

# UCSF ChimeraX - I - Overview

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```
## Warning: package 'knitr' was built under R version 3.5.2
```

## 1 Workshop goal

Even though this workshop can be attended by complete novices, previous workshops on PyMOL or UCSF Chimera would be very beneficial.

This **ChimeraX** session is planned to be an overview of the software (that is still in beta development) and explore some of the new features implemented for the display of large molecules and Cryo-EM data.

### 1.1 Learning objectives

- Launching **ChimeraX**
- Review **ChimeraX** interface and tools
- Open a 3D coordinate file directly from RCSB Protein Data Bank
- Move & interact with displayed molecule
- Show/Alter representation as ribbons, surfaces, etc.
- Atom selection
- Save and image
- Display biological assembly
- Close and quit

## 2 Introduction

UCSF ChimeraX (or simply **ChimeraX**) is the next-generation molecular visualization program from the Resource for Biocomputing, Visualization and Informatics (RBVI), an NIH Biomedical Technology Research Resource (Goddard et al. 2018).

In the long run it is intended to replace UCSF Chimera (Pettersen et al. 2004) for molecular graphics visualization. **ChimeraX** has a new interface and also new capabilities such as “ambient occlusion lighting” for realistic shadows.

**ChimeraX** can work with a variety of formats, notably crystallographic data from the Protein Data Bank and Cryo-EM maps.

**ChimeraX** exists for the 64 bit operating systems of MacOS, Windows 10 and Linux. **ChimeraX** is free for academic use and is available for download at <https://www.rbvi.ucsf.edu/chimerax/download.html> but is already installed on the classroom iMacs under the Macintosh OS.

## 3 ChimeraX vs Chimera features

**ChimeraX** will retain a large number of features and capabilities of **Chimera** but since the current implementation is still a “beta release” (as of this writing it is **ChimeraX** version 0.5) many commands and features are only available *via* line-command only rather than mouse click interface.

## 3.1 Features

Citing the web site: Compared to Chimera, ChimeraX has a more modern user interface, better graphics, and handles large structures much faster.

Although similar in many aspects, ChimeraX is not backward compatible with Chimera and does not read Chimera session files.

Amongst various improvements and advantages of **ChimeraX** over **Chimera**:

1. the fast rendering of large number of atoms
2. interactive ambient occlusion lighting modes
3. fast and robust solvent excluded surfaces

## 3.2 Missing features

While **ChimeraX** has several completely new features and other advantages, it will not substantially replace the functionality in **Chimera** for quite some time. It currently has a limited set of features and few user-interface dialogs; most capabilities are implemented as commands only.

Missing features include a long list detailed on the web site. However “daily builds” of the application may bring them to life at any time.

## 3.3 Main difference

One important difference between the two software is that **Chimera** opens many ancillary, separate windows as commands are given while **ChimeraX** functions within a *single window pane*. However, embedded windows can be *undocked* and separated from the main window.

Another difference is that **ChimeraX** has a **built-in browser** that can open pages containing active links to be run within **ChimeraX**. This is the case in particular for the **Tutorials** pages.

## 4 Set-up

If you are using the iMac for the first time you may need to review and update the mouse button assignment by going to the “Apple” menu at the top left:

**Apple > System Preferences... > Mouse**

“Standard” setting should be set as follows (if you are right-handed) :

- Left: Primary Button
- Wheel: Button 3
- Right: Secondary Button

*Note:* If you are left-handed inverting Left and Right assignments might work better for you.

*Note:*

### TASK

This button will invite you to act on **suggested actions** as we go along the workshop.

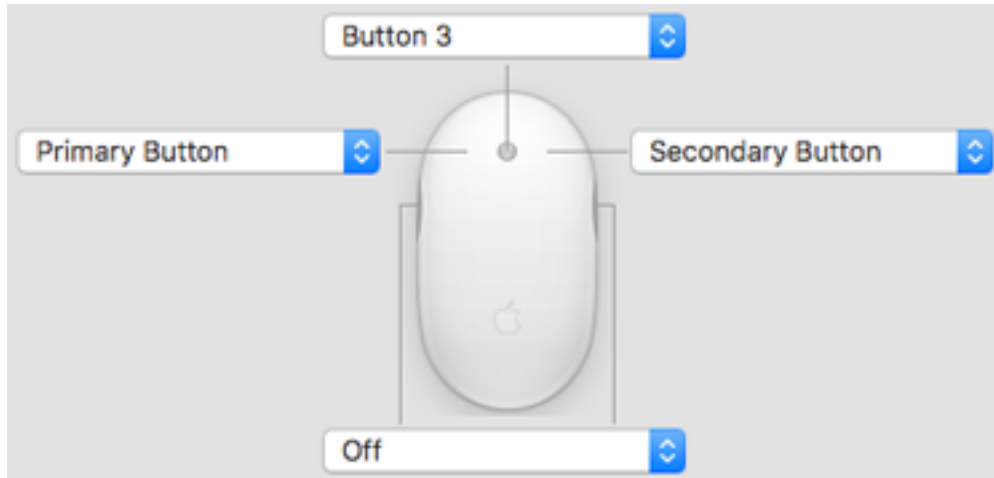


Figure 1: “*Verify mouse settings in System Preferences.*”



Figure 2: “*ChimeraX icon.*”

## 5 Finding and Launching ChimeraX

### 5.1 ChimeraX Location

If you are following this workshop live in the classroom, the iMac in front of you has **ChimeraX** installed within the /Applications directory.

You can also find **ChimeraX** by using Spotlight Search: the “magnifying glass” icon on the *top right* of the Macintosh screen.

On a Windows computer you would type **ChimeraX** in the search area next to the Start button or within a “magnifying glass” text entry, also bottom left, with “Cortna” helper in Windows 10.

If you are using your own computer **ChimeraX** can be found in the same way.

### 5.2 Launch ChimeraX

#### TASK

If **ChimeraX** has not launched automatically, double-click on its icon:

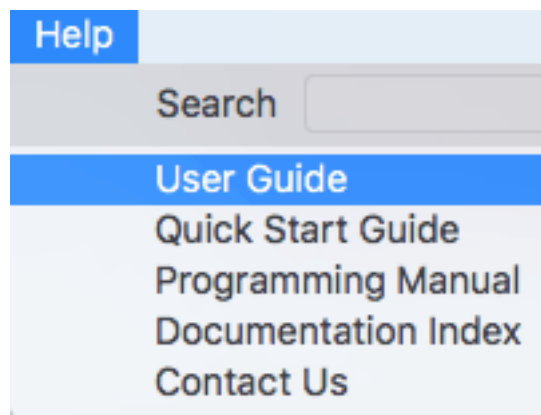


Figure 3: “*ChimeraX Help menu.*”

## 6 Documentation and help

### 6.1 Online

**ChimeraX** documentation can be found online as links from the **ChimeraX** home page<sup>1</sup> within the “Quick Links” section at the top left as:

- Documentation<sup>2</sup>
  - User Guide<sup>3</sup>
  - Tutorials<sup>4</sup>

### 6.2 Built-in

The same documentation is available built-in **ChimeraX** and can be accessed from the **Help** menu:

Calling this help will open a built-in internal browser that is integrated with **ChimeraX**. This is particularly useful for tutorials as commands can be clicked-on directly. However, for this session please do not open the tutorials.

## 7 ChimeraX interface

**ChimeraX** opens with an all-in one window interface split in 2 main panels accompanied by toolbars at the top and on the left side.. Many of the

From the web page:

ChimeraX has an all-in-one window interface in which various *panels* can be shown, hidden, and repositioned. Panels can also be detached (undocked) from the main ChimeraX window and subsequently reinserted (docked). The overall window also contains the *main window* for 3D graphics, a *title bar* across the top, and a *status line* for transient messages across the bottom. At the bottom right are small icons\*:

<sup>1</sup><http://www.rbvi.ucsf.edu/chimerax/>

<sup>2</sup><https://www.cgl.ucsf.edu/chimerax/docs/>

<sup>3</sup><http://www.rbvi.ucsf.edu/chimerax/docs/user/index.html>

<sup>4</sup><http://www.rbvi.ucsf.edu/chimerax/tutorials.html>

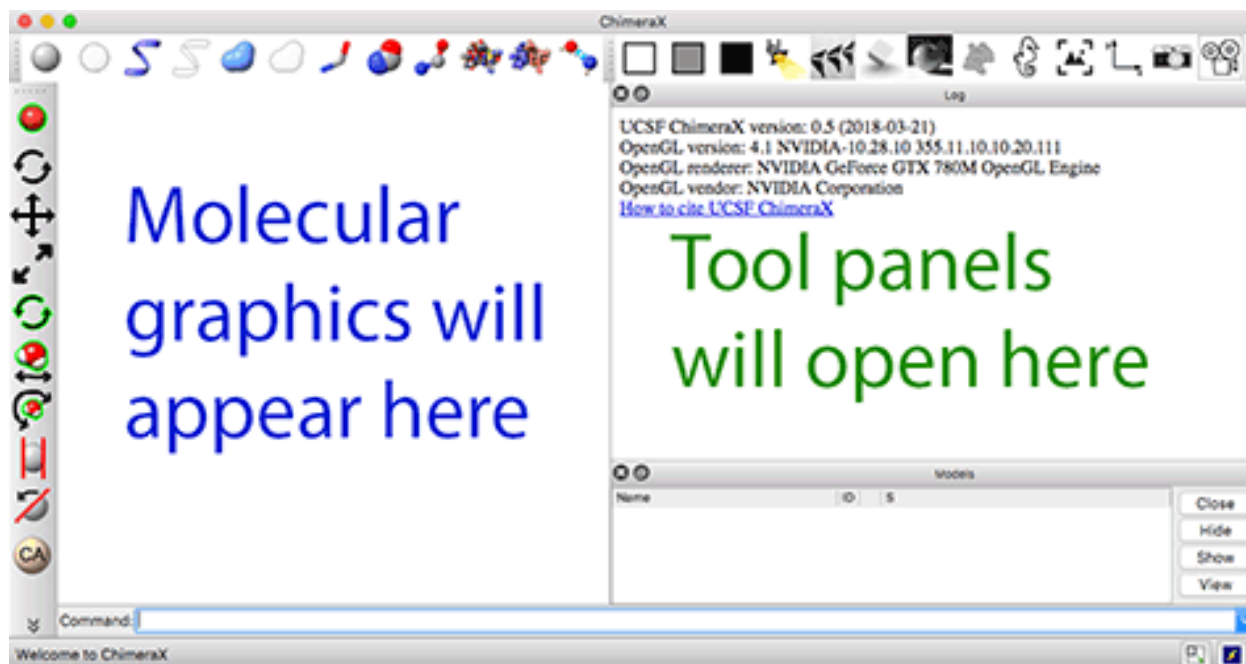





Figure 4: “*ChimeraX all-in one window.*”

-  - toggle main window to fill overall window
-  or  - toggle main window between 3D graphics and **Rapid Access**.

The **Tools > Toolbar >** menus can turn on and off the top and side bars for the control of:

- Density Map (not active by default)
- Graphics (top right)
- Molecule Display (top left)
- Mouse Modes for Right Button (vertical, left side)

The **Density Map Toolbar** controls display of electron density maps

The **Graphics Toolbar** controls the background color, lightings, sketch outline, image and movie making.

The **Molecule Display Toolbar** controls the display of atoms, ribbons, surfaces, sticks, spheres, ball-and-sticks, color atoms by elements, color atoms by chain, and display hydrogen bonds.

The **Mouse Modes for Right Button** (vertical to the left) provides advanced features to manipulate the molecular display by allocating functions to the right-mouse button.

More information on using the all-in-one **ChimeraX** window is detailed on the documentation web page [The ChimeraX Window](https://www.rbvi.ucsf.edu/chimerax/docs/user/window.html)<sup>5</sup>.

## 8 Tools menu

The **Tools** menu is used to engage various options. We just used the menu cascade **Tools > Toolbar >** above to toggle the display of the control toolbars within the all-in-one window.

<sup>5</sup><https://www.rbvi.ucsf.edu/chimerax/docs/user/window.html>

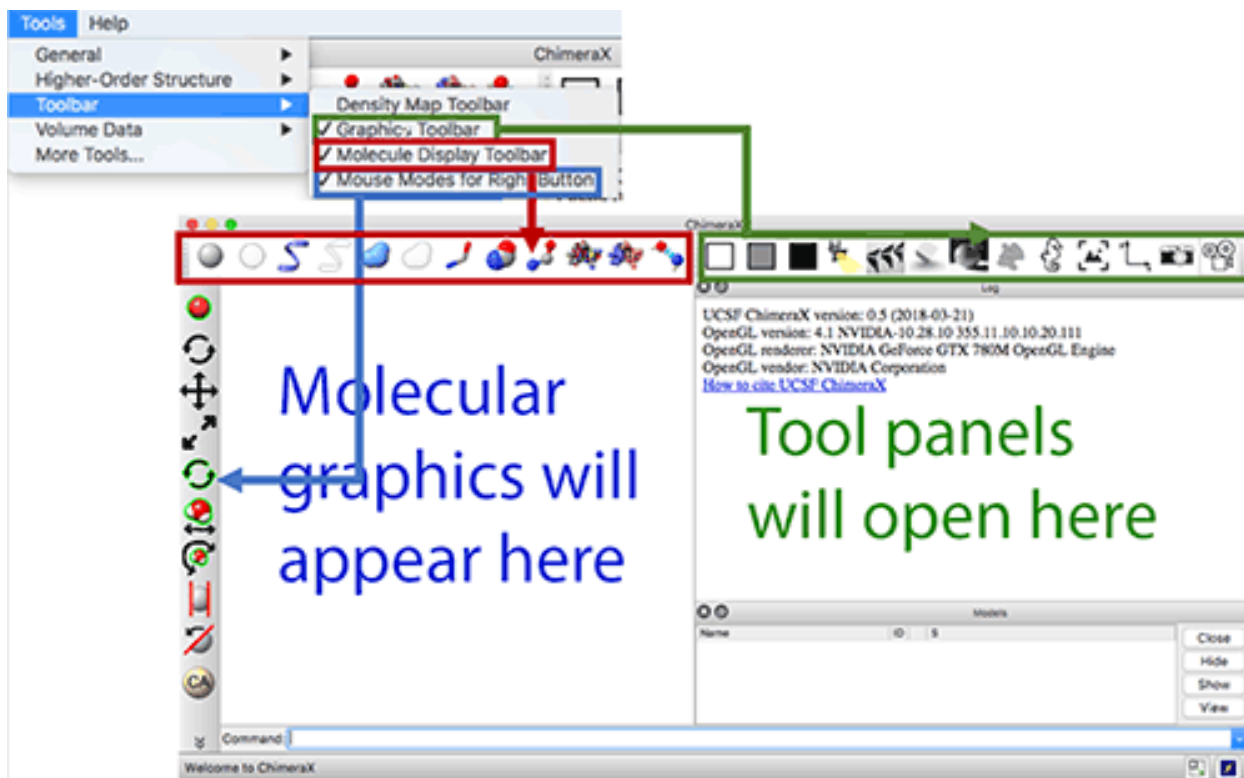


Figure 5: “*Tools > Toolbar > menus toggle toolbars on all-in-one window.*”

The menu cascade **Tools > General** > offers important tools that need to be turned on if they are not yet present.

In the section below we will turn on the line-command.

## 8.1 Line command

It is useful to turn on the line-command if it not yet turned on.

### TASK

Follow the menu cascade:

**Tools > General > Command Line Interface**

You should now see a text area at the bottom of the all-in-one window preceded with the word *Command:*.

## 9 Open a 3D structure

In this section we will use a simple example file: *1mbo. Structure and refinement of oxymyoglobin at 1.6 angstroms resolution* (Phillips 1980).

**ChimeraX** can open a structure in 2 ways:

- directly on the Internet with the command **open**
- with the menu cascade **File > Open...** if the file is already saved on your computer.

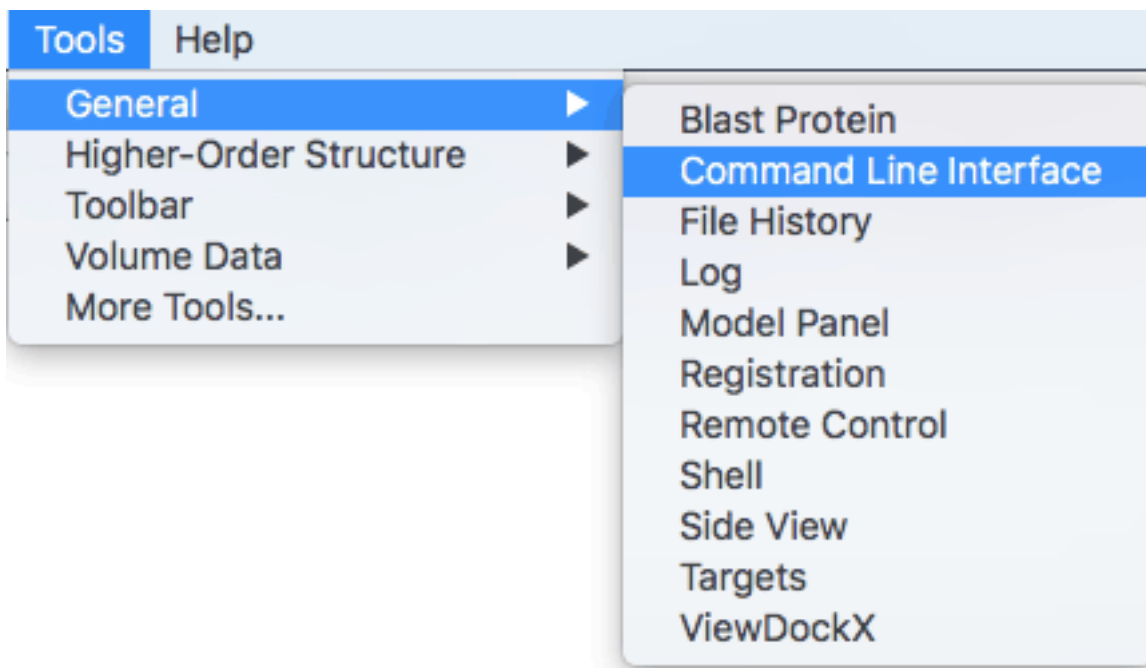


Figure 6: “*Tools > General > menus.*”

In both cases you would need to know the PDB ID code of four characters gleaned *e.g.* from the PDB site or a publication.

*Note:* When the structure is loaded, it is presented in a default preset mode that depends on the number of chains contained within the file (more info below.)

#### TASK

**On the command line type the following: open 1mbo and press Return on your keyboard.**

**ChimeraX** will *fetch* the file from the Protein Data Bank web site in the *cif* format and save it within your **Downloads** folder by default. On a Macintosh the file will be saved in: */Users/YOU/Downloads/ChimeraX* where **YOU** is your username. On other operating systems the file would be saved in a similar way and location.

The structure will be displayed on the left within the molecular graphics panel. On the right pane, summary information about the structure will be displayed below a reminder of the command issued.

The summary information will be most useful for complex structures and will display the name of chains. Here there is only chain **A**. The citation provided is the **primary citation** of structure publication.

Finally, information about number of atoms and bonds are provided.

Here: *Opened mmCIF data containing 1601 atoms and 1296 bonds*

*Note:* The *Model Panel* will open automatically at the bottom right. It can be closed by clicking the (x) button and can be “detached” by clicking the other button. If closed it can be recalled with the menu cascade: **Tools > General > Model Panel**. The buttons on the right can affect the model: **Close, Hide, Show, View**

#### TASK

**To make your display similar to the following image, simply click the *white square* within the *Graphics Toolbar* at the top right. This will change the background to white.**



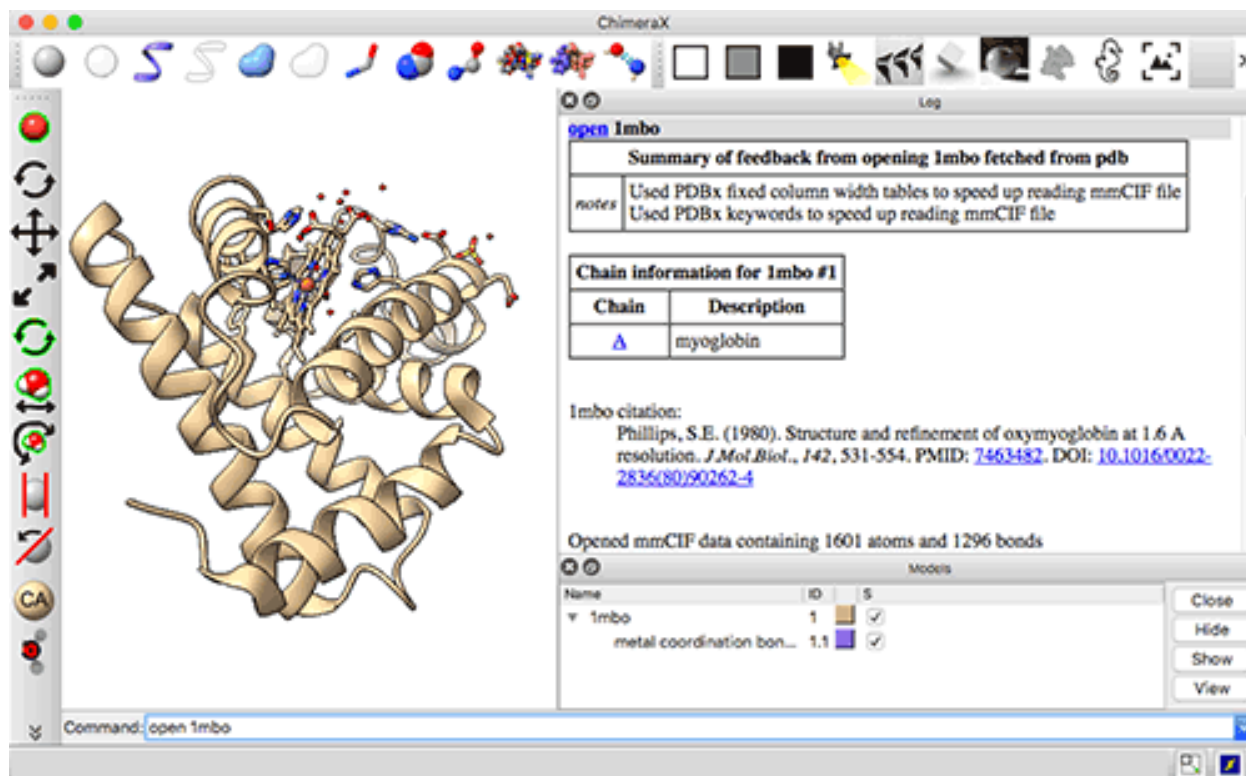


Figure 7: “Myoglobin protein in 1mbo opens as ribbons; ligands as sticks. Hovering the mouse over will reveal amino acid info.”

*Important Note:* When a button is clicked, its line-command equivalent is immediately displayed on the right panel.

For the background color change this would have echoed `set bgColor white` onto the panel. Note also that the command is highlighted in blue and is a hypertext link to the help pages. Clicking on such a link will open the **ChimeraX** internal browser to display this information.

#### TASK

Explore briefly the current display.

To rotate the structure: click on the left mouse button and move.

Table 1: Summary of the graphics mouse control

Mouse button	Control
left	rotate molecule when clicking within the space occupied by molecule
left	rotate around Z axis when clicking on corners
right	upward: zoom out. downward: zoom in
wheel	click: translate molecule
wheel	rotate wheel to zoom in and out

You should easily note the following:

- protein: shown as ribbon
- ligands (heme and SO<sub>4</sub>) : shown as sticks
- chelated iron ion (FE) : shown as sphere; hydrogen bonds internally and to His and OXY
- oxygen atoms (OXY) : shown as sticks; hydrogen bonds to FE
- residues within close distance to ligands: shown as sticks.
- a few HOH water molecules: shown as small red spheres.

*Important Note:* **ChimeraX** automatically adjusts the appearance and style of the structure, based on rules that take into account the number of chains contained in the structure. For example for 1mbo there is only one chain and therefore the structure is presented as a **ribbon**. This can explain that different structures

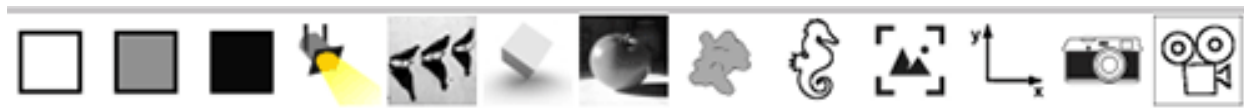


Figure 8: “The Graphics Toolbar”



Figure 9: “The *Flat lighting* and *Silhouette edges* buttons”

## 10.1 Background color

The first three square items change the background color. There are more fancy colors that could be used, but these three choices are the most useful.

The command `set bg_color` can be used for more dramatic colors (not recommended for publication!) See next section for color names.

## 10.2 Light and shadows

### TASK

*On your own* select the next four items. They pertain to lighting and shadows:

- simple lighting (projector)
- single shadow (shadow)
- soft lighting (cube)
- full lighting (apple)
- flat lighting (gray blob)

*Note:* the *soft* and *full* lighting use *ambient occlusion* shadows to provide a life-like aspect. This is a rather modern method and requires light sources from multiple directions. **ChimeraX** uses 64 lights by default, reduced to only 16 for structures that are very large (more than 250 chains.)

## 10.3 Edges outline (silhouettes)

When you press the “flat” lighting (gray blob) button, you may note that there is a slight black outline on the edges of the drawing. This is controlled by the next button “Silhouette edges” that looks like a hippocampus (9th button from the left.)

### TASK

- Click on the “flat” lighting button
- Then click on the “Silhouette edges” button

Note how the outline disappears and makes the molecule contours harder to discern.

The silhouette can be further altered by line command, for example to change the color or the width of the outline.

### TASK

Change the silhouette defaults with the following commands:



Figure 10: “*Artistic depiction?*”

```
color list
No custom colors.
248 builtin colors: alice blue , aliceblue , antique white , antiquewhite ,
aqua , aquamarine , azure , beige , bisque , black , blanched
almond , blanchedalmond , blue , blue violet , blueviolet , brown ,
burly wood , burlywood , cadet blue , cadetblue , chartreuse ,
```

Figure 11: “*Output of command color list.*”

- `set silhouettes true` : this is equivalent to clicking on the “Silhouette edges” button
- `set silhouetteWidth 5` : this changes the width of the line
- `set silhouetteColor blue` : this change the color of the line

In some cases, these kind of setting for both silhouette and flat lighting can provide “artistic” depictions.

*Note:* There are many colors built-in **ChimeraX** (currently 248 colors are defined.) The name of the colors can be listed with the command: `color list` or `color list builtin`. This will show a small square of color followed by the color name.

## 10.4 Change molecule color

The “Model Panel” (described above) is useful for selecting all or portions of the molecular display (more on that later) but also provides an easy way to alter the color of the representation(s).

The small, colored squares represent the current color of the described item. Clicking on any of those squares will open a color editor where color can be altered.

### TASK

**Change the ribbon color:** click on the brown square to open color editor.

## 10.5 Orientation, snapshot and movie

The last four buttons of the Graphics Toolbar have the following name:

- View all.

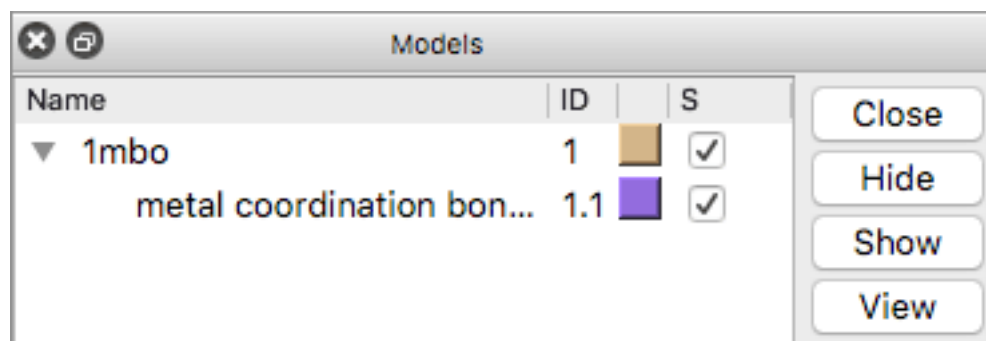


Figure 12: “*Model Panel window after automatic initial display.*”



Figure 13: “*Color editor.*”



Figure 14: “*Last 4 buttons of Graphics Toolbar.*”

```

view
view orient
save ~/Desktop/image1.png supersample 3
movie record
turn y 2 180
wait 180
movie encode ~/Desktop/movie1.mp4
Movie saved to /Users/jsgro/Desktop/movie1.mp4

```

Figure 15: “*Commands echoed on right panel.*”

- Standard orientation.
- Save snapshot to desktop.
- Record spin movie.

**View all** will “shrink” (zoom out) the size of molecules so that all fit within the molecular graphics panel. There is no rotation involved.

**Standard orientation** will reorient the molecule to the position where it was first opened.

**Save snapshot to desktop** will save a .png image of the current molecular graphics panel, with the same dimensions, directly onto the desktop for easy finding. All options will be default options, such as the smoothing of lines.

**Record spin movie** will save a movie of 180 frames in .mp4 format with a 360 degrees rotation (hence 2 degrees increment.) The file is also saved directly onto the desktop.

#### TASK

*On your own* try these four buttons and note the equivalent commands displayed onto the right panel.

This is what you should see: 1 line each for the first 3 buttons, and 4 lines for the movie button.

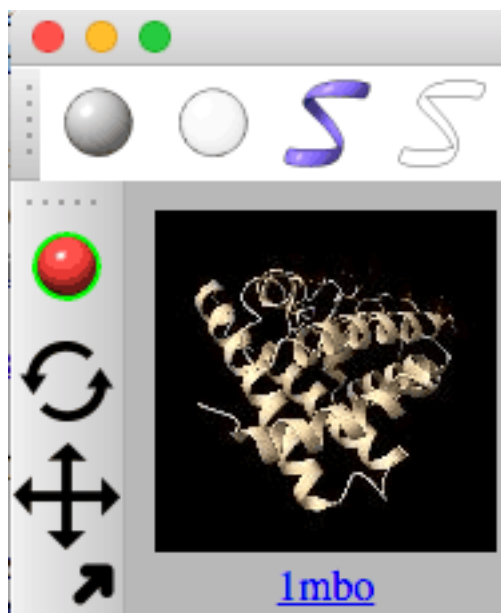


Figure 16: “*Rapid Access square representation.*”

## 11 Molecular display toolbar

### 11.1 Restart

For this section it is best to quit and restart **ChimeraX** to ensure that everything is reset and facilitate the next exercises.

#### TASK

##### Quit and restart ChimeraX

*Note:* as you restart you may note that a mini representation of the previously opened molecule(s) is visible within the left panel.

The “lightning” icon at the bottom right of the The ChimeraX Window will toggle on/off between the 3D molecular graphics (left panel) and the **Rapid Access** display showing mini representations of previously opened molecules.

If you have not opened any other molecule there will only be one for **1mbo** present.

#### TASK

##### Reopen 1mbo by clicking on the Rapid Access square representation

The **ChimeraX** window will now show the molecule again in the default view.

### 11.2 Molecular display toolbar buttons

The molecular display toolbar will alter, show or hide the following representations: atoms, ribbons, surface, stick, sphere, ball-and-stick, atom color by element, atom color by chain, and hydrogen bonds.

The name of the Molecular display toolbar can be seen by hovering the mouse over each button:

- Show atoms
- Hide atoms



Figure 17: “Molecular display toolbar. Atoms, ribbon, surface etc.”

- Show molecule ribbons
- Hide molecule ribbons
- Show molecular surface
- Hide molecular surface
- Show molecule in stick style
- Show molecule in sphere style
- Show molecule in ball and stick style
- Color atoms by elements
- Color atoms by chain
- Show hydrogen bonds

It is important to remember that the 3D coordinate file will contain **ATOM** records for protein and nucleic acid atoms, and **HETATM** records for “heteroatoms” *i.e.* atoms that are *other than* protein and nucleic acid. These are usually ligands, solvents, metal ions, and water molecules.

During the *default* view display, **ChimeraX** will recognize these distinctions and prepare the protein as a **ribbon** (depending on number of chain present, see above.) Then it will show ligands as sticks, ions as spheres, and amino acids close to ligands also as sticks. This is what we see here for the default display of 1mbo.

We are now going to alter, hide or show various representations. However, we shall **NOT** start with the atom buttons (the first 2 buttons.)

#### TASK

**Click button on the Molecular display toolbar but NOT the first two (Show/Hide atoms) for now!**

It is better if you click in the order from left to right (again, NOT touching the first 2.)

The table below summarizes what you should see if you click the buttons from the molecular display toolbar in the order they appear on the bar (except the first 2.) The result is also linked to which atoms are currently selected (see next section.)

Table 2: Table summarizing what you should see

Click on button	See this
Show molecule ribbons	Nothing will change as the ribbon is already visible!
Hide molecule ribbons	Ribbon disappears. Only sticks (ligands and close amino acids) and sphere (ion) will remain.
Show molecular surface	Molecular surface will show for protein. Ligands are outside of surface as sticks.
Hide molecular surface	Surface disappears. Only sticks (ligands and close amino acids) and sphere (ion) will remain.
Show molecule in stick style	Ion sphere becomes small sphere. No other changes
Show molecule in sphere style	Ligands and close amino acids, water molecules shown as spheres.
Show molecule in ball and stick style	Ligands and close amino acids, water molecules shown as ball and sticks.
Color atoms by elements	No change. Already colored that way.
Color atoms by chain	All become the same color (purple) as there is only one chain.

Click on button	See this
Show hydrogen bonds	Add H-bonds to visible ball-and-stick models

### 11.3 Show and hide atoms


*Note:* Here it may again be useful to quit, restart, and reopen **1mbo**.

When a molecule is first open, as already mentioned above, **ChimeraX** creates an initial display based on *Automatic Styling* sometimes referred as *Smart Initial Display*.

However, as soon as one uses the “Show atoms” and “Hide atoms” buttons this display is altered in a way that is not easily reconstructed without knowing more about **ChimeraX**.

This behavior is related to the **current** selection of atoms as understood by **ChimeraX**.

One easy method is to quit and restart.

Another method is to toggle off the right-hand panel with the bottom right toggle button . However, this would open a second version of that molecule and the “Model Panel” could then be used to close the first to reveal the newly opened molecule.

### 11.4 Atom selection

#### 11.4.1 Definitions

Which atom(s) are currently selected will determine the effect of many buttons (*e.g.* on Molecular display toolbar) or command lines.

While selected atoms will appear highlighted in green outlines on the graphics window, there are sometimes “internal” selection that occur as we experienced with the “Atom display” earlier.

Selection can be accomplished by line command, or by mouse click or drag. The help pages on selection<sup>7</sup> and the `select`<sup>8</sup> command offer a more complete description.

The line command selection itself relies heavily on the atom specification<sup>9</sup> to designate complete models, chains etc.

When a molecule is opened, it is given a model number. This number appears also within the “Model panel” (see above.)

The following summary table shows the “hierarchical specifiers” for models, chains and atoms (simplified from the atom specification page.)

Table 3: Table listing “hierarchical specifiers” for **atom specification**.

Symbol	Reference Level	Definition	Examples
#	model	model number assigned in ChimeraX	#1 #1.3
/	chain	chain identifier	/A
:	residue	residue number OR residue name	:51 :glu
@	atom	atom name in PDB file	@ca @nz

<sup>7</sup><http://www.rbvi.ucsf.edu/chimerax/docs/user/selection.html>

<sup>8</sup><http://www.rbvi.ucsf.edu/chimerax/docs/user/commands/select.html>

<sup>9</sup><http://www.rbvi.ucsf.edu/chimerax/docs/user/commands/atomspec.html>



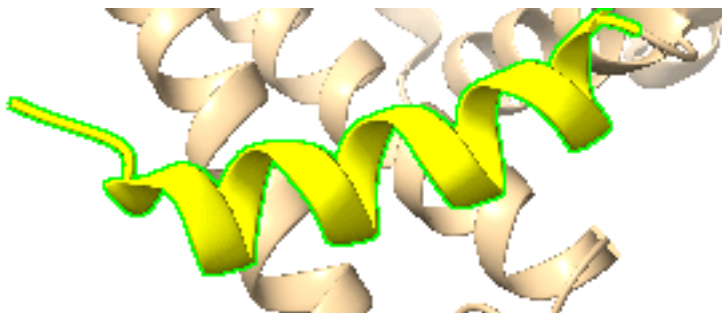


Figure 18: “*Select and color with selection command.*”

The atom specifications can be combined; here are a few examples from the atom specification page:

Table 4: examples of atom selection by hierarchical specifiers

Example	Meaning
<code>#1</code>	all atoms in model 1
<code>#1/B-D,F</code>	chains B, C, D, and F in model 1
<code>#1,2:50,70-85@ca</code>	atoms named CA in residues 50 and 70-85 in models 1 and 2
<code>/a,d-f:43-256</code>	residues 43-256 in chains A, D, E, and F
<code>:12-25,48@ca,n</code>	atoms named CA and N in residues 12-25 and 48
<code>:lys,arg</code>	lysine and arginine residues
<code>:lys,arg@cb</code>	atoms named CB in lysine and arginine residues

There are many more examples, including much more complex examples on the atom specification page.

#### TASK

Use the `select` command with a definition above to color the first 18 amino acids of `1mbo`.

On the command line type the following commands:

- `sel #1:1-18`
- `sel` is short for `select` - this will select amino acids 1 through 18 for model 1. On the display the selection will be highlighted by a surrounding green outline.
- `color sel yellow` (this will color the selection yellow.)
- To release the selection: `Ctrl-Click` the left button anywhere on the background.

#### 11.4.2 Built-in classifications; atoms and heteroatoms

Interestingly, there is no built-in command for selecting all “heteroatoms” (HETATM records; if you are familiar with `PyMOL` the selector in that software is `hetatm`.)

However, `ChimeraX` offers a range of useful premade selectors referred to as “classifications.” (See middle section of atom specification page.)

### 11.5 Models

Every time a molecule is opened, it is given a model number and shows as an entry in the “**Model Panel**” (See image above in section **Change molecule color**.)

The model number appears under the column **ID** while column **S** means “Show” and can be used to hide the structure.

## 12 Biological Assembly

### 12.1 Coordinates files

The PDB files solved by X-Ray crystallography contain the solution to solving the “**asymmetric unit**” *i.e.* the smallest portion of the crystal necessary to reconstruct the whole crystal by symmetry. However, that does not necessarily reflect the biologically active form, monomeric or multimeric form of the **biologically functional assembly**.

A biological assembly may be built from<sup>10</sup>:

- one copy of the asymmetric unit
- multiple copies of the asymmetric unit
- a portion of the asymmetric unit

The coordinate file (which will be downloaded automatically) will contain information for the rotational and translational transformations to build a biological assembly. This takes form as a 3x4 (rotation/translation) matrix.

If the file format is **.pdb** the matrices will be listed in the **REMARK 350** entries in the header. For example, the PDB file 1DUD is a monomer as an asymmetric unit, but a trimer as a biological assembly. Three matrices, including the *identity matrix* will be provided:

```
[...]
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
REMARK 350  BIOMT1  1  1.000000  0.000000  0.000000      0.000000
REMARK 350  BIOMT2  1  0.000000  1.000000  0.000000      0.000000
REMARK 350  BIOMT3  1  0.000000  0.000000  1.000000      0.000000
REMARK 350  BIOMT1  2 -0.500000 -0.866025  0.000000     43.320000
REMARK 350  BIOMT2  2  0.866025 -0.500000  0.000000     75.032444
REMARK 350  BIOMT3  2  0.000000  0.000000  1.000000      0.000000
REMARK 350  BIOMT1  3 -0.500000  0.866025  0.000000    -43.320000
REMARK 350  BIOMT2  3 -0.866025 -0.500000  0.000000     75.032444
REMARK 350  BIOMT3  3  0.000000  0.000000  1.000000      0.000000
```

If the file is downloaded as the newly used CIF format (**.cif**) the matrices in the header will follow some `loop_` definitions such as `_pdbx_struct_assembly_prop.biol_id` and `_pdbx_struct_oper_list.symmetry_operation` amongst many others. The matrices will not appear as neatly organized to the human eyes (!) without the presentation in columns:

```
[...]
_pdbx_struct_oper_list.matrix[3][3]
_pdbx_struct_oper_list.vector[3]
1 'identity operation'      1_555 x,y,z      1.0000000000  0.0000000000  0.0000000000  0.0000000000
1.0000000000  0.0000000000  0.0000000000  0.0000000000  0.0000000000  1.0000000000  0.0000000000
2 'crystal symmetry operation' 2_665 -y+1,x-y+1,z -0.5000000000 -0.8660254038 0.0000000000 43.3200000000
-0.5000000000 0.0000000000 75.0324409839 0.0000000000 0.0000000000 1.0000000000 0.0000000000
3 'crystal symmetry operation' 3_565 -x+y,-x+1,z -0.5000000000 0.8660254038 0.0000000000 -43.3200000000
-0.5000000000 0.0000000000 75.0324409839 0.0000000000 0.0000000000 1.0000000000 0.0000000000
```

<sup>10</sup><https://pdb101.rcsb.org/learn/guide-to-understanding-pdb-data/biological-assemblies>

<b>sym #1</b>		
<b>1dud mmCIF Assemblies</b>		
<b>1</b>	<b>author_and_software_defined_assembly</b>	<b>3 copies of chain A</b>

Figure 19: “Symmetry information output”

In the next section we’ll briefly review how **ChimeraX** allows the display of either versions, asymmetric unit or biological assembly, for 2 common cases.

## 12.2 1DUD trimeric assembly

The first example will show how to create a the biological assembly, a trimer, from the single monomeric structure structure (*asymmetric unit*) contained within the coordinate files. As stated above the file will contain the necessary information to build the biological assembly.

This structure is an *Escherichia coli* dUTPase in complex with a substrate analogue (dUDP) (Larsson, Svensson, and Nyman 1996).

### TASK

**Close all models (e.g. with the *close* button on the Models Panel, or restart. Then open structure 1dud.**

- To open the structure type command: **open 1dud**. You will see a single ribbon structure.
- To inquire about possible symmetrical constructions, type command **sym #1** (assuming model #1 contains that structure.)

Since there is only one solution the following table will appear with one entry:

The solution is a trimer of chain A as specified in the last column.

- Create biological assembly with command: **sym #1 assembly 1**. This request that symmetry be applied to model 1 (#1) to create the assembly versio 1 (which in this case is the only one described within the file.)

*Note:* that the Models Panel now contains 2 entries:

- 1dud with ID of 1 - which is now hidden (**Show** button is off)
- 1dudasembly1 with ID of 2, which is shown.

*Note:* it is possible to request that the biological entity be part of the same model by adding **newmodel false**. The above command could be re-written as: **sym #1 assembly 1 newmodel f**

## 12.3 2BIW monomer

2BIW contains the *Crystal structure of apocarotenoid cleavage oxygenase from Synechocystis, native enzyme* (Kloer et al. 2005).

The *asymmetric unit* consists of **4 monomers** of the enzyme while the biological assembly consists of only one monomer. Therefore the coordinates file contains four times the amount of information relevant to the biologist.

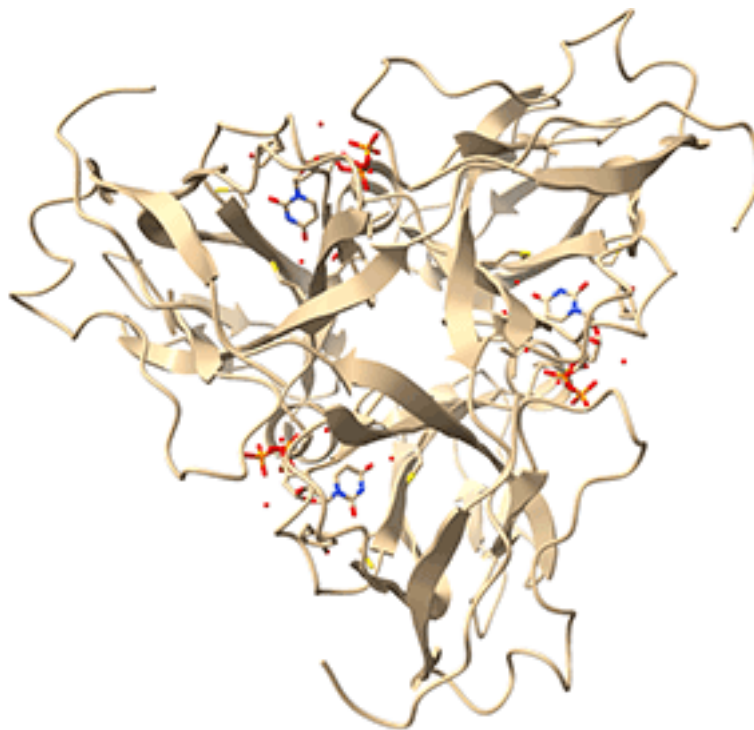


Figure 20: “*Trimeric assembly of 1dud.*”

Currently **ChimeraX** will download the complete coordinates file, and the user will call the biological assembly as we have done above.

For this structure

#### TASK

Close all models (*e.g.* with the *close* button on the Models Panel, or restart. Then open structure 2biw.

- **open 2biw**
  - optionally click on the top bar button to “color atoms by chain” (11th button from the left on the molecular display toolbar.)
- Call symmetry options with **sym #1** (change 1 to the model number if different.) As we established above there are 4 monomers, each of them is a biological assembly.

We’ll display only the second one, and hide the others, and keep everything within the same model:

- **sym #1 assembly 2 newmodel f**

However, it may be easier (as in the previous example) to let **ChimeraX** create a new model, as just clicking on the “show ribbon button” (3rd button from the left on the molecular display toolbar) will show all monomers again!

## REFERENCES

Goddard, T. D., C. C. Huang, E. C. Meng, E. F. Pettersen, G. S. Couch, J. H. Morris, and T. E. Ferrin. 2018. “UCSF ChimeraX: Meeting modern challenges in visualization and analysis.” *Protein Sci.* 27 (1):

**sym #1**

<b>2biw mmCIF Assemblies</b>		
<a href="#">1</a>	author_and_software_defined_assembly	1 copy of chain A
<a href="#">2</a>	author_and_software_defined_assembly	1 copy of chain B
<a href="#">3</a>	author_and_software_defined_assembly	1 copy of chain C
<a href="#">4</a>	author_and_software_defined_assembly	1 copy of chain D

Figure 21: “*Symmetry information output*”

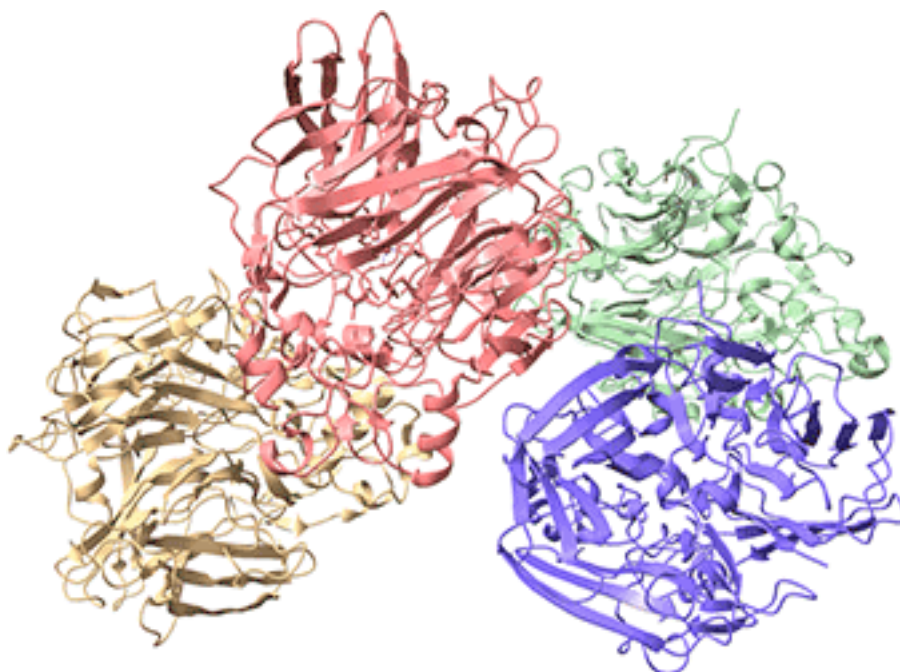


Figure 22: “*Four monomers of 2biw make the asymmetric unit.*”

14–25. <https://doi.org/10.1002/pro.3235>.

Kloer, D. P., S. Ruch, S. Al-Babili, P. Beyer, and G. E. Schulz. 2005. “The structure of a retinal-forming carotenoid oxygenase.” *Science* 308 (5719): 267–69. <https://doi.org/10.1126/science.1108965>.

Larsson, G., L. A. Svensson, and P. O. Nyman. 1996. “Crystal structure of the Escherichia coli dUTPase in complex with a substrate analogue (dUDP).” *Nat. Struct. Biol.* 3 (6): 532–38. <https://doi.org/10.1038/nsb0696-532>.

Pettersen, E. F., T. D. Goddard, C. C. Huang, G. S. Couch, D. M. Greenblatt, E. C. Meng, and T. E. Ferrin. 2004. “UCSF Chimera—a visualization system for exploratory research and analysis.” *J Comput Chem* 25 (13): 1605–12. <https://doi.org/10.1002/jcc.20084>.

Phillips, S. E. 1980. “Structure and refinement of oxymyoglobin at 1.6 Å resolution.” *J. Mol. Biol.* 142 (4): 531–54.