


## Tutorial One: Create Project, Load Structure, Prepare, Viewer, Compare Structures



**Estimated time: 30 minutes**



This tutorial will instruct users on how to begin working with a structure in Cyrus Bench including the different ways structures can be displayed, and how structures can be compared to each other. The Prepare tool, Structure Viewer, display modes, inverse selector, Compare tool, Scores, and the Superpose function will be introduced.

### 1) Open or create a project



From <https://cad.cyrusbio.com>, click on **Projects**  if you are running this tutorial in a new project. Then enter a name and click **Create project**. Or click on an existing project.

### 2) Load structures

If the [Structure Loader](#) is not already open in the center window, click **Structure Loader** . A tab in the center window should appear that is titled **Structure Loader** .

Under **Inputs**, enter this PDB ID   and click . The structure will appear in the list in the middle, lower window:

#	Name	Source
1	1P68	RCSB 

The spinning  indicates that the structure is loading and will become a  when it is done. After structures have loaded, they will be listed in the left window like this:

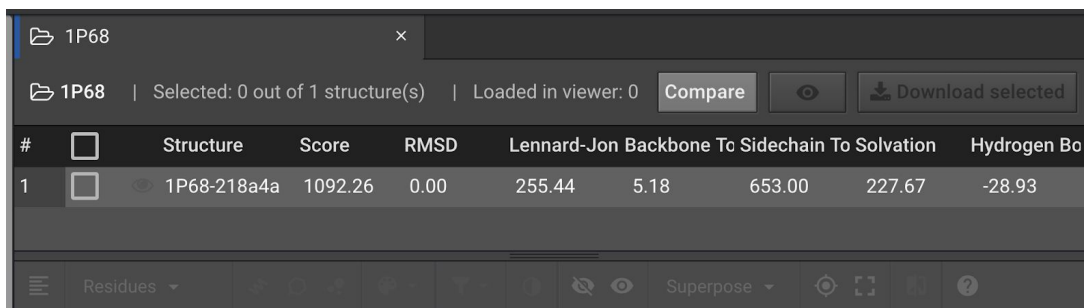


Repeat the process to load PDB ID 2JUA which will be used at the end of this tutorial 2JUA is a 77% homolog to 1P68 and will be used to show the structural similarities.

### 3) Prepare structures

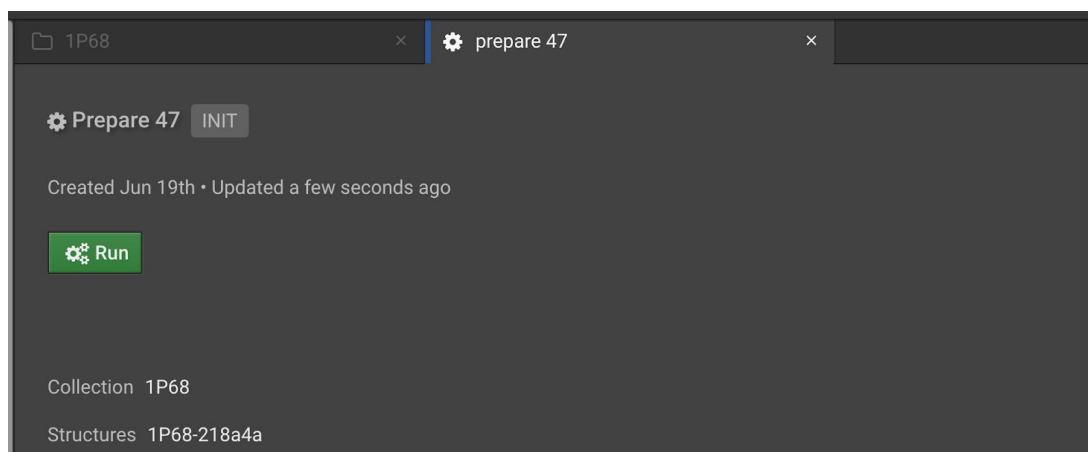
Many structures will require further processing before you can have confidence that it is optimal. One of the simplest way to improve a structure is to run Prepare. For more information on Prepare, click [here](#).

First, Prepare will be run on 1P68. Click on the 1P68 folder in the left window in order to bring it into the center tab...



#	Structure	Score	RMSD	Lennard-Jon	Backbone To Sidechain	To Solvation	Hydrogen Bo	
1	1P68-218a4a	1092.26	0.00	255.44	5.18	653.00	227.67	-28.93

Click the  to the left of the structure name in order to select it. Then in the right window, click **Prepare**. This will open a Prepare tab in the center window:

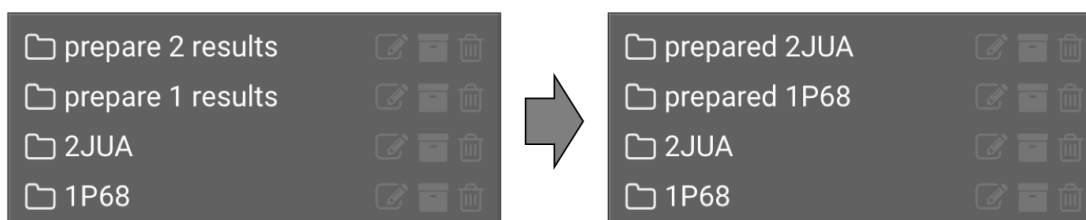


Click **Run**. Repeat this procedure for 2JUA.

The job will appear in the right window in the Task section:

Task	Updated			
prepare 2	2 minutes ago	✓		
prepare 1	2 minutes ago	✓		

The will appear once the job is finished. The finished jobs will appear in the left window. It may take a few minutes for this to run. Click the to the right of the prepare results files and rename them like below:



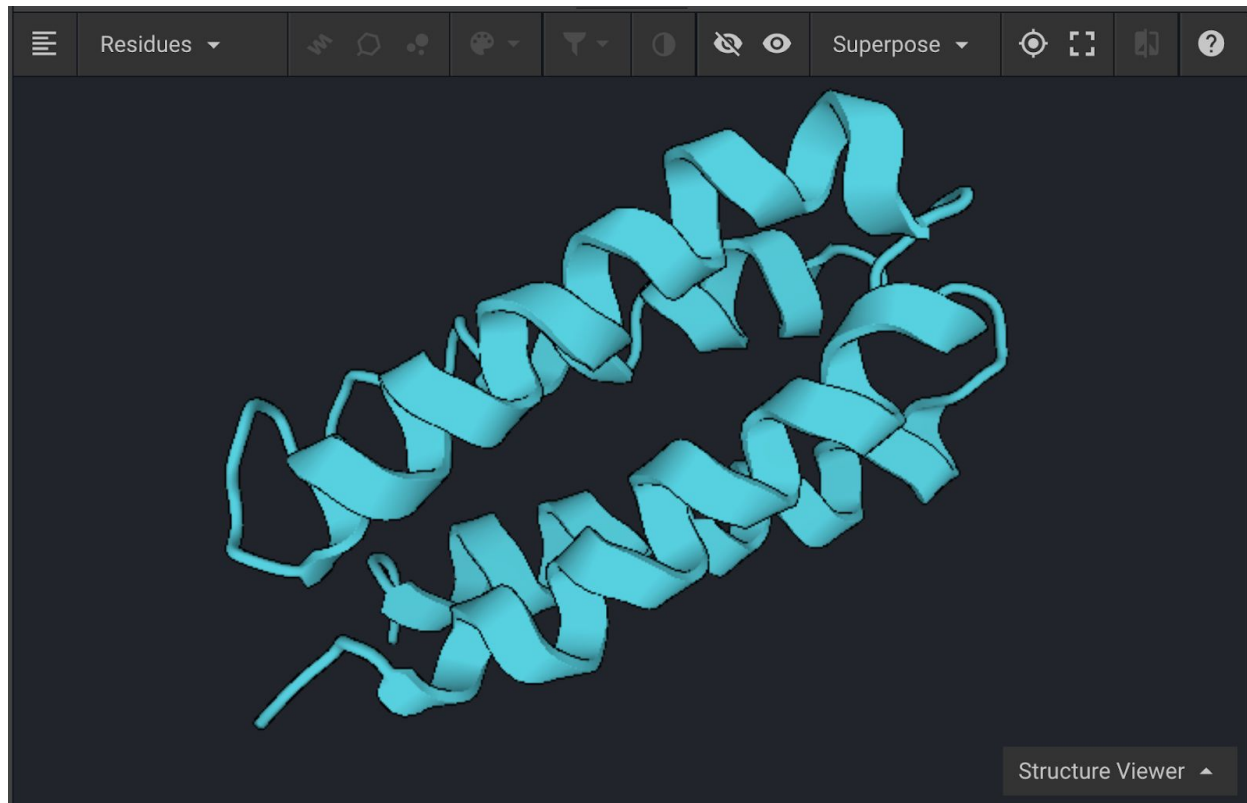
#### 4) View structures

In the left window, click in order to bring it into the center tab:


#	Structure	Score	RMSD	Lennard-Jo	Backbone T	Sidechain T	Solvation	Hydrogen B
1	structure 1	305.13	0.23	-229.86	9.98	365.34	215.48	-35.72

The screenshot shows a window titled 'prepared 1P68'. Below the title bar, there is a sub-header 'prepare 1 results' and a status bar 'Selected: 0 out of 1 structure(s)'. There are buttons for 'Compare', 'View' (eye icon), and 'Download selected'. The table above shows the data for the selected structure. At the bottom, there is a toolbar with 'Residues' dropdown, 'Superpose' dropdown, and other icons.




To the left of the word structure 1, click the in order to bring the structure into the [Structure Viewer](#) in the lower center window as shown on the next page:

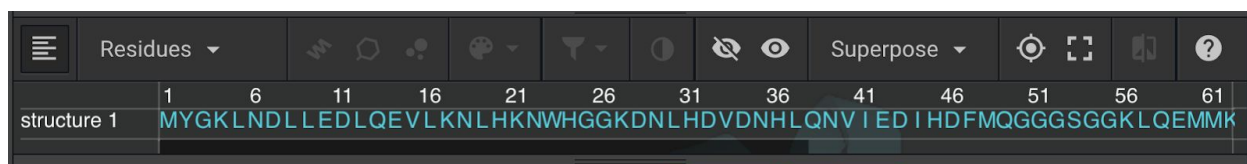


Above the structure is a bar with several buttons that will be described in detail in this tutorial.


You can increase the size of the Structure Viewer by dragging the  above that bar upwards as indicated below:

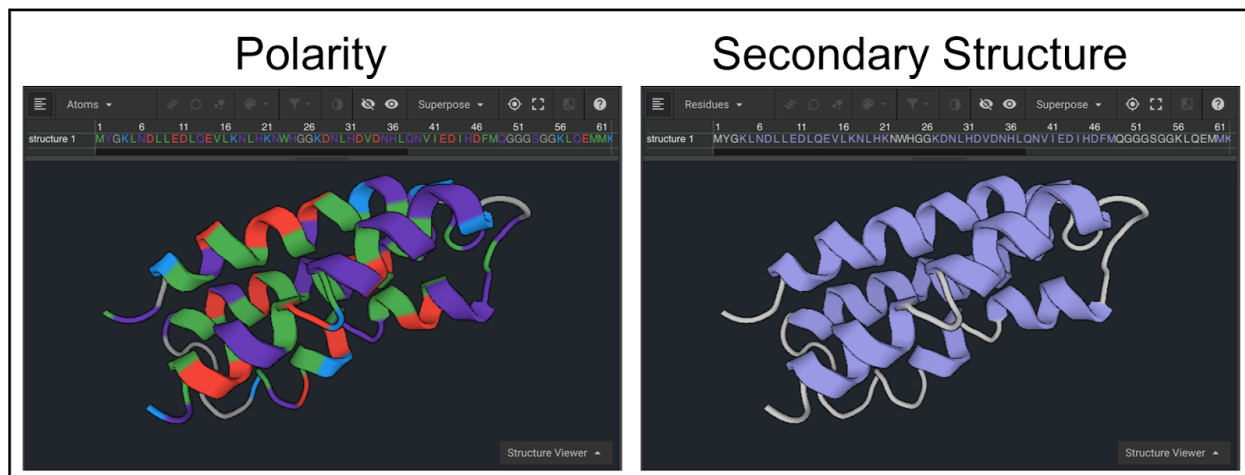




You can also enter Full Screen mode by clicking . Exit by hitting Esc. If the protein is not centered in the Viewer, click . Click and drag inside the Structure Viewer in order to change the protein's orientation. Click  in order to bring the sequence into view.

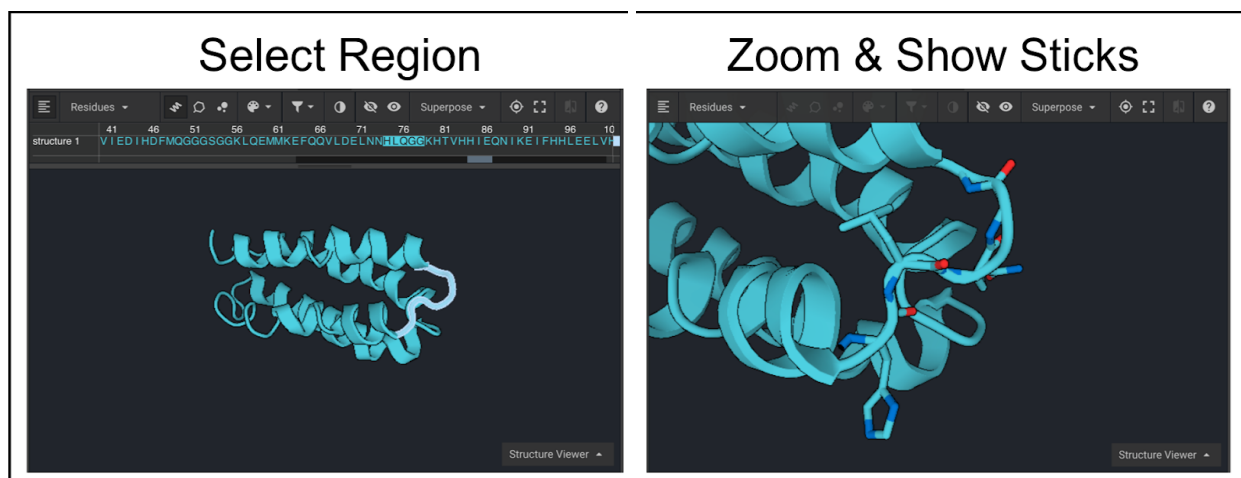




## Change Structure Display Mode and Color



Once the sequence is in view click the sequence name, **structure 1**, in order to highlight the entire protein. You can also do this by double-clicking anywhere on the structure in the Structure Viewer. Click  to bring a drop down window that allows you to color by CPK, Secondary Structure, Polarity, or choose a color. Select Polarity (below left) and Secondary Structure (below right), one at a time, to see each color setting. Click on empty space to deselect everything.

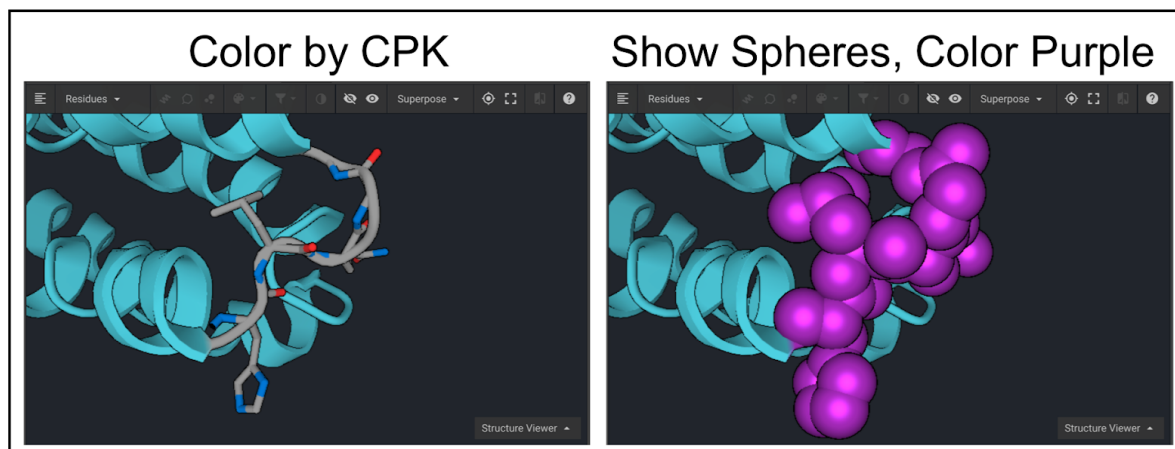


Next, scroll to the right half of the sequence and select residues 74-78 using the dark scroll bar under the sequence (shown below left) and click  in order to center the loop. To present residues 74-78 as sticks once they have been selected click  (shown below right).





The sequence can be hidden from view by clicking  as shown above. Select residues 74-78 from the structure again and click . To see atomic coloring select CPK from the drop down



menu (shown below left). To display the atoms as colored spheres click  and then click  to select a color (shown below right).






## Resetting Structure Viewer

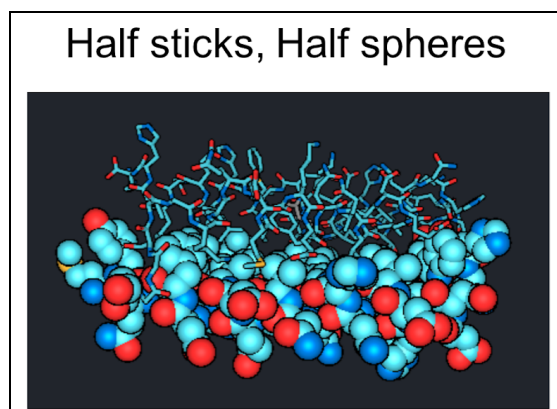
To reset the Structure Viewer close out the  tab to close the window. Select the structure again from the list in the left window and click  in order to bring the structure into the Structure Viewer in the lower center window.

## Using the Inverse Selector to Display Structure

Highlight residues 51-102 and click  in order to hide the cartoon mode for this region. Click  to present the residues as sticks instead.

Click , which will reverse your selection to the remaining residues 1-50. Click  in order to hide the cartoon mode for this region and click  to show spheres.


Half of the structure should now be displayed as sticks and the other half should be displayed as spheres as shown in the image to the right.

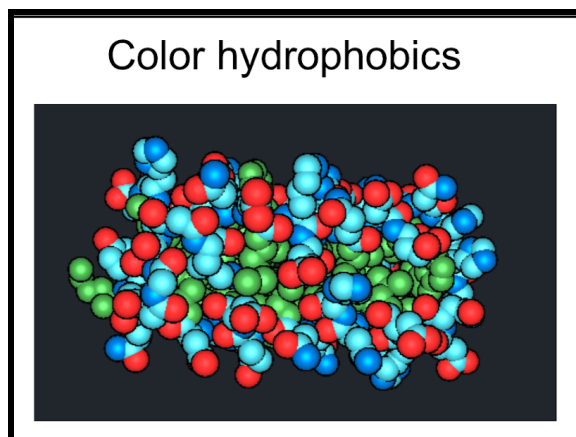


## Display Structure through Filter

Select the entire structure and click  in order to change everything to spheres. Click .

This opens a drop down window that allows you to display only side-chains, backbone, cysteines, hydrophobics, polar, or positively or negatively charged residues.


Select hydrophobic residues. Click  and select a color; hydrophobic residues are shown in green in the figure below.



## 5) Compare structures

You can either compare structures based on their Scores or by visually comparing the structures in the Viewer.

### Comparing Energy Scores between Two Structures

To use the [Compare](#) tool for the original PDB structure for 1P68 to the structure generated after running Prepare, select 1P68 on the left and click .



In the drop down window, select prepared 1P68.

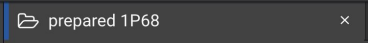
#	Structure	Score	RMSD	Lennard-Jone	Backbone	Tor	Sidecha
1	1P68-218a4a	1092.26	0.00	255.44	5.18	653.00	
prepared 1P68   Loaded in viewer: 1							
#	Structure	Score	RMSD	Lennard-Jone	Backbone	Tor	Sidecha
1	structure 1	305.13	0.23	-229.86	9.98	365.34	



The comparison above shows that after the Prepare function was run the Score for the energy of the 1P68 structure was lowered from a score of 1092.26 to 305.13 [Rosetta Energy Units](#)

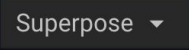

(REUs). The individual components for the REU Score are listed to the right. In this example the decrease in the Lennard-Jones and Side-Chain component scores were the major contributors to the lower REU score. This indicates that the atomic proximity and side-chain rotamers moved into more favorable positions.

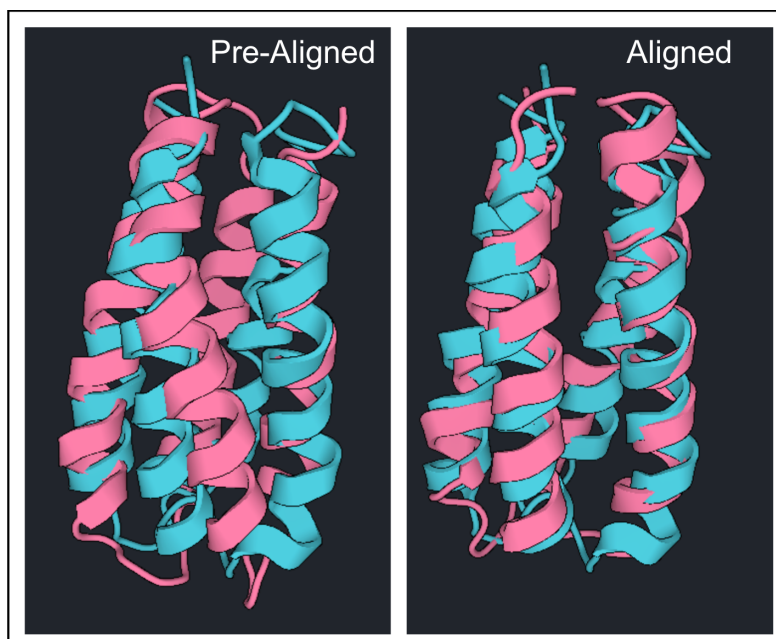
## Using the Structure Viewer to Compare Structures

To visually compare two structures using the Structure Viewer click the  to the left of the structure ID to ensure that both structures are visible. Click  to show the sequences and ensure that the structures are displayed in two different colors such as green and purple as shown above.



To compare structures originating from different PDBs they must first be aligned. Here the prepared structure of 1P68 will be compared to the prepared structure of 2JUA. Reset the Structure Viewer for prepared 1P68 by closing the  tab.

Select prepared 1P68 from the left window and click , then select prepared 2JUA. Be sure that both structures are visible by clicking the  and make sure they are not the same color.

In order to align them select both structures by double clicking one structure and then holding down the command (Mac) or Control (PC) and double clicking on the other structure. Click  to open a drop down, then click .





The differences between these two structures can be highlighted by clicking . Click  to show the differences as side chains as shown below:

