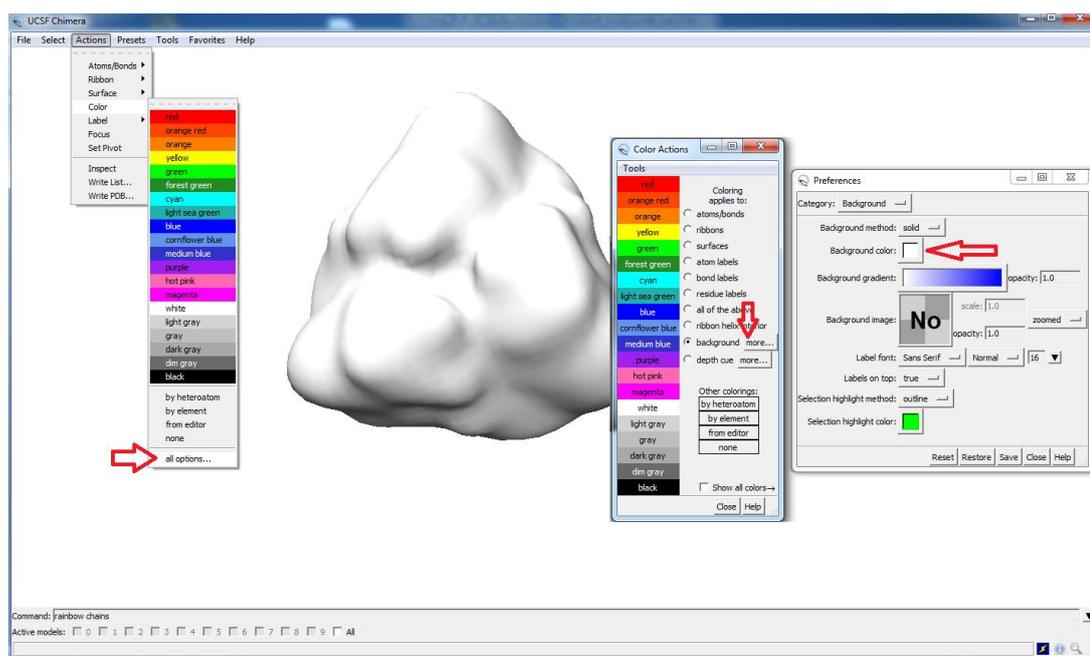


## STEP 12 RECORDING A MOVIE FROM SIMULATION

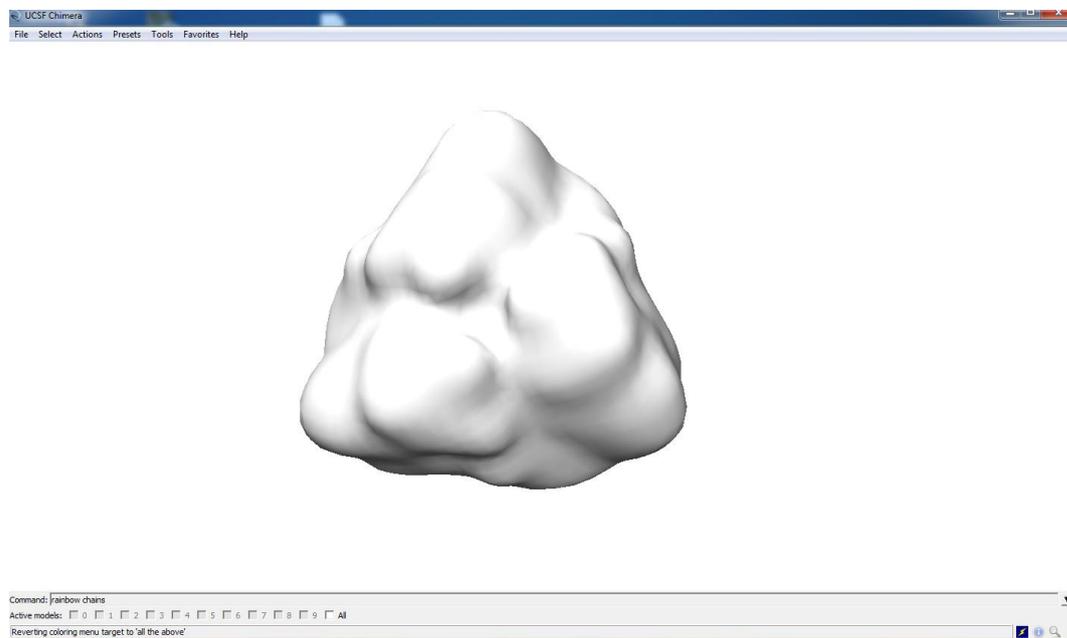
The PyRy3D UCSF Chimera Extension allows to record a movie presenting structures generated by the program in consecutive steps of simulation. Thus far you can observe how PyRy3D was testing a conformational space of solutions and which structures were tested.

In our tutorial (**STEP 7**), we performed a short simulation that took 100 steps. In this step of the tutorial we will record a movie from structures generated during this modeling.

1. First, close your UCSF Chimera graphics window.
2. Open new Chimera session.
3. Using UCSF Chimera's menu (**File→Open**), open the electron density map that you used to perform the simulation (**1nic.mrc**).
4. Change the map's volume threshold to **20.0** using the **Volume Viewer** tool (**Tools→Volume Data→Volume Viewer**).
5. Change the map's transparency to 0.5 and brightness to 10 (**Volume Viewer→Features→Brightness and Transparency**)
6. Set the background white (**Actions→Color→all options→background→ white**)

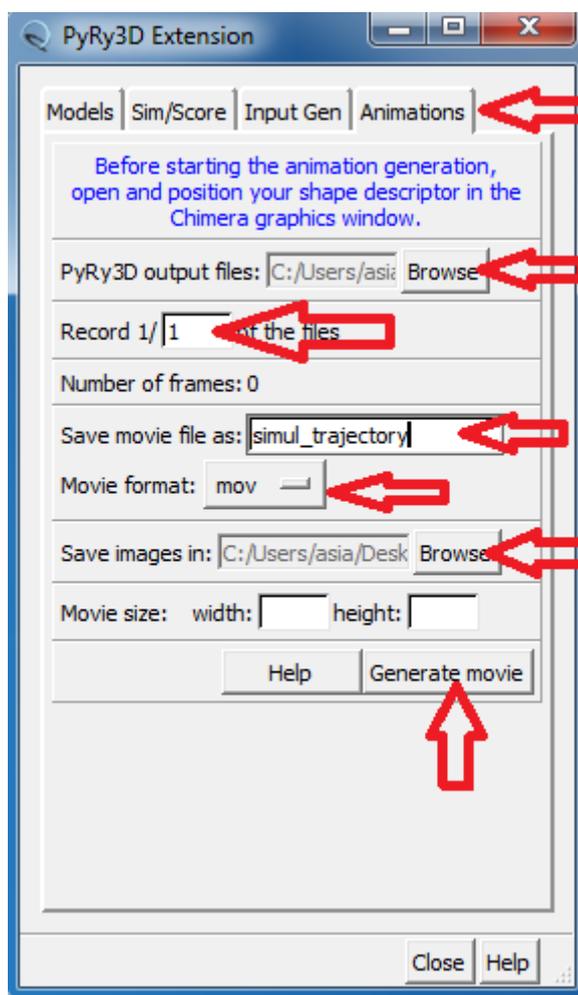


7. Zoom the view in or out to the point where the electron density map is large.

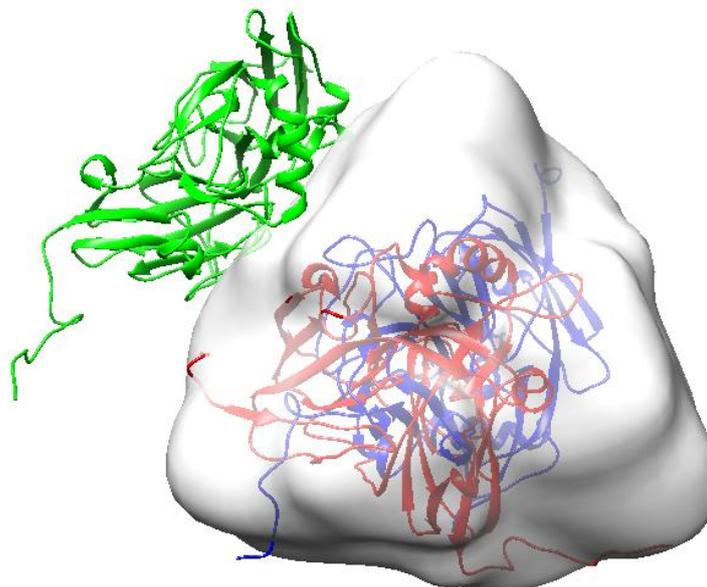


8. Go to the **Animations** tab in PyRy3D Extension's interface.
9. Use the **PyRy3D Output Files:** entry to point to the directory that contains output files from the simulation performed in **STEP7**.
10. The **Record 1/x frames** entry lets you decide what fraction of the output files should be recorded. This is useful mostly for longer simulations. **1/1** means that all generated structures will be used to record a movie,  $\frac{1}{2}$  that 50% (every second file) etc. In case of simulation we performed in **STEP7** which was pretty short, we can record all frames. Please select **Record 1/1 frames**
11. **Save movie file as:** – write a path to folder where you would like to store a video file with simulation results including a name for file with a movie eg. **“C:\video\_pyry\simulation”**. Next select one of the video formats below (\*.mov is set by default).
12. **Save images in:** - lets you choose a place where temporary movie frames (parts of the movie) will be saved during the movie recording. Before encoding a final movie, UCSF Chimera saves a sequence of .png screenshots which might take some disk space.

13. Leave the **Movie size** fields empty – the size of the movie will be adjusted to your screen.
14. Click **Generate Movie** to start. The video recording might take some time, but please be patient. You can easily check the modeling process step by step afterwards! Most of the formats can be played in any software capable of playing videos (like **Windows Media Player**, or **Totem**) .



15. While film is recording you will see new complexes appearing on the Chimera screen. These are structures saved on disc during simulation



16. After the recording is over in a **Model Panel** you will have several objects loaded which refers to: single chains of best complex generated by the program (**\* A, \* B, \* C**) and structure of the whole best model as one object (**\*best\_simulation\_complex\*.pdb**). \* refers to name of pdb file given by PyRy3D program.

