

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

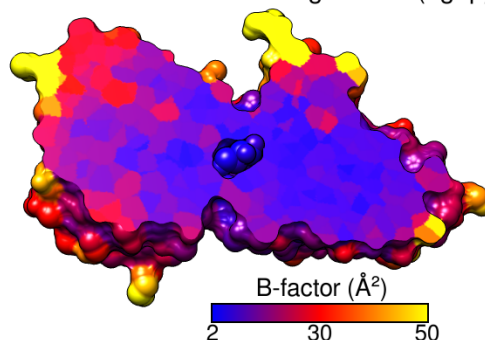
Start [Render by Attribute](#) (under **Tools... Depiction**) and make sure it is set to show the [attributes](#) of **atoms**. Look in the **Attribute** list to see what is available: **bfactor** and **occupancy**, which were read from the input PDB file. Choose **bfactor**; a histogram of the values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