

Getting Started With Your Chime Tutorial

Things Needed (included in Chime_Tutorial.zip)

This manual

Your favorite PDB file (this package contains de-oxy hemoglobin as an example).

Template files (templateframe.html, templatebuttons.html, and templateleft.html)

Make sure the Chime plug-in has been installed on your computer. It can be downloaded at <http://www.mdlchime.com/chime/>.

How to Download a PDB File:

Go to <http://www.pdb.org>

Use the search tool to search for the protein you want.

If you get hits, the page will show a list that looks like this:

<input type="checkbox"/> 1HC1	Deposited: 15-May-1991 Exp. Method: X-ray Diffraction Resolution: 3.20 Å	{ EXPLORE }
Title	Crystal structure of hexameric haemocyanin from Panulirus interruptus refined at 3.2 Å resolution.	
Classification	Oxygen Transport	
Compound	Arthropodan Hemocyanin (Deoxygenated) Subunit 1 Refined Using Non-Crystallographic Symmetry Restraints	
<input type="checkbox"/> 1HC2	Deposited: 15-May-1991 Exp. Method: X-ray Diffraction Resolution: 3.20 Å	{ EXPLORE }
Title	Crystal structure of hexameric haemocyanin from Panulirus interruptus refined at 3.2 Å resolution.	
Classification	Oxygen Transport	
Compound	Arthropodan Hemocyanin (Deoxygenated) Subunit 2 Refined Using Non-Crystallographic Symmetry Restraints	

If the protein you want is in this list, click on the red **Explore** on the right. This will take you to the page for that protein. This page gives you the name of the document that accompanies this PDB file, if available, as well as a brief description of the molecule and what is depicted in the PDB file. On the left you will see a menu, with the items, “summary information, view structure, download display file, etc.” If you choose “View Structure” you will be taken to a page which accesses a number of Chime plug-ins. You can use these to preview your protein before you download. To download the protein’s PDB file, go to “Download Display File.” Scroll down until you see this menu:

Download the Structure File:

Choose from the following file and [compression formats](#):

	file format	
compression	PDB	mmCIF
none	X	X
Unix compressed	X	X
GNU zipped ("gzipped")	X	X
ZIPped	X	X

Mouse over the X under Column “PDB” and Row “none.” Right click and “save target as” to the folder of your choice. You have now downloaded your PDB file and can use it for your Chime tutorial.

Let’s Begin:

Make sure all 4 files (PDB + 3 template web pages) are all in one folder. If you want to explore, the 3 web pages are already somewhat configured to show a simple tutorial for

deoxyhemoglobin. Exploring these web pages using “View Source” may be useful in helping you to become comfortable with way they are organized. In order to make your own tutorial, you must add your own PDB file to this folder. These can be downloaded at <http://www.pdb.org>.

It is important to remember that this process does not employ any sort of web editor such as Frontpage or Dreamweaver. We will be working with the html itself. If you are new to html, don't be intimidated. Minimal knowledge of html is necessary.

Now we can get started. Open [templateframe.html](#). You will see a two-frame web page, with the PDB file in the left frame, and the area for text and buttons in the right frame. Go to the “View” pull-down menu. Select “Source.” This will open notepad. Here you will see, among a lot of other html, the following text:

```
<frameset cols="70%, 30%"><!-- "*" , "*" means 2 equal-sized columns -->
  <frame src="templateleft.html" name="chimeleft">
  <frame src="templatebuttons.html" name="chimeright">
</frameset>
```

Basically, this is showing us that contents of the frames are derived from other html files. This [templateframe.html](#) page does not really contain any content, other than these directions and a title.

You will also notice the following:

```
<!-- A simple 2-frame page -->
```

The `<!-- *** -->` notation allows you to type within the arrows without that information being displayed on the website. This is useful for making notes to oneself. You will notice hints and directions have been inserted throughout the source codes of the three websites using this notation.

You can now close this notepad file.

Editing the Left Frame:

Right click on the left frame, and select “View Source.” The first modification you will learn how to make is changing the page's title. At the top, find the line

```
<title>*3D Structure of *A PROTEIN*</title>
```

Replace `*A PROTEIN*` with the name of your protein.

Next, you will insert your own PDB file.

Here you will see the following text:

```
<embed src="1a3n.pdb" align=center bgcolor="#000000"
width="450" height="450"
name="myfavorite"></embed></div>
```

“1a3n.pdb” is the file for deoxy-hemoglobin. Within the quotes, replace 1a3n.pdb with the name of *your* PDB file. Also, notice the line ‘name=”myfavorite”’ It is a good idea to change this to something that relates to the protein whose PDB file you are displaying, for instance, “hemoglobin”. Remember what you put down here because you will need it again for the right frame.

Now click “File” and select “Save As”. Save the file under a name related to your protein; keep it short if possible. You may also want to add the suffix “left” to the name, for example: “hemoglobinleft.html”. This helps with organization but is not required. This window can now be closed.

Editing the Frame Set/Editing the Right Frame/Adding a script

Bring back the templateframe.html page. Move the mouse over the right frame, and right click. Select “View Source.” Once again, another Notepad window will open, so that you can edit the html.

First, go to “File” and choose “Save As.” Once again, give name this file *.html. Following the same logic as above, you may want to make it *buttons.html.

Bring the templateframe.html back up. Select the “View” pull-down menu from the top menu. Select “source.” Once again, choose “Save As” and name this file in a similar fashion as before. Now we are going to direct the frameset to the two web pages that will be seen inside the right and left frames.

Remember this from earlier:

```
<frameset cols="70%, 30%"><!-- "*" , "*" means 2 equal-sized columns -->
  <frame src="templateleft.html" name="chimeleft">
  <frame src="templatebuttons.html" name="chimeright">
</frameset>
```

Using the names you designated for your left and right frames, replace “templateleft.html” and “templatebuttons.html”, respectively.

Click “File.” And “Save.” You can close this notepad. You can also close templateframe.html. Open the website that designates your frameset.

Mouse over the right frame. Right click, and select “View Source.”

The default title reads

```
<title>MY FAVORITE PROTEIN</title>
```

You can change this to the title of your choice. Slightly lower you will see:

```
<h2>3D Structure of **A PROTEIN**</h2>
```

You can change this too. Scroll down a bit, and you will see some notations made using the <!-- * --> format.

After some text, you should also see the following command:

```
<embed type="application/x-spt" width=13 height=13 button=push target="myfavorite"
```

script="

Go ahead and replace “myfavorite” with the name that I told you to remember from earlier. Remember to leave the quotes. This command directs the button to the chime-plugin window located in the left frame.

One line down you will see “reset”, “slab off”, etc. This is the beginning of the script that I wrote for hemoglobin as a demo. Starting with “reset”, select this text and scroll down so that you have highlighted all the text between “reset” and “select all”. Delete this text. You will now see:

Let's display the molecule as four distinct peptide chains. Click <embed type="application/x-spt" width=13 height=13 button=push target="myfavorite ←(you will have changed this by now, hopefully)" script="

"> here.

You can replace my text (“Let’s...Click.”)with your own, remembering that what will appear in the text instead of <embed.....”> is a little grey button. You will probably want to type something that explains the way your molecule is depicted in the Chime window, sort of like a caption.

Now go back to your frameset and manipulate your Chime protein to the desired depiction. Once you have achieved this, right click on the Chime window. Scroll down to “Edit” and select “Copy Chime Script.”

Now go back to the html code for your right frame. Place the cursor between the quotation marks, right click and paste the script into this area. The script is now located within the “embed” command. You are not done yet, though. Scroll back up to the beginning of your script. Remember, that scripts are sometimes very long, so be sure you scroll to beginning of the correct one.

At the beginning of the script, you will see this:

```
#!/rasmol -script
# File: \s3ds.
# Creator: Chime Version 2.0
```

```
set load check on
load pdb "1msw.pdb"
background [0,0,0]
set ambient 60
set specular off
```

Delete all of this. You must do this every time you create a new button and copy a script, or else the button will not appear and every bit of the script's text will appear on your web page. Now you are ready to test and see if your script worked. Click on file and save your work.

Bring back your frameset and refresh the page. Hopefully your page appears with some text and a button. Click on the button to see if the script executes correctly.

Adding More Text and Buttons

Remember you can add a blank line between blocks of text using

```
<br>
```

```
<br>
```

You can begin a new paragraph using

```
<br>
```

When you want to add another button, simply type in the desired text, and copy and paste

```
<embed type="application/x-spt" width=13 height=13 button=push target="myfavorite" script="
```

from somewhere else in the html. The skip several lines and add this:

```
“>
```

followed by any text that you want to occur after the grey button. Then go back to your PDB image, manipulate it to the desired depiction, and copy the Chime script using the procedure above. Paste the chime script between the quotation marks and remember to delete the top lines that look like this:

```
#!/rasmol -script  
# File: \s3ds.  
# Creator: Chime Version 2.0
```

```
set load check on  
load pdb "1msw.pdb"  
background [0,0,0]  
set ambient 60  
set specular off
```

Using the procedure described above, you can make a page using any number of combinations of text and buttons.

In addition to the parameters available within the Chime plugin, there are programs available which can assist you in manipulating the PDB file in more advanced ways. One such program is called RASMOL and is available for download at this website:

<http://www.umass.edu/microbio/rasmol/getras.htm>

Tips for Advanced Display

Changing the size of the Chime window plug-in:

In the event that the chime window of this template is too big or too small, you can change the size of the window by changing the following values:

```
<embed src="1a3n.pdb" align=center bgcolor="#000000"  
width="450" height="450"  
name="myfavorite"></embed></div>
```

Notice that the values given for height and width are both 450. These values can be changed according to your application.

Potential problems with complicated molecule depictions (and suggestions on how to fix them):

Oftentimes, after copying a script into your html and inserting a button into the right frame, you will notice that a) the script is very long and b) it takes longer after clicking the button for the chime window to depict the molecule in the proper orientation.

Here is an example:

Imagine that you have a Chime file of a protein consisting of two distinct chains, A and B. Let's say you select chain A and display it with the "spacefilling" option. Likewise, you select chain B and display it as "wireframe." If you copy the chime script into notepad after the

```
<embed type="application/x-spt" width=13 height=13 button=push target="myfavorite"  
script="
```

and before the

```
">
```

you will notice that this script is very large (sometimes several thousand lines long!). This lengthy script makes it not only cumbersome to navigate around your html code but also results in the plug-in taking a long time to load your chosen orientation. You can imagine with larger proteins that this can become quite a nuisance. This situation can be remedied, although it is often on a case-by-case basis.

Here is an example (you may want to try this for practice):

Let's say you want to depict your protein as mostly wireframe, but you wish to depict all of the alanine residues as spacefilling. Using the menus and options available to you by right-clicking the Chime window, you succeed in capturing this display. Now you want to create a button in your right frame that will orient the molecule in this manner, so you copy and paste this command:

```
<embed type="application/x-spt" width=13 height=13 button=push target="myfavorite"  
script="
```

followed by ">\

Now you right click on the Chime window and "Copy Chime Script." You now paste your script between the quotation marks, but the script is really long! How can you clean this up?

Look for this text or something similar:

```
# Atoms
```

```
colour atoms cpk
select all
spacefill off
select (atomno>=29) and (atomno<=33)
spacefill on
select (atomno>=82) and (atomno<=91)
spacefill on
select (atomno>=130) and (atomno<=134)
```

you will notice that the “select (atomno>130 etc...” command goes on for quite some time. Beginning with “select all” you can delete everything from there until the next # sign, which usually says “#bonds”
Once you have deleted this, you can simply replace it with

```
select ala
spacefill on
```

and have the same effect as the previous string of commands. Now, suppose you want to color the alanine residues green. Simply type

```
color green
```

directly after “spacefill on”. Hopefully with practice, your ability to manipulate chime scripts will become more intuitive. One way to do this is to download RASMOL and familiarize yourself with the various Chime commands.

For now, here is a brief list of Chime Commands that you can use:

Command	Possible values
Select (use this command to specify the target of other commands).	all, DNA, amino, nucleic, ala, cys, aromatic, hetero, etc.
Color	green, red, blue, magenta, etc.
spacefill	on, off, a value such as 100 or 500 (500 having a larger radius)
wireframe	on, off, 100, 399
reset	n/a
hbond	on, off

Remember to save your work.

Have fun and good luck!

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