rectangular boxes) with [PipesAndPlanks](#), and adjusting the lighting to decrease contrast. See also: [Axes/Planes/Centroids](#), [presets](#), [tips on preparing images](#)

[Start Chimera](#) and show the [Command Line](#) (for example, with **Favorites... Command Line**). Fetch Protein Data Bank entry [2mnr](#):

Command: [open](#) 2mnr

The structure is the enzyme mandelate racemase, containing an N-terminal $\alpha+\beta$ domain and a C-terminal β/α -barrel domain. [Move and scale](#) the structure as desired throughout the tutorial.

The window can be resized by dragging its lower right corner with the mouse or by using a command, for example:

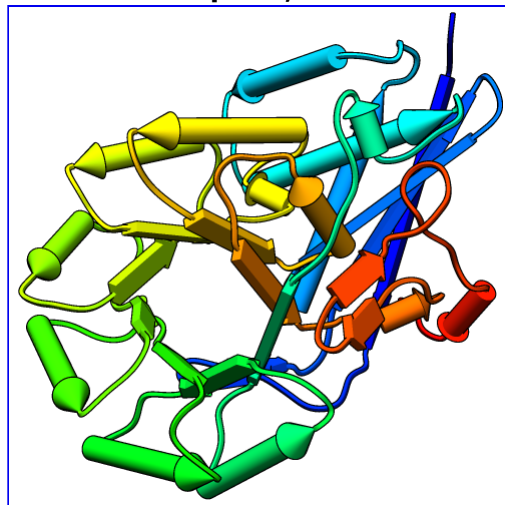
Command: [windowsize](#) 500 500

Rainbow-color-code the protein chain from blue at the N-terminus to red at the C-terminus:

Command: [rainbow](#)

Start [PipesAndPlanks](#) (under **Tools... Depiction** in the menu), and click **Apply** to generate the pipes-and-planks representation with default settings. **Helix color**, **Strand color**, and **Coil color** settings of “No color” indicate that each pipe, plank, and stretch of coil should be colored using the ribbon color of its first residue.

default: two-point, contrast 0.83



The pipes-and-planks representation is shown in addition to the ribbon, rather than replacing it. Hide the ribbon and atoms:

Command: [~ribbon](#)

Command: [~disp](#)

Apply publication preset 1, which sets the background to white and turns on black outlines (silhouette edges):

Command: [preset](#) apply pub 1

The first example image was saved with the current settings, including default lighting.

Decreasing the Contrast

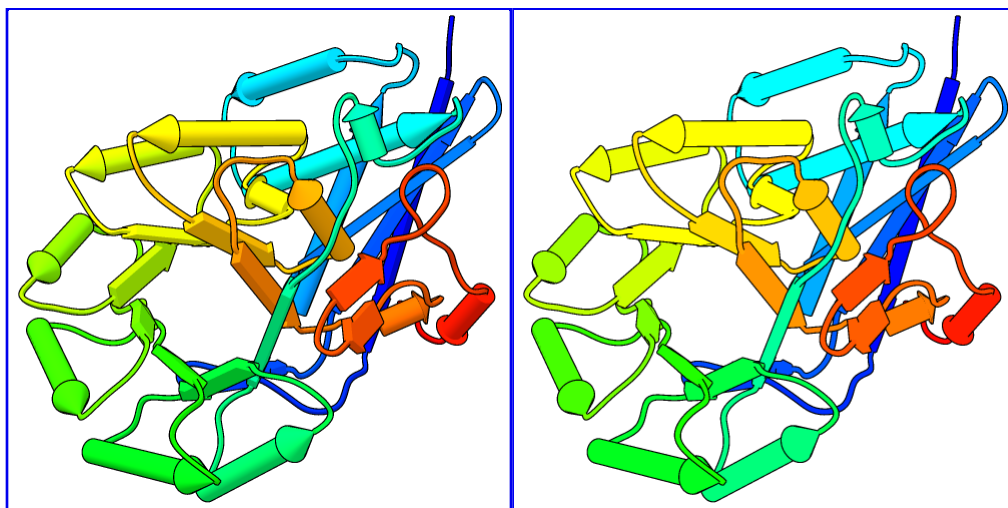
While shading can enhance the perception of depth, shapes, and

two-point, contrast 0.4

ambient-only

orientations, it can also make colors muddy and images harder to interpret. One way to lighten the shading is to decrease the contrast, for example:

Command:
light contrast
0.4



The default lighting mode, **two-point**,

includes two directional lights and ambient (nondirectional) light. Decreasing the contrast increases the ambient light and gives a flatter appearance.

A yet flatter appearance, similar to a line drawing, can be achieved by changing the lighting mode to ambient-only:

Command: **light mode ambient**

The lighting mode and contrast can also be adjusted in the **Lighting** tool (under **Tools... Viewing Controls** in the menu), along with other related settings.

Additional Outlines

In the ambient-only lighting mode, some of the object contours are lost. However, more black outlines can be added using **edge color** settings in the **PipesAndPlanks** dialog. The last example image was saved in the ambient-only lighting mode after setting the **Helix edge color** and **Strand edge color** to black, but leaving the **Coil edge color** as "No color."

A color setting can be changed by clicking the square [color well](#) and using the resulting **Color Editor**. The current color can be changed by moving the sliders or by entering a [color name](#) (for example, **black**) in the **Color name** field. The active color well should change concurrently, but drag-and-drop from the **Color Editor** to a color well or between two color wells will also work.

Click **Apply** in the **PipesAndPlanks** dialog to apply your changes. The edges may look quite fuzzy in the Chimera window, but image [supersampling](#) (on by default) will make them smoother in saved images. All images in this tutorial were saved using **File... Save Image** with default settings.

Try other changes if you wish; adjustable settings include pipe radius, plank width, and whether to show helix and strand N→C directionality with arrowheads.

ambient-only, more outlines

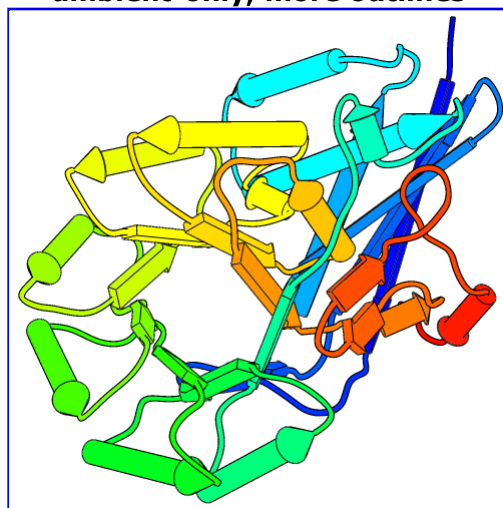


Image Tutorial: Similar Binding Sites

Background

β -1,4-glycanase (gold, Protein Data Bank entry [1exp](#)) and cellobiohydrolase I (cyan, Protein Data Bank entry [1cel](#)) have different folds but a similar pattern of amino acids near a glucose residue. This possible example of convergent evolution was identified in Table 5 of:

[Detection of protein three-dimensional side-chain patterns: new examples of convergent evolution.](#) Russell RB. *J Mol Biol.* 1998 Jun 26;279(5):1211-27.

Image How-To

The recipe here is just an example; there are usually many routes to the same or similar results. Not all of the steps can be done with commands – for example, there is no substitute for interactively finding the best views – but commands for much of the setup below are collected into the Chimera command file [convergent.com](#).

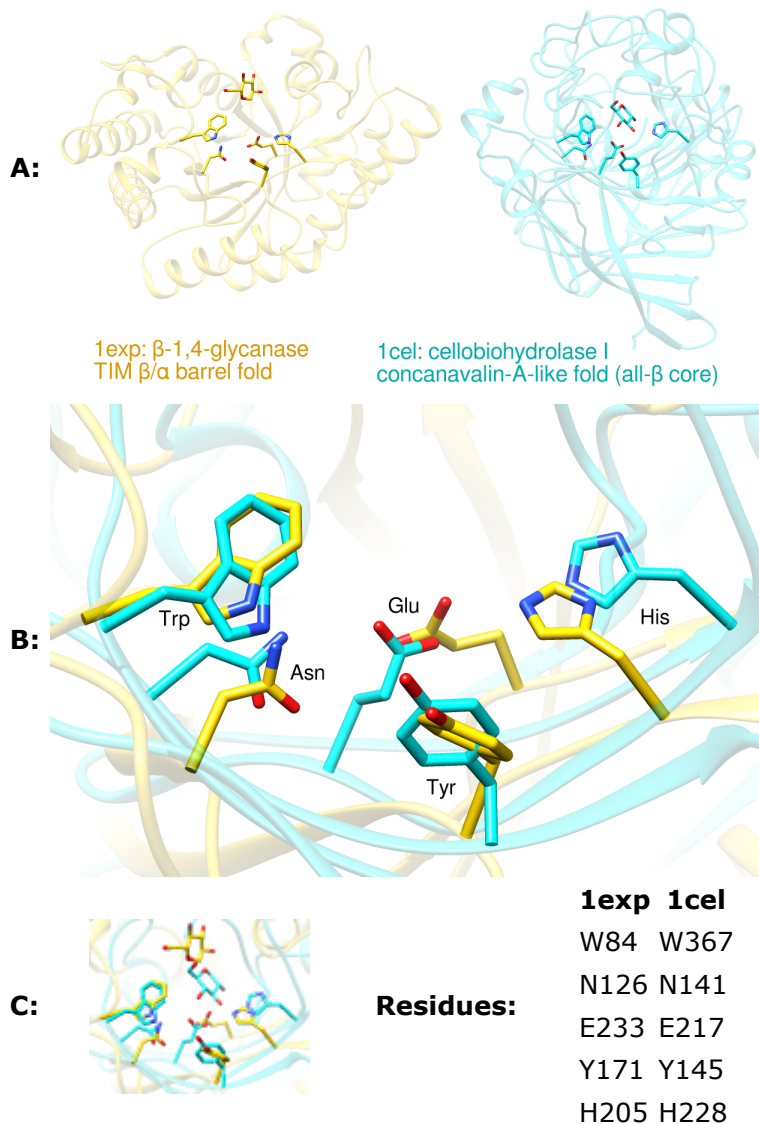
See also: [presets](#), [tips on preparing images](#)

The images show (A) the two proteins side by side, (B) a closeup of the superimposed sites without glucose, and (C) a thumbnail of the superimposed sites. Often it is best to create a set of views that, while different, are consistent or related to each other by only simple transformations. We will generate the view shown in B first and then base the others upon it.

[Start Chimera](#) and enlarge the window as desired. Show the [Command Line](#) (for example, with **Favorites... Command Line**). Fetch **1exp** and then **1cel** from the [Protein Data Bank](#):

Command: [open](#) **1exp**
Command: [open](#) **1cel**
Command: [focus](#)

Similar binding sites in different protein folds



Move and scale the structures [using the mouse](#) and the **Side View** as you wish throughout the tutorial.

1cel includes two copies of the protein, chains A and B; one copy can be deleted:

Command: [delete](#) **:.b**

Command: [focus](#)

Use the ribbons preset, and for now, hide all atoms and bonds:

Command: [preset](#) **apply int 1**

Command: [~disp](#)

Set up the basic coloring scheme and white background:

Command: [color](#) **gold #0**

Command: [color](#) **cyan #1**

Command: [background](#) **solid white**

Display the residues identified by Russell and use them to superimpose the structures:

Command: [alias](#) **site1 #0:84,126,233,171,205**

Command: [alias](#) **site2 #1:367,141,217,145,228**

Command: [alias](#) **both site1 | site2**

Command: [disp](#) **both**

Command: [match](#) **iterate 2.0 site2 site1**

Command: [focus](#) **both**

Command: [color](#) **byhet**

The aliases in the above [match](#) command specify entire residues. The match command requires equal numbers of atoms from the two structures, specified in the same order. In this case, the residues are of the same types (thus containing the same numbers of atoms) and the atoms of each residue will be in the same order because they are automatically sorted by name.

Make the sticks and ribbons smoother by increasing subdivision:

Command: [set subdivision](#) **10**

De-Emphasizing the Ribbons

The display is still quite “busy,” in part because the two proteins have different folds. We will de-emphasize the ribbons by making them transparent and slimmer. Make the ribbons 75% transparent (25% opaque):

Command: [transparency](#) **75,r**

The **,r** part indicates that only ribbons should be affected, not atoms, bonds, surfaces, *etc.*

By default, transparent surfaces (including objects as well as surfaces proper) appear more opaque when viewed edge-on as compared to face-on. The transparent ribbons will be less obtrusive with *non-angle-dependent* transparency:

Command: [set flatTransparency](#)

The sidechain sticks terminate as rounded “nubbins” inside the ribbon. To make these ends flat

instead:

Command: [repr wire @ca](#)

The ribbon dimensions can be adjusted in [Ribbon Style Editor](#). Start that tool (under **Tools... Depiction** in the menu) and adjust the **Ribbon Scaling** values:

2° Structure	Width	Height
Coil	0.20	0.20
Helix	0.60	0.20
Sheet	0.60	0.20
Arrow (base)	1.0	0.20
Arrow (tip)	0.20	0.20

The **Nucleic** values only pertain to DNA and RNA. Click **Apply** to adjust the ribbon scaling (secondary-structure-specific dimensions). Click **Save As...** to name and save the scaling for later use. For example, if the scaling is named **slim**, it could also be applied with:

Command: [ribscale slim](#)

Generating Positions (Views)

The displayed sidechains are somewhat obscured by other parts of the proteins. Rotate, translate, and scale the structures, and in the [Side View](#), adjust the front and back clipping planes to simplify the view. You may also want to adjust the window dimensions. After generating a good view of the set of displayed residues (such as in [figure B](#)), save the position:

Command: [savepos closeup](#)

It does not have to be perfect; the same command can be used again later to re-save the position after further adjustments. You may also wish to [save the session](#) (see the **File** menu) at this stage and whenever you are pleased with your previous work and want to ensure it will not be lost.

Next, generate and save positions for the other two figures. The intent is to preserve the orientations in the **closeup** position while possibly translating up/down and left/right and changing the scale.

1. position for [figure C](#), closeup with glucose molecules:

Display the glucose residues, both named BGC (**Note**: older versions of these PDB entries used the name GLC instead):

Command: [disp :bgc](#)

If you have changed the view from the **closeup** position, restore it:

Command: [reset closeup](#)

Scale and translate everything (avoiding rotation) so that the glucose molecules are visible, optionally adjust the clipping planes in the [Side View](#), and then save another position:

Command: **savepos closeup2**

Scaling can be done [with the mouse](#), or with the command **scale**, or by moving the small square in the **Side View**. Translations (up/down, left/right) can be performed [with the mouse](#) or with the command **move**. If you make a mistake, you can simply revert to the **closeup** position and start over.

2. position for [figure A](#), the two proteins side by side:

Again we wish to leave the orientation of the structures the same as in the **closeup** position, but separate them and zoom out so that all parts are visible. Restore the **closeup** position:

Command: **reset closeup**

Zoom out (scale down) and turn off clipping by unchecking the **Clip** option in the **Side View**. Scale and vertically translate the structures as needed to leave room for a title at the top and other text at the bottom. The proteins are still superimposed, in the middle of the window. Translate one structure to the left and the other to the right:

Command: **move x -25 models #0**

Command: **move x 30 models #1**

The exact translation distances needed will differ according to your starting position. When a satisfactory side-by-side view has been achieved, save the position:

Command: **savepos sidebyside**

Adding Labels and Saving Scenes

Chimera [scenes](#) are similar to positions but contain more information such as colors, display styles, and which atoms and labels are displayed. If scenes are saved and restored, it will not be necessary to manually display and undisplay the glucose residues and the appropriate labels between saving the different images. However, a drawback of scenes is that they increase session file size.

Start **2D Labels** (under **Tools... Utilities**) to annotate the images.

1. [figure B](#):

Command: **reset closeup**

Command: **~disp :bgc**

and then use **2D Labels** to label the residues. Click to start a label and type to enter its contents. Click the [color well](#) to set label color, in this case **black**. The appropriate font size depends on the size of the window; use what you think looks best. Each label can be repositioned by dragging. When done creating the labels for this view, save the scene:

Command: **scene sceneB save**

Next, hide all of these labels using the **Shown** checkboxes in the **2D Labels**

dialog.

2. [figure C](#):

Command: [reset](#) **closeup2**

Command: [disp](#) :bgc

Command: [scene](#) **sceneC save**

We will not make the window thumbnail-sized until right before saving the image.

3. [figure A](#):

Command: [reset](#) **sidebyside**

and then use [2D Labels](#) to add a **black** title above the structures and color-coded descriptions below them. The label color for the gold structure was first set to gold (by clicking the [color well](#) and entering the name **gold** into the [Color Editor](#)) and then darkened until suitably visible on the white background. The label color for the cyan structure was similarly derived from **cyan**. Symbols such as Greek letters can be inserted using the menu in the [2D Labels](#) dialog. When done creating the labels for this view, save the scene:

Command: [scene](#) **sceneA save**

Now all of the work other than saving the images is done. You should definitely [save the session](#) (see the **File** menu) at this point; it will include the labels, saved positions, and saved scenes. The images can be saved now or later, after quitting from Chimera, restarting Chimera, and [restoring the session](#).

Saving the Images

- [figure A](#):

1. as needed, [start Chimera](#) and [restore the session](#) (for example, using **File... Restore Session**)
2. restore the corresponding scene:

Command: [scene](#) **sceneA reset**

3. choose **File... Save Image**, specify file location, name and type (**PNG** was used), adjust size as desired (width 1200 pixels was used), and click **Save**

- [figure B](#):

1. restore the corresponding scene:

Command: [scene](#) **sceneB reset**

2. choose **File... Save Image**, specify file location, name and type (**PNG** was used), adjust size as desired (width 1200 pixels was used), and click **Save**

- [figure C](#):

1. restore the corresponding scene:

Command: [scene](#) **sceneC reset**

2. it was decided that this thumbnail image for the [Chimera Image Gallery](#) should be 110 by 87 pixels, a different aspect ratio than the window in the session. Resize the window to the planned thumbnail size, then scale as needed:

Command: [window size](#) **110 87**

Command: [scale](#) **1.2**

Of course, the scaling could have been done interactively with the mouse, but instead a scale factor was determined empirically (by resetting and trying different values) and written down so that the thumbnail could also be reproduced exactly from the session that had already been saved.

3. choose **File... Save Image**, specify file location, name and type (**PNG** was used), and click **Save**; in this case, the size was kept the same as the Chimera graphics window (width 110 pixels, height 87 pixels)

Image Tutorial: Surface Properties

This tutorial describes generating high-quality images of a protein surface colored to show [hydrophobicity](#) and [electrostatic potential](#). Note there are several routes to the same or similar results. See also: [presets](#), [tips on preparing images](#)

[Start Chimera](#) and show the [Command Line](#) (for example, with **Favorites... Command Line**). Fetch Protein Data Bank entry [3eeb](#):

Command: [open](#) **3eeb**

The structure is a toxin that is activated by binding inositol hexakisphosphate (IHP), a highly negatively charged small molecule. As might be expected, the binding site is polar and lined with many positively charged groups. This can be illustrated by coloring the surface to show its properties.

[Move and scale](#) the structure as you wish throughout the tutorial. Delete one of the copies of the structure, chain A, and solvent:

Command: [delete](#) **:.a**

Command: [del](#) **solvent**

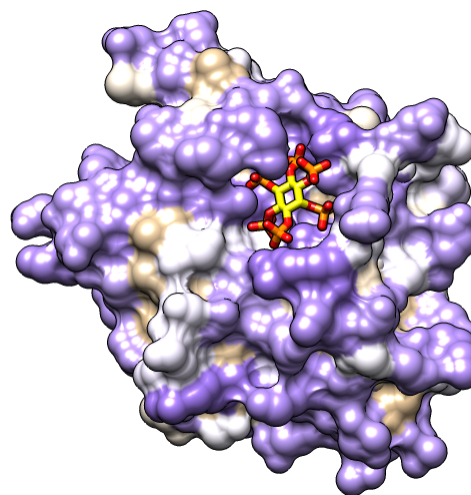
Resize the window as desired, either by dragging its lower right corner with the mouse or by using the command [window size](#). The window dimensions define the aspect ratio (width:height) of output images, but image resolution (pixel dimensions) can be specified independently when an image is saved.

Amino Acid Hydrophobicity

Use the "hydrophobicity surface" preset to display the molecular surface colored by amino acid hydrophobicity:

Command: [preset](#) **apply int 3**

Colors are mapped to [Kyte-Doolittle hydrophobicity](#): from **dodger blue** for the most hydrophilic, to **white**, to **orange red** for the most hydrophobic. The IHP molecule looks somewhat like a distorted snowflake. The IHP-binding pocket is primarily blue, indicating its hydrophilic character. However, as shown in the figure, we will use different colors than in the preset.



A nearby sodium ion and the heteroatoms in IHP are [colored by element](#). Hide the ion, make the sticks fatter, and make ligand carbons yellow:

Command: [~disp](#) **ions**

Command: [setattr](#) **m stickScale 2**

Command: [color](#) **yellow ligand & C**

Different colors can be mapped to this **kdHydrophobicity** attribute of residues using the command [range color](#):

Command: **[rangecol](#) kdHydrophobicity min medium purple 0 white max tan**

Now the most polar residues are **medium purple** and the most hydrophobic are **tan**. (The same thing can be done in the **[Render by Attribute](#)** graphical interface; for a similar process, see the **[B-Factor Coloring](#)** image tutorial.)

The built-in colors can be viewed **[here](#)** or by choosing **Actions... Color... all options** from the menu and in the resulting dialog, checking the option to **Show all colors**. Additional colors can be created with the command **[colordef](#)**.

Use a publication preset for nice image settings, including white background, black outlines, and increased smoothness:

Command: **[preset](#) apply pub 1**

The example image was saved from a 500x500-pixel window using **File... Save Image** with default settings.

Electrostatic Potential

If not already done, show the molecular surface and use a publication preset:

Command: **[surf](#)**

Command: **[preset](#) apply pub 1**

Start **[Coulombic Surface Coloring](#)** (under **Tools... Surface/Binding Analysis**), choose the surface model, and click **OK**.

The publication presets provide a nice starting point, but you might want to adjust some settings, such as the thickness of the black outlines:

Command: **[set silhouetteWidth](#) 3**

If you prefer a simple "line drawing" appearance, try ambient-only lighting:

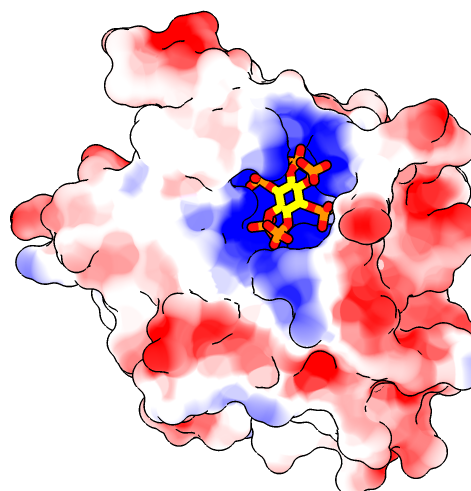
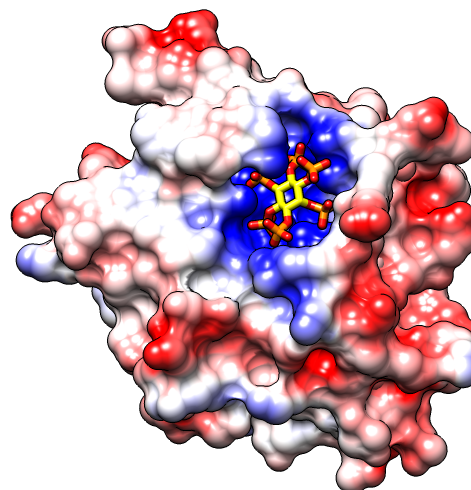
Command: **[light](#) mode ambient**

To restore the default lighting mode:

Command: **[light](#) mode two-point**

The example images were saved from a 500x500-pixel window using **File... Save Image** with default settings.

There is a limit to how thick lines such as silhouette edges, wire, and mesh can be drawn while rendering an image. If supersampling is done, the image is initially drawn at a larger size than requested (3x3 by default) and then sampled back down to the final size. In large and/or supersampled images, lines may be thinner than expected. The **File... Save Image** dialog reports the effective maximum linewidth. It may be possible to achieve the desired thickness by



reducing the supersampling level and/or the pixel dimensions of the image.

Chimera itself does not perform Poisson-Boltzmann electrostatics calculations, but it can read a grid file or “map” of electrostatic potential values output by another program such as [DelPhi](#), [APBS](#), or [UHBD](#). Chimera also includes interfaces for running some of these programs: the [APBS](#) tool uses a web service, whereas [DelPhiController](#) requires a local (user-installed) copy of [DelPhi](#). Surfaces can be colored by the potential map values using [Electrostatic Surface Coloring](#) or the command [scolor](#). An example map file ([3eebB.phi](#), calculated with DelPhi for the same structure as in the tutorial above) is provided for those who wish to try this approach.

meng-at-cgl.ucsf.edu / September 2012

Molecular Visualization with UCSF Chimera: Making Movies

- Presentation and follow-along tutorial
-

Chimera Movie Making

Tom Goddard
October 3, 2012

This tutorial shows how to make animations using Chimera for use on web sites, in journal articles, and talks. We will use maltotriose binding protein, PDB [2gha](#), and Chimera 1.7 snapshot version from September 2012 for our examples.

Topics

- Spinning a molecule.
- Special effects: silhouette edges, shadows, background color.
- Movies with several motions. Command scripts.
- What to show in an animation. Morphing example.
- Saving your work. Use a session file to setup the initial scene.
- Optional: How to put an animation in a web page.

Spinning a molecule

- Open 2GHA.pdb.
- Delete chain B. *Select / Chain / B and Actions / Atoms / Delete*
- Color ribbon. *Preset / Interactive ribbons*
- Highlight ligand. *Select / Structure / Ligand and Actions / Atoms / Sphere*

- Rotate 360 degrees. *Favorites / Command-Line*
turn y 1 360
- Record "spin" movie.
movie record ; turn y 1 360 ; wait ; movie encode
- Semicolons separate commands on one line.
- **movie record** starts capturing images.
- **wait** prevents going to the next command until motion finishes.
- **movie encode** writes the images to a movie file.



Special effects: silhouette edges, shadows, background color

- Background white. Command **set bg white**.
- Silhouette edges. *Tools / Viewing Controls / Effects*.
- Enable shadows.
- Background gradient. *Favorites / Preferences*, category Background, background method gradient
- Gray gradient. Click background gradient color well.
- Set window size. Command **window size 640 480**.
- Record movie, 2 degree steps, supersample to smooth edges.

movie record supersample 3 ; turn y 2 180 ; wait ; movie encode



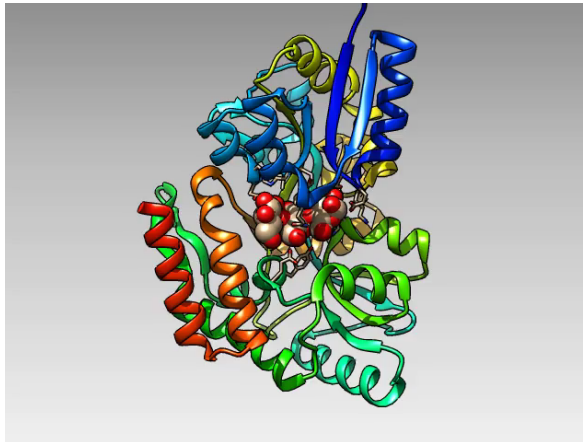
Movies with Several Motions: Command scripts

- To make more complex movies put commands in a plain text file and run it.
- Try this using Text Edit on Mac, or Note Pad on Windows, or any text editor.

```
movie record
turn y 2 180
wait
movie encode
```

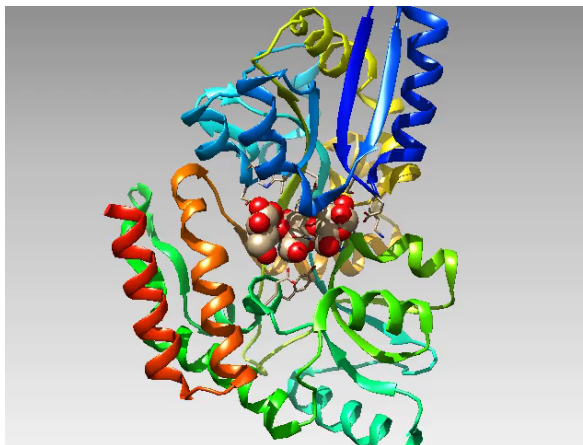
- Zoom in on ligand and do second spin.
- Interactively try this command: **scale 1.02 80**
- Make rotation about center of ligand. Select central ligand atom. *Actons / Set Pivot*

```
movie record
turn y 2 180
wait
scale 1.02 80
wait
turn y 2 180
wait
movie encode ~/Desktop/spin3.mp4
```



- Fade out ribbon so it does not block view of ligand.
- Interactively try this command: **transp 80,r**
- Turn off silhouettes to deemphasize ribbon.
- To make duller transparency try: **set flat**
- To smoothly fade to transparent ribbon use: **movie crossfade 25**

```
movie record
turn y 2 180
wait
scale 1.02 80
wait
movie crossfade 25
transp 80,r ; set flat
turn y 2 180
wait
movie encode ~/Desktop/spin5.mp4
```



What to show in an animation. Morphing example

Many of the commands useful in making movies are demonstrated on the [Movie Examples](#) page on [Chimera web site](#) under [Documentation](#).

Morphing is one of the most useful kinds of animation, making it easier to see differences between two conformations of a molecule.

- Open 2ghb.pdb, no maltotriose ligand bound.
- Delete chains B and C.
- Use MatchMaker to align 2ghb to 2gha. *Tools / Structure Comparison*
- Color 2gha ribbon pink. Command **color pink,r #0**
- Morph using *Tools / Structure Comparison / Morph Conformations*
- Hide original structures with *Favorites / Model Panel*
- Show ligand from 2gha: **~ribbon #0 ; ~display #0 ; display ligand**
- Show morph residues near ligand: **disp #2 & ligand zr<5**
- Use MD Movie dialog *File / Record Movie...*
- To use morph in a command script: **coordset #2 1,41**



Structure superposition.



Morph movie.

Saving your work. Use a Session File to Setup the Initial Scene

To save your movie making work, save a Chimera session that sets up the scene, and use a command script that records the movie.

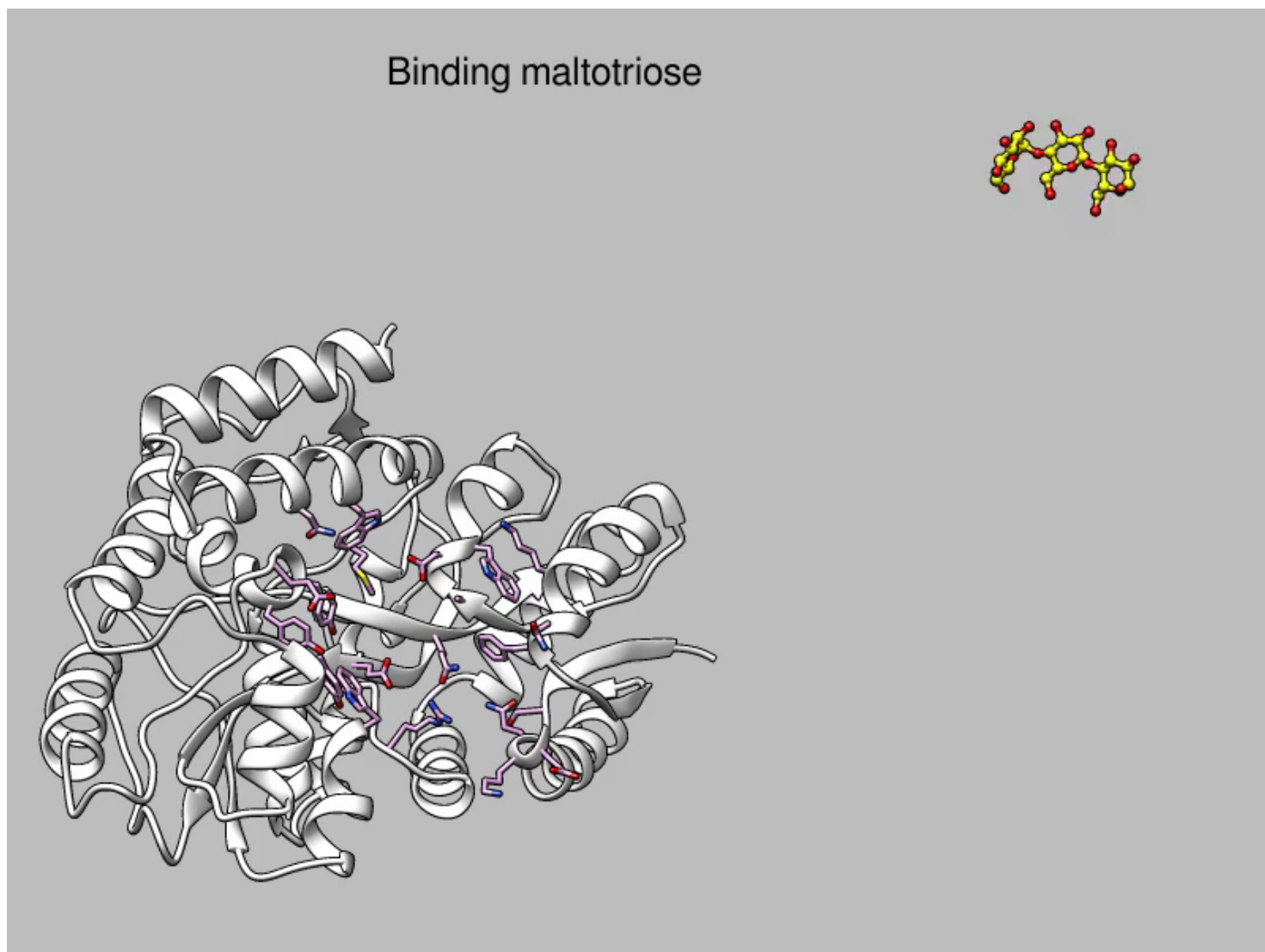
- Save session with calculated morph. *File / Save Session As...*
- Save command script that records the movie.

```
movie record
coordset #2 1,41
wait
movie encode
```

- For each movie you make keep 3 files: the Chimera session, the command script, and the movie (**morph.py**, **morph.cmd**, **morph.mp4**).
- This allows you to later improve the movie, change its size, etc. with little effort.

A Fancier Movie Example

Includes titling (**2dlabel**), ligand fly in (**savepos / reset**), hydrogen bond display (**hbond**), surface display (**surf**).



Other example animations are on the Chimera [Animation Gallery](#) web page.

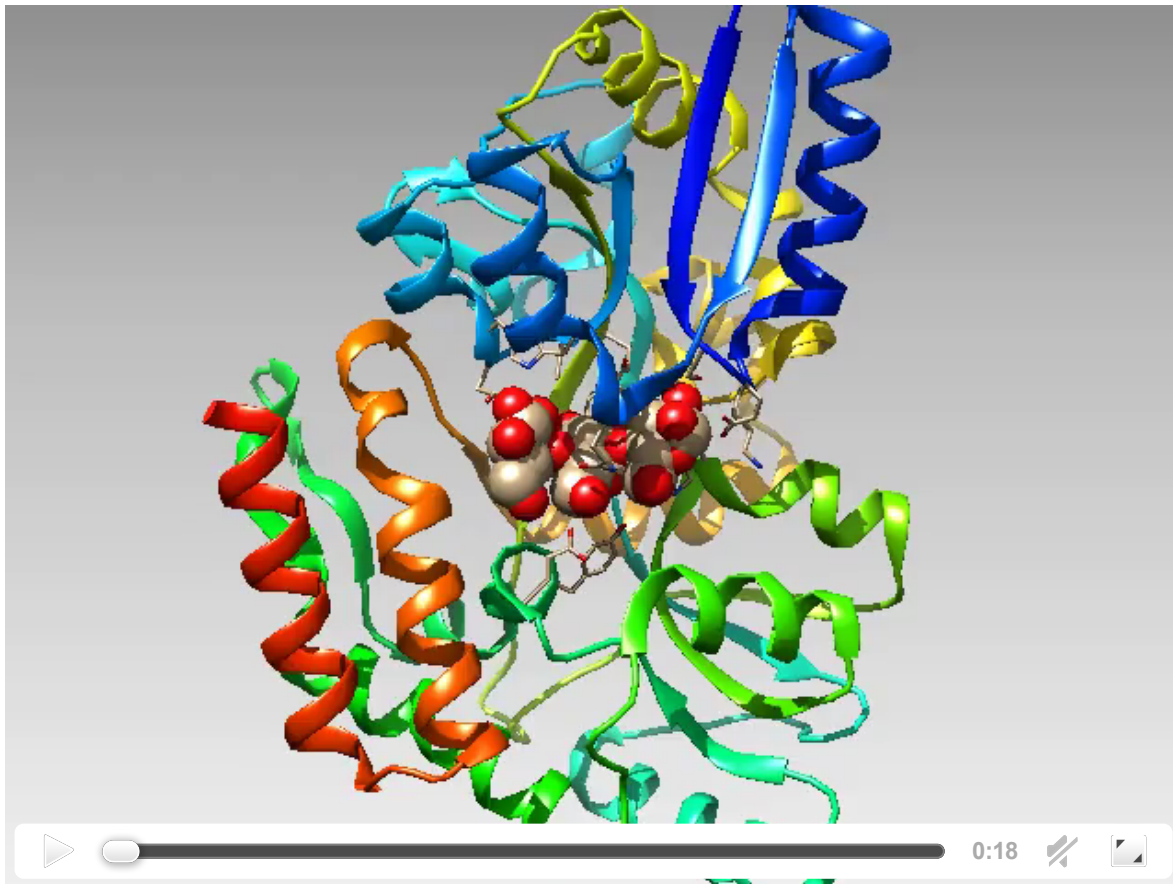
How to put an animation in a web page

- Use HTML5 video tag to embed a movie in a web page.

```
<html>
<body>

<video width="640" height="480" controls="controls">
  <source src="movie.mp4" type="video/mp4" />
  Your browser does not support the video tag.
</video>

</body>
</html>
```



- Chimera records movies in H.264 format by default.
- Safari and Chrome and Internet Explorer 9 web browsers will play this.
- Firefox does not play H.264. Encode a second format (Ogg Theora) to play in Firefox without plug-ins.

Molecular Visualization with UCSF Chimera: Question & Answer Session

- New features in Chimera 1.7:
 - Improved graphics
 - performance increase for newer video cards
 - higher default frame rate for smoother motions
 - glossy lighting
 - interactive shadows
 - New tools
 - PDB2PQR - assignment of atomic partial charges and radii
 - APBS - continuum electrostatics calculation
 - AutoDock Vina - molecular docking
 - Model/Refine Loops - interface to Modeller
 - Notepad - save user-entered descriptive text with sessions
 - New image/movie features
 - export in HTML/WebGL format for interactive web viewing
 - Animation tool for creating simple movies
- Future directions:
 - Chimera 2.0 - web- and desktop-based application
 - Web-based application using modern web standards (HTML5, JavaScript, WebGL)
 - Desktop-based application using modern cross-platform toolkits (Qt, OpenGL)
 - Performance from parallelization (threads, GPU)
 - Integration with web services (databases, computation, storage)
 - interface to cloud computing infrastructure such as Amazon Web Services
 - Access to extensive computational resources
 - Minimize cost for hardware setup and maintenance
 - Pre-made system images for common tasks (molecular dynamics, virtual screening)
- What is a feature you would like to see in Chimera?
 - Tell us now
 - Mail suggestions to chimera-users@cgl.ucsf.edu later