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.

A:

B:

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**
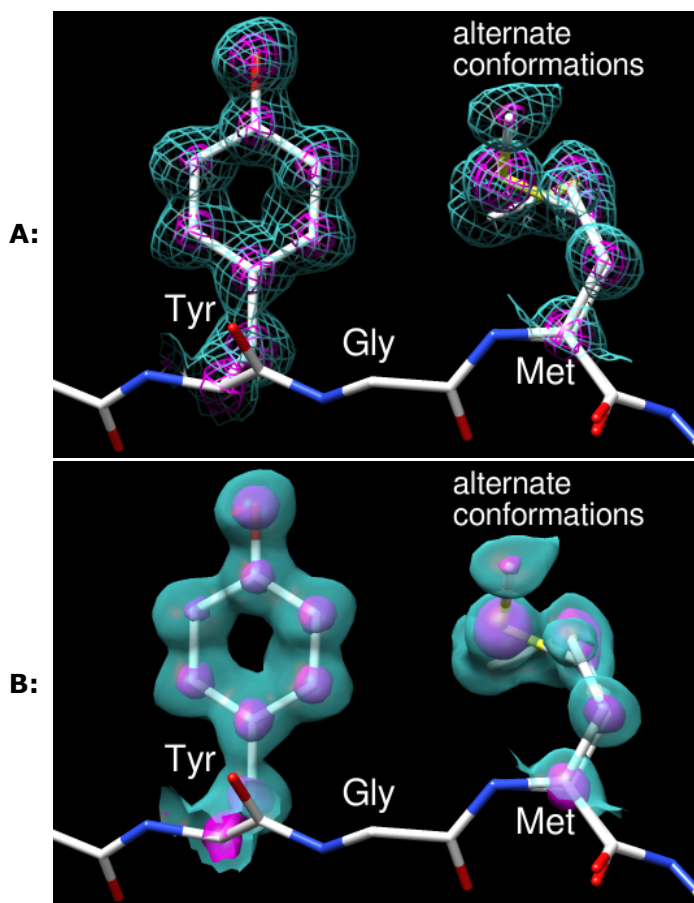
> *Command*: **show** **:168-170**
> *Command*: **focus**
> *Command*: **disp** **:167,171@n,ca,c,o**

Change to the stick representation and make the sticks thinner:

> *Command*: **rep** **stick**
> *Command*: **setattr** **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;
   - 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)
   - 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
   - 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

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