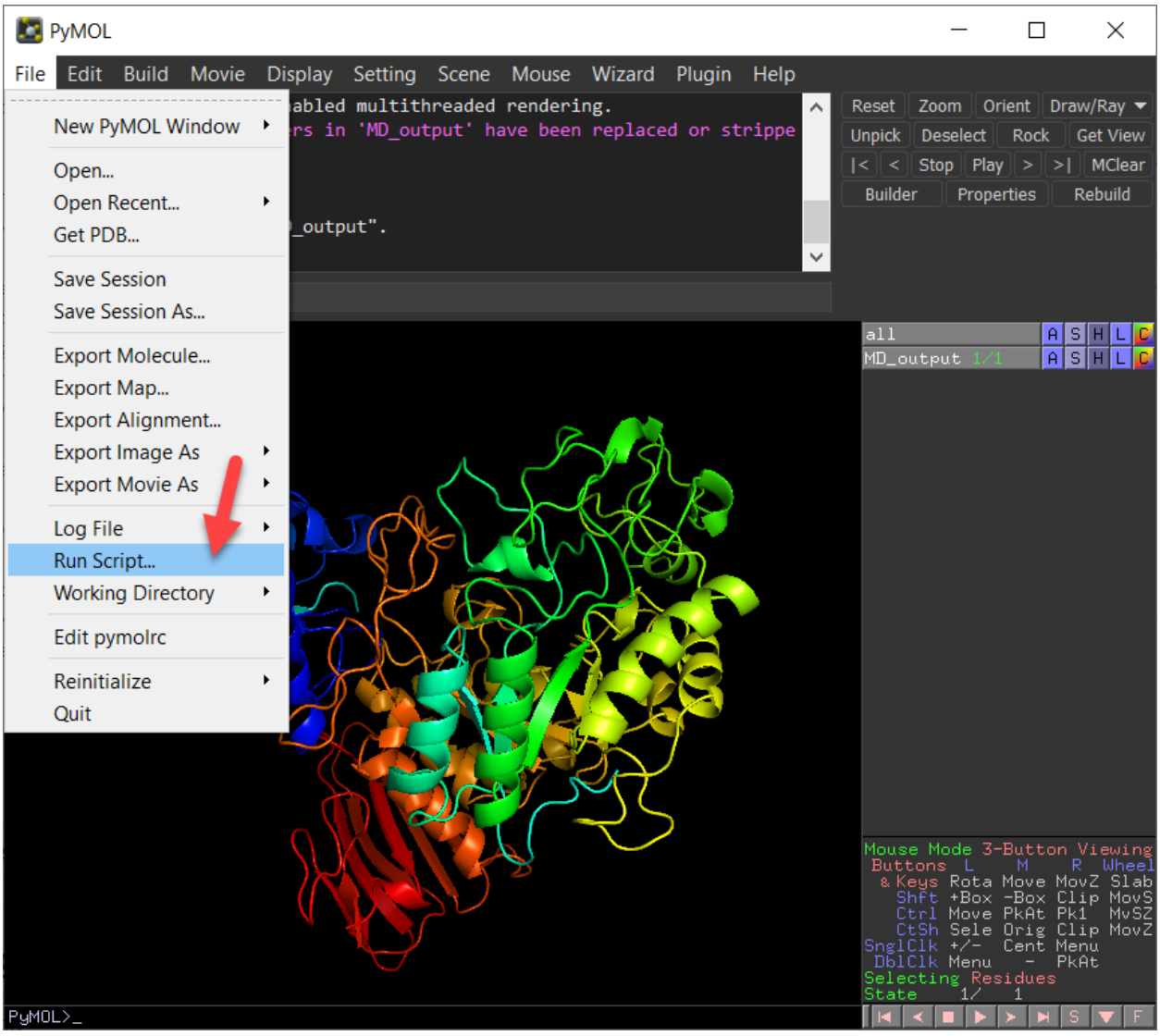
Showing interactions using PyMOL

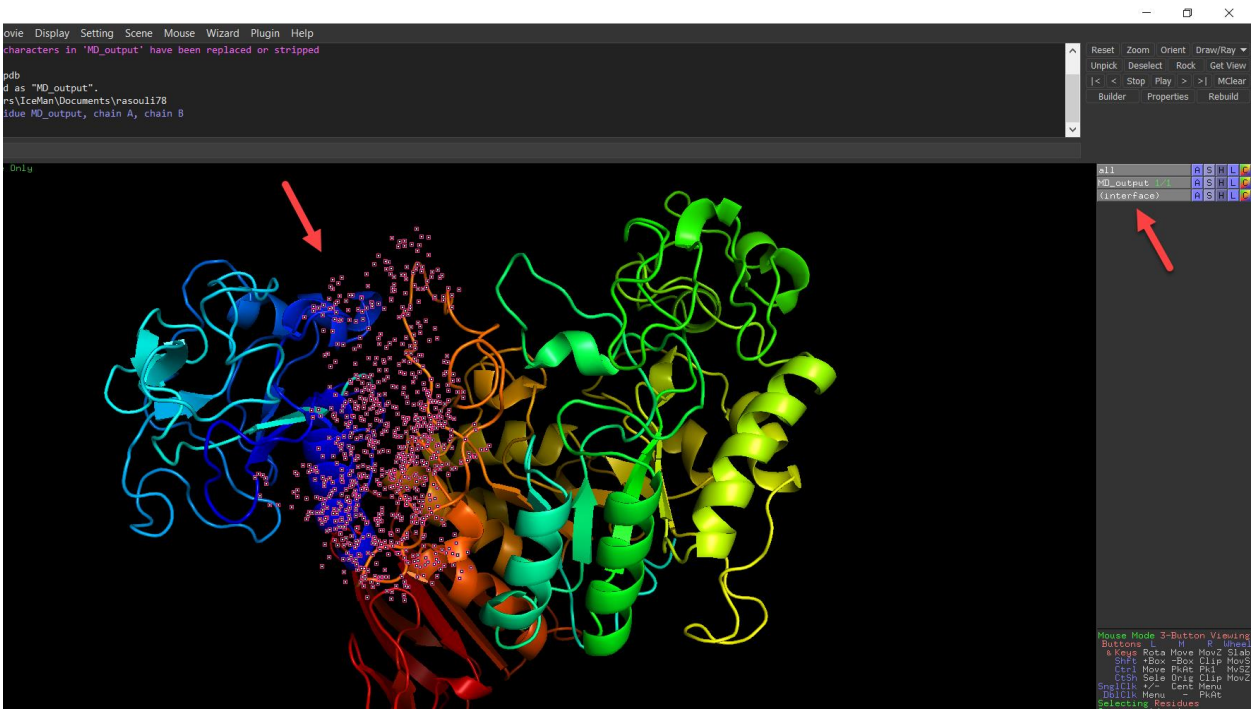
1. Install PyMOL (https://pymol.org/2/).
2. Run PyMOL.
3. Extract your protein complex from MD trajectories.
4. Open the complex in PyMOL. I inserted an output of protein-protein MD simulation in this folder. You can use it as an example to show its interactions.
5. Go to PyMOL file menu as shown below and then select [Run Script] option. Then orient the PyMOL to where your [InterfaceResidues.py] is and run this script.



6. Run the following command:

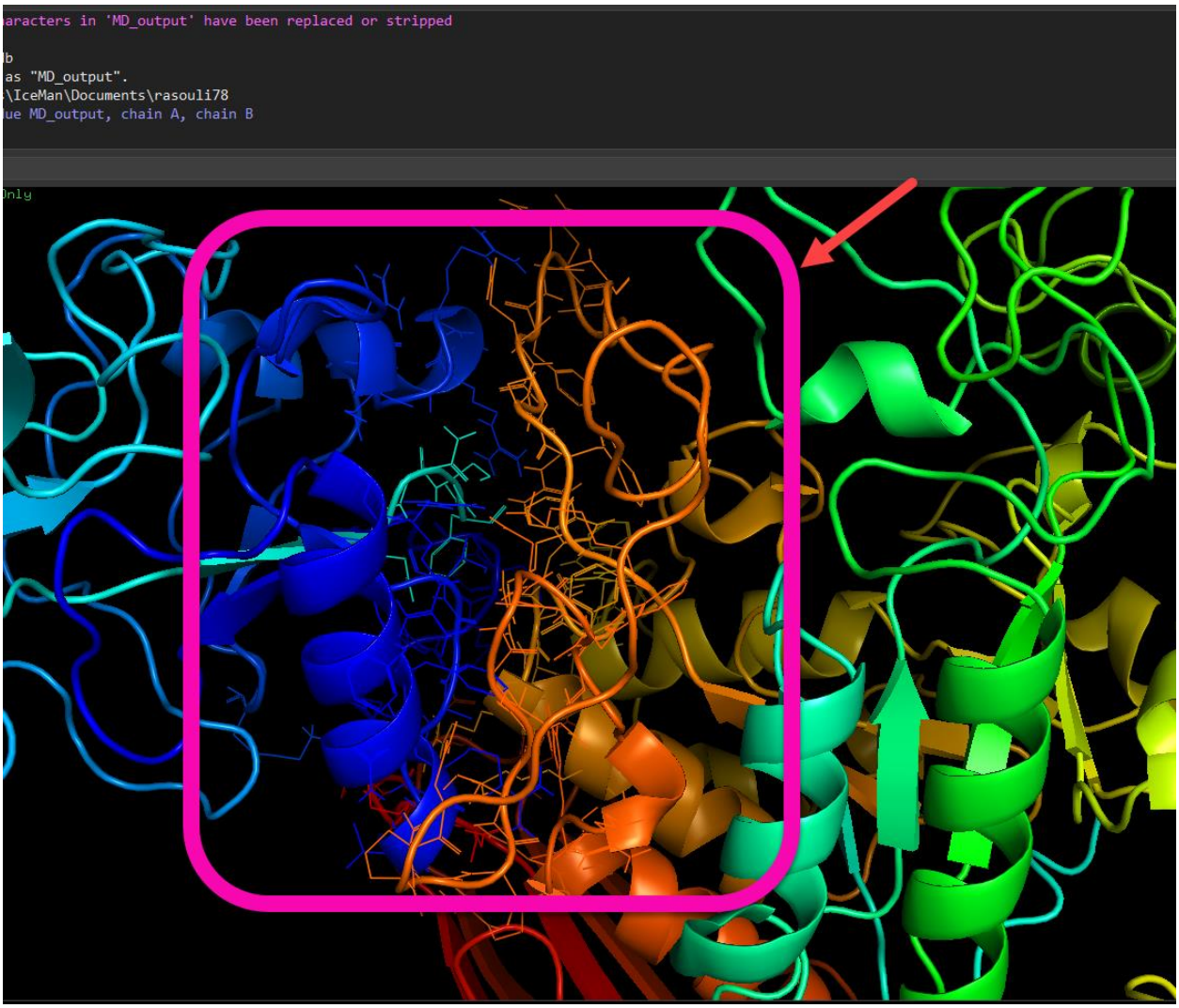
```
interfaceResidue MD_output, chain A, chain B
```

You can assign any name to your complex. Here my complex name is [MD_output]. So, you can define your own name. After running, you your PyMOL interface will change as below:

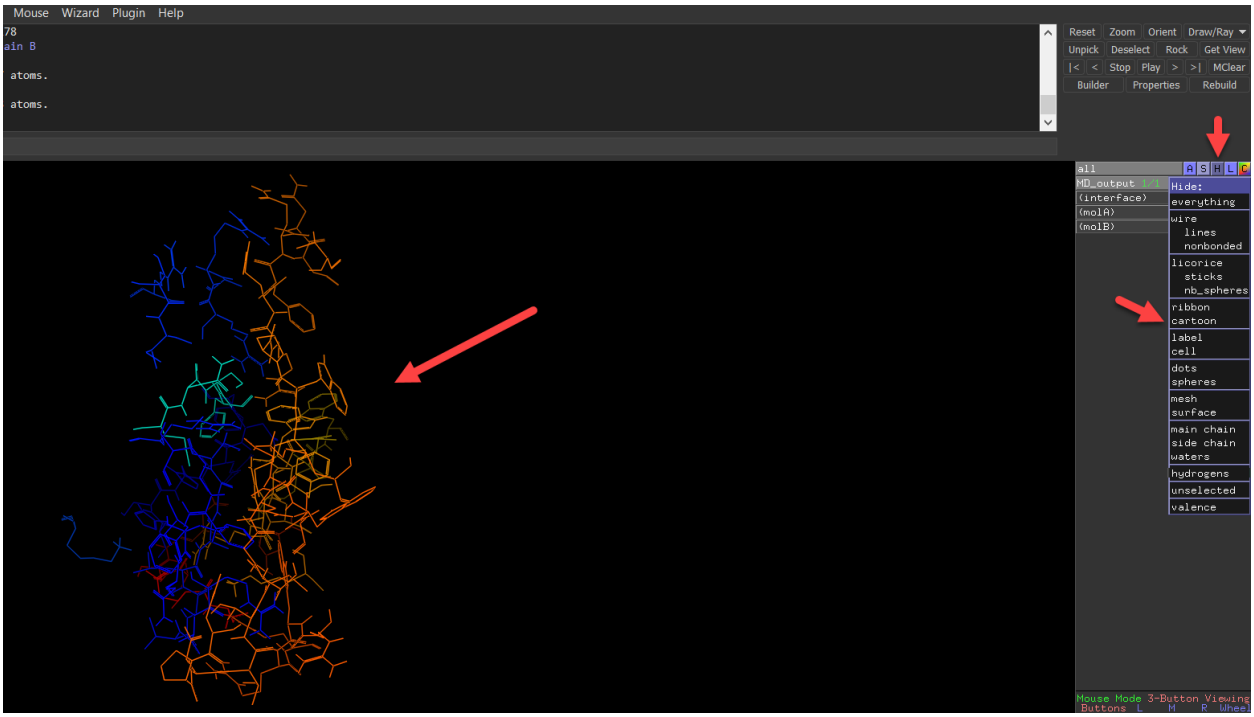


Now you should use PyMOL options to render your protein and display lines mode in the interface panel that highlighted by an arrow in the below figure.

Then, you will see the following changes in your PyMOL interface.

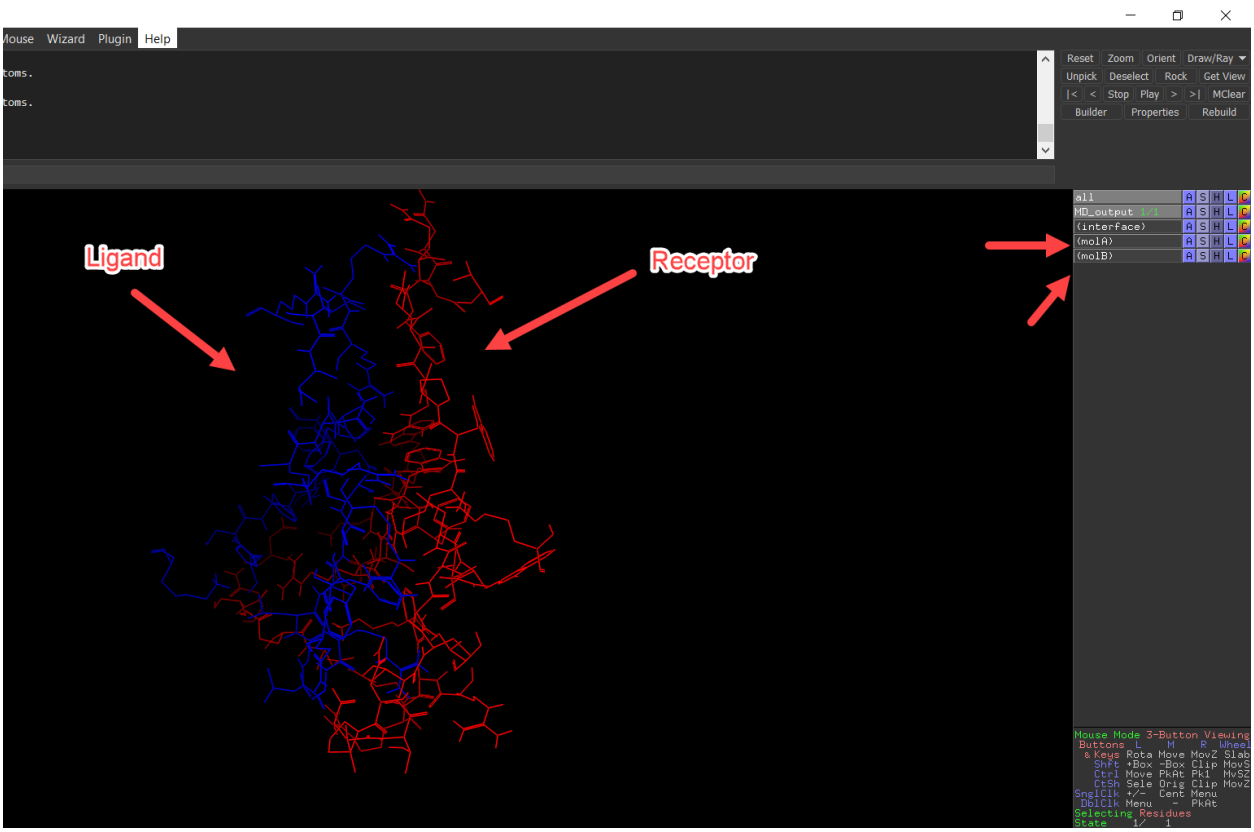


7. Hide the cartoon mode of whole complex using PyMOL action menu (H) option and select cartoon to hide the whole complex. You should see the below figure:

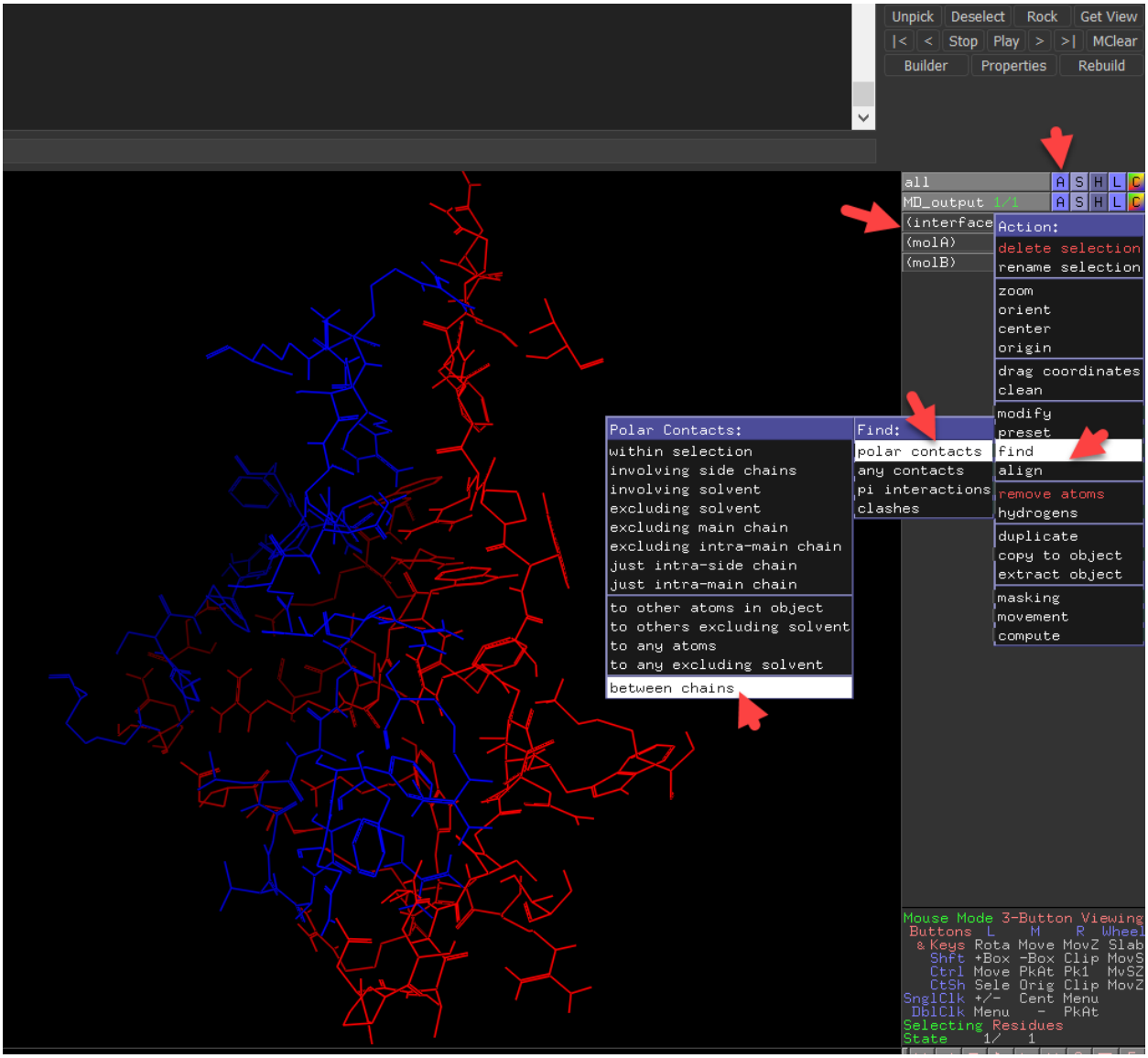


8. Using following commands and (C) option in PyMOL action interface you can change the color of both chains of your complex. I select red for chain A and Blue for chain B using PyMOL options. You can also change background color using [Display] menu in PyMOL.

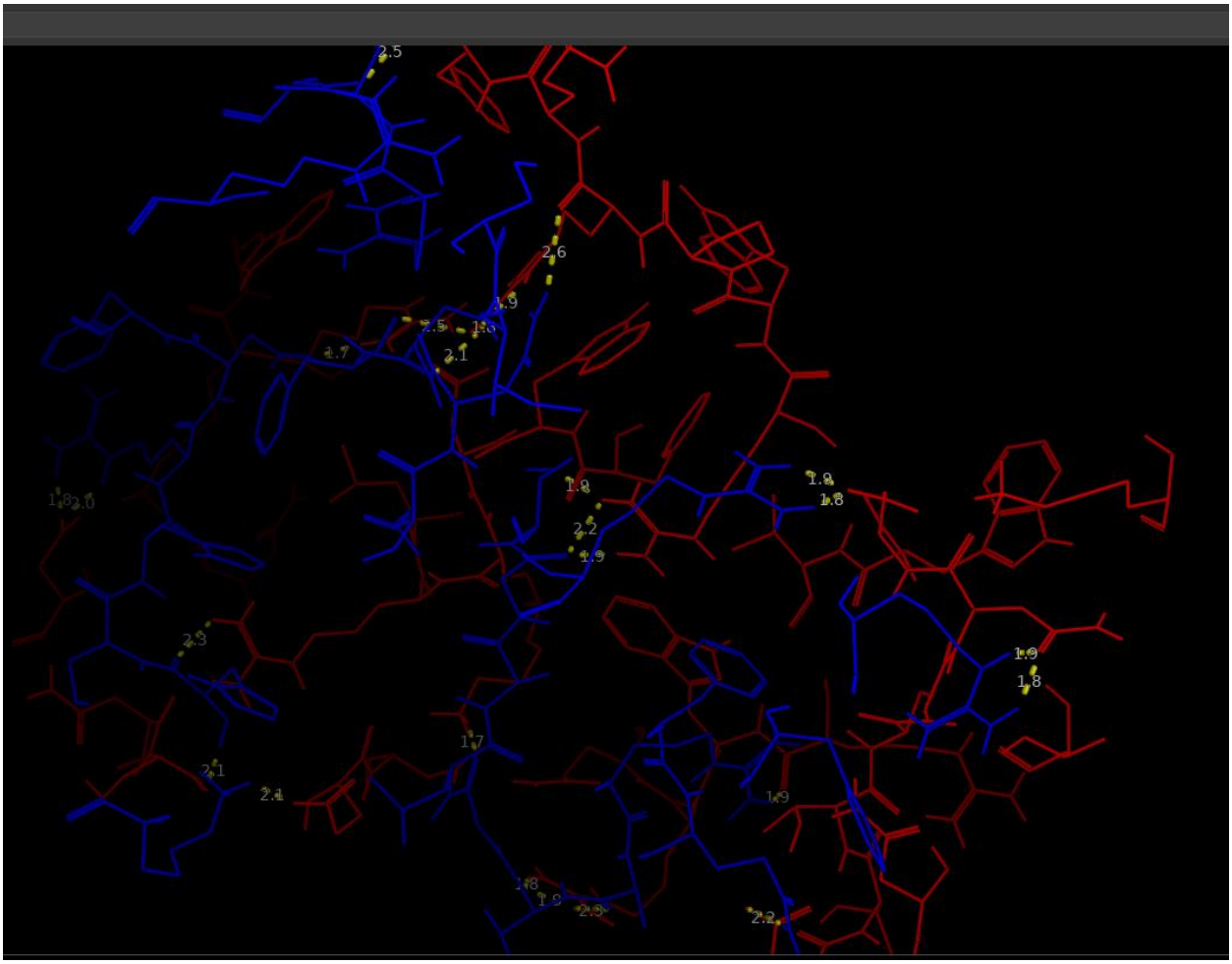
```
select molA, chain A
select molB, chain B
```



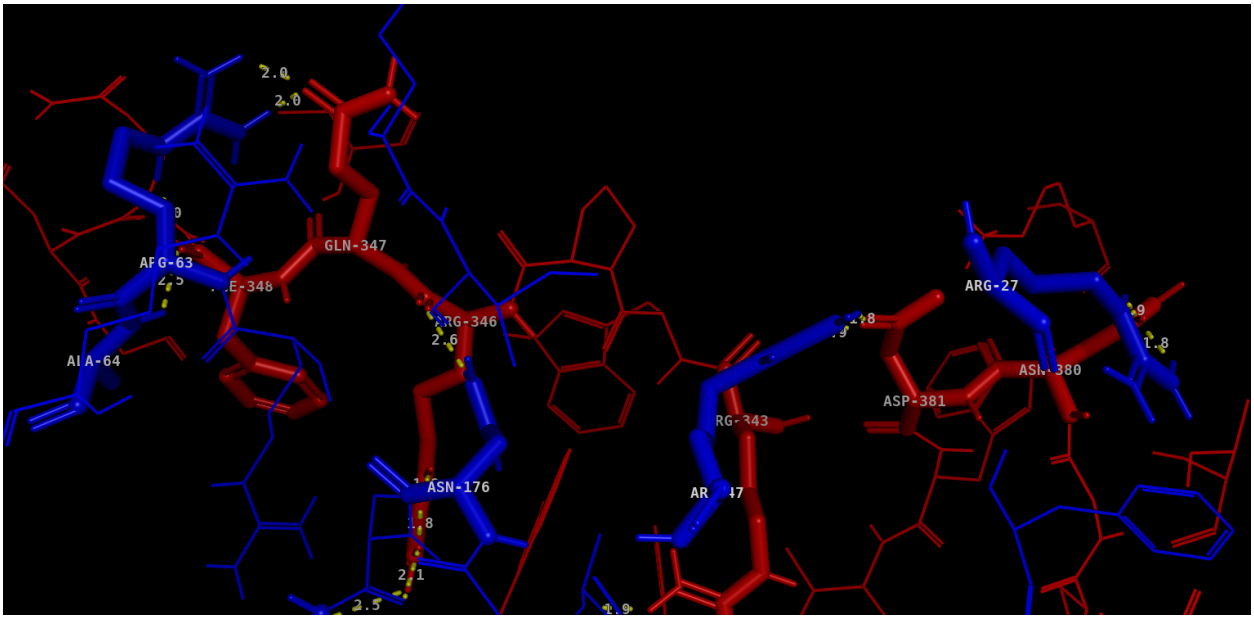
9. In the [interface panel] select action menu (A), then [Find], then [polar contact], and next [between chains] as shown in the following figure.



Then you will see the following figure. As shown, the H-bonds between chains will appear in yellow color. These interactions are key residues in both chains that interacted to each other. You can change the representation mode of these interactions from lines to sticks or shperes to see the target residues in detail.



10. You can hide [line] mode of other residues that are not involved in H-bonds. As shown, you can see the list of important residues participated in receptor-ligand interactions. You can use PyMOL coloring function to select the best illustration mode of observed interactions. You should compare the results of MD interactions and Docking outputs before MD to see the occured changes among interactions that receptor/ligand complexes can build before/after MD.



You can show the interactions between ligand and receptor by displaying protein surface for your complexes after/before MD and interpret the surface of interactions.