Tutorial on using QChromosome Visualizer (QCV) software for chromatin model simulations

In this tutorial you will learn the main functions of QChromosome Visualizer (QCV), starting from loading a molecule, through modifying the parameters of the visualisation of the molecule and ending up with rendering high-quality molecule images and movies.
In this tutorial we use as an example the trajectory of a model of first part (1000 pseudoatoms) of the chromosome arm 2L of *Drosophila melanogaster* that was generated by our implementation of the Strings and Binders Switch (SBS) model. The **2chr_PolII.pdb.gz** file with *Drosophila* chromatin MC trajectory is provided on our web server with the tutorial at the following URL: http://regulomics.mimuw.edu.pl/~bartek/QCV/chr2_polII.pdb.gz. The file is using a standard PDB format with each frame bracketed by MODEL and ENDMDL records. The single chromosome segment consists of four types of pseudoatoms, representing 20 kbp of DNA each. Pseudoatoms with the ability to interact with Polymerase II are named BOU (as in bound), pseudoatoms that interact with lamin (chromatin sites that bind suppressor of hairy wing Su(Hw)) are named LAM, other chromatin pseudoatoms are named UNB. Polimerase II is represented by freely diffusing pseudoatoms that are named BIN (as in binder). The simulation was obtained using our implementation of the SBS model described by Barbieri et all. 2012.

In this tutorial, we will go through the main functions of the QCV software, opening a project, importing a pdb file, viewing the simulation, changing the view parameters, saving high quality snapshots and animations, including 360 videos and saving the project files.

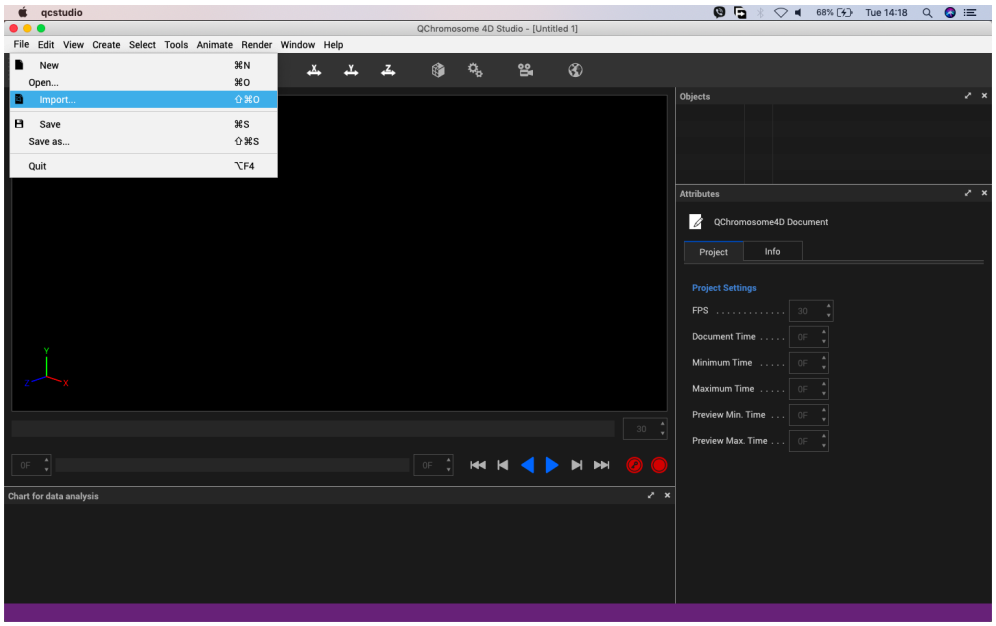
Starting the application

After installation procedure, described in the readme file of the source code distributed on github at https://github.com/regulomics/ChromosomeVisualizer, in order to run QCV just write in the terminal:

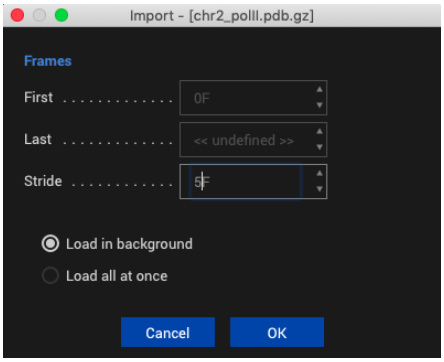
```
$ qcstudio
```

Once we have started the application, the main window appears with an empty project allowing us to load the data and start setting the parameters of the visualisation

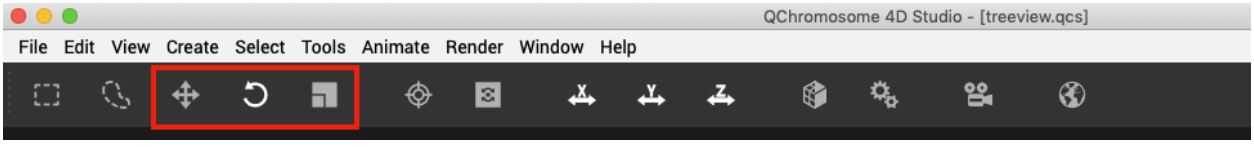
Loading the trajectory
To load the new trajectory to the program just choose **File** → **Import** and find the pdb file you want to open.



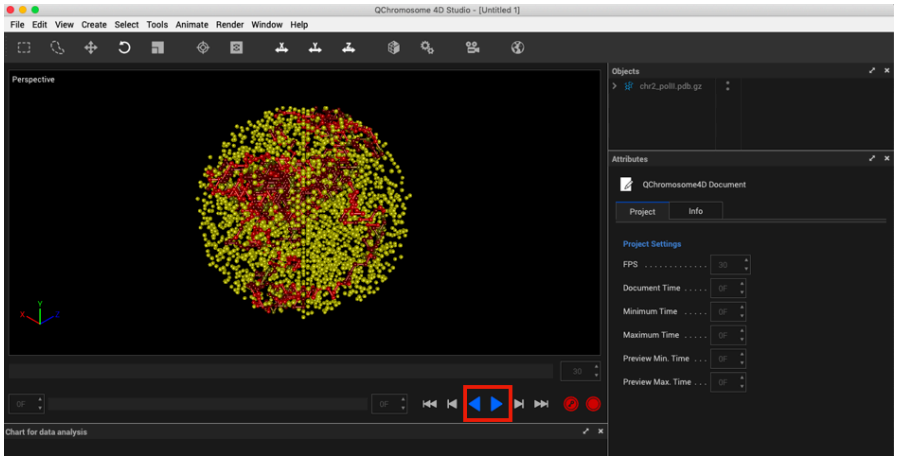
Another window named **Import - [2chr_polII.pdb.gz]** will appear and let choose the range of the frames to load (**First** and **Last**) and a number of frames skipped (**Stride**) between the loaded steps (this is useful if we are loading from large files with many small steps recorded). Changing the **Stride** value to 5 means that every fifth frame from the trajectory will be loaded into the QCV program. If you want to load all chosen trajectory steps at once immediately, select **Load all at once** option. This is however, impractical for large files, as it takes up more memory than it is necessary. In order to avoid that and have more control over the loading process (e.g one can stop the loading and restore it again), we recommend to select **Load in background** option and press **Ok**. This will make the program only read frames to memory as they need to be shown.



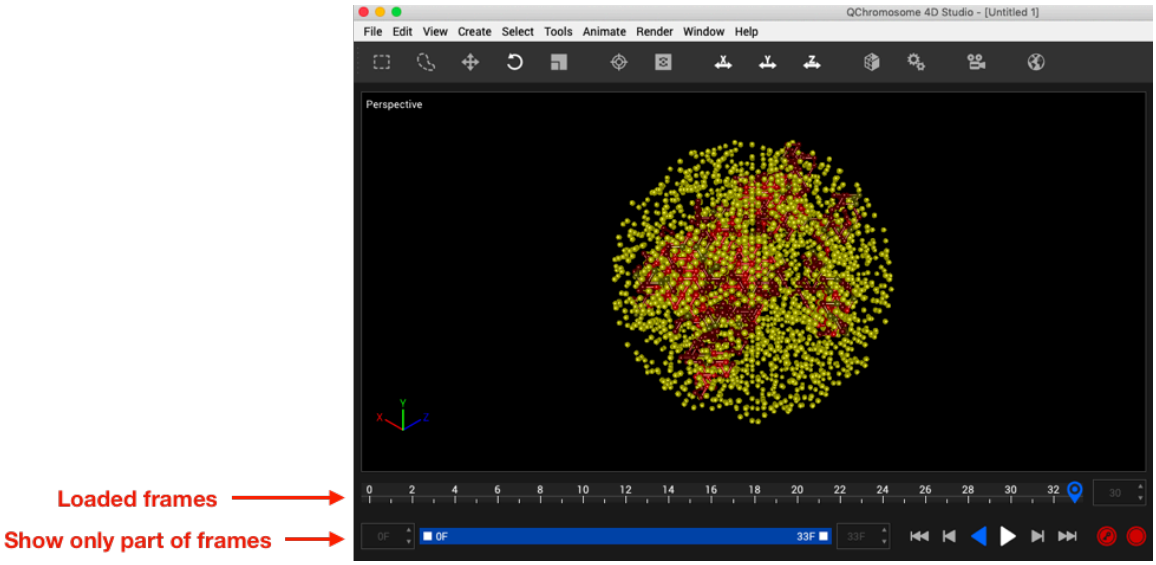
First step of chr2 trajectory is showed in the main QCV window. You can manipulate (rotate, translate, scale) the molecule by using an appropriate bottoms on the **Menu tool**.



Load next steps of simulation and stop loading any time you want by pressing **Play/Stop** button.



During the loading process two line appears in the **Animation toolbar**. Upper one shows the number of loaded steps, as well as marks of the state that is displayed in the main window. Lower one allows to play/render only an appropriate range of the trajectory.



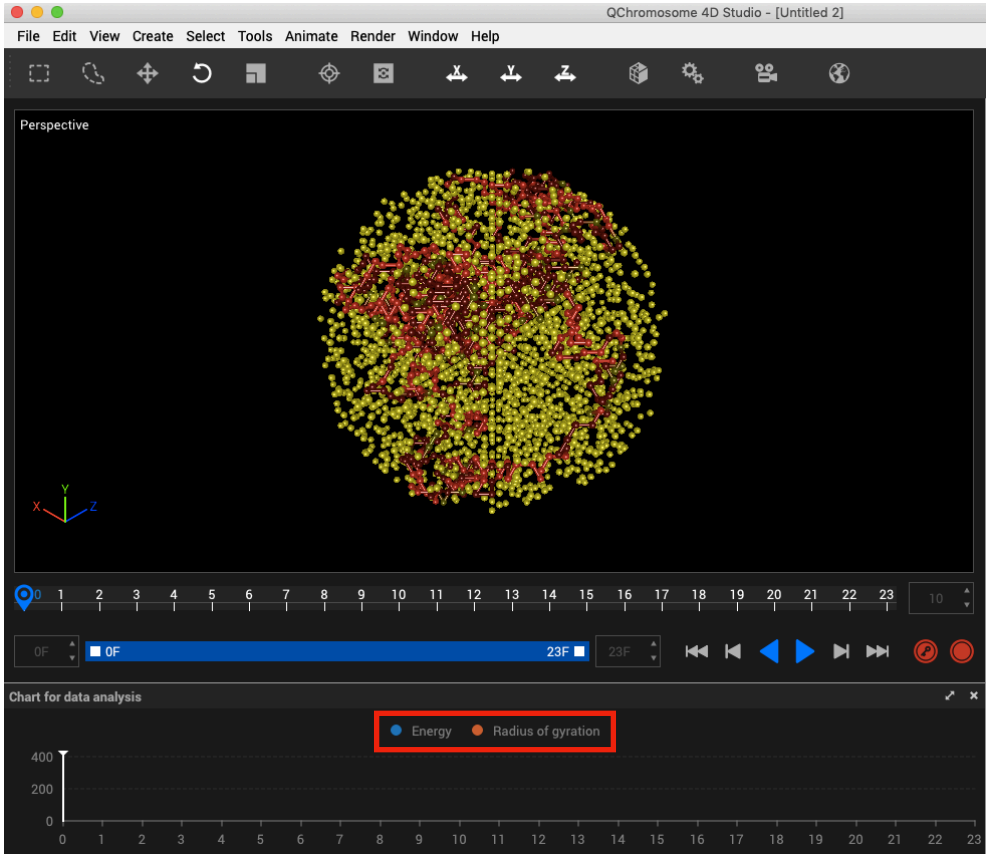
Loading the data that describe the simulation

Using QCV you can easily make charts for data that describe the progress of the simulation, like energy, radius of gyration, temperature etc. All data can be given in one text file in xvg format, where first column will be ignored by the QCV program while second and next columns are interpreted as Y values for different sessions. In the first lines, you can put the name of each session after the **@** sign in the format **@ sNR legend "NAME OF THE SESSION"**, like on the picture below.

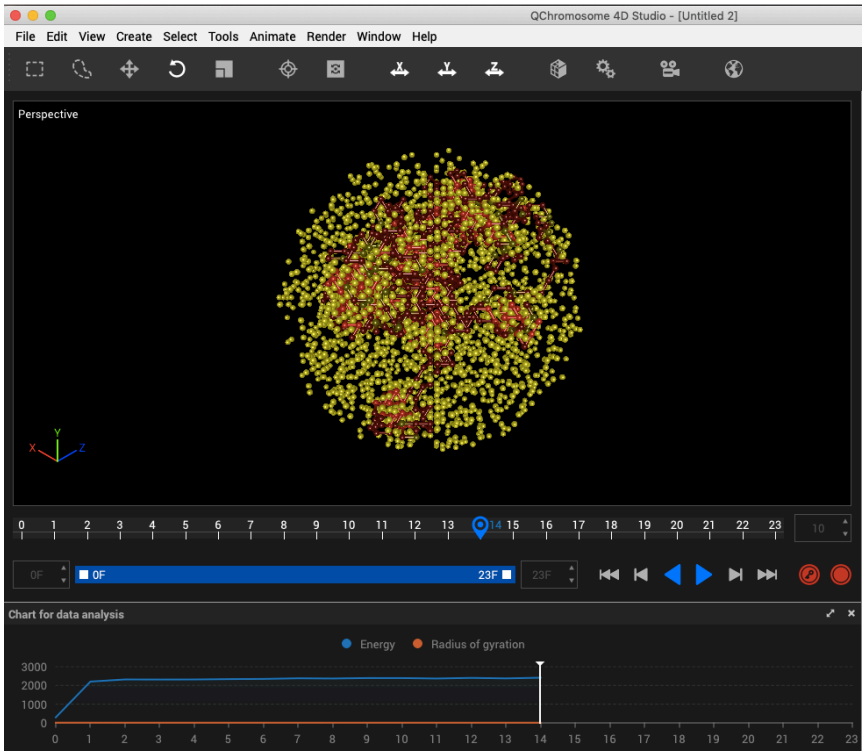
```
@ s0 legend "Energy"
@ s1 legend "Radius of gyration"
0 296 13.40
48000 2119 13.1305959566
49000 2102 13.1474147444
98000 2245 13.1072714402
147000 2210 13.0155478152
196000 2207 13.1675712809
245000 2290 13.3274470254
294000 2261 12.9360890073
343000 2272 12.8291177056
392000 2283 12.7518929649
441000 2321 12.6150562994
490000 2343 12.4971246043
539000 2344 12.5378091015
588000 2321 12.7281976817
637000 2358 12.5498794424
686000 2317 12.5867054186
735000 2342 12.3984896226
784000 2322 12.3823122676
```

In our case the first column describes the frame number in our trajectory, second column is a score or “energy” while third is a radius of gyration.

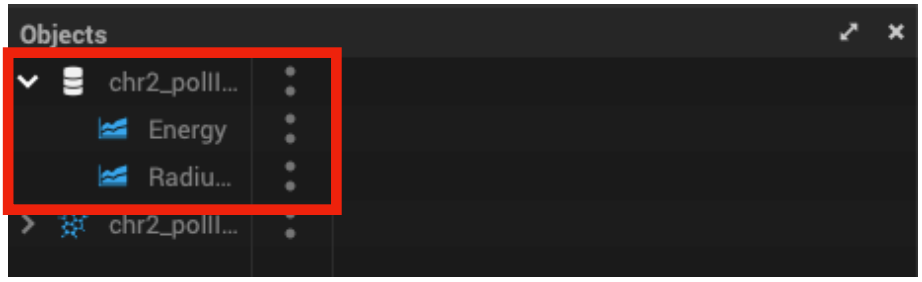
To load data for making charts just choose **File** → **Import** and find the xvg file (in our case chr2_polII.xvg) corresponding to the loaded trajectory. Press **Open** button.



The legend appears in the **Chart of data analysis** window and the indicator of the currently displayed frame has returned to the beginning of the trajectory. The name of the loaded file appears in the **Objects** window. Press **Play** button to load data from the xvg file.

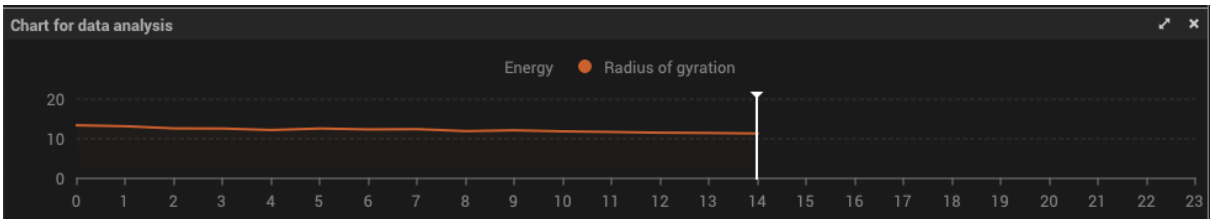


It i s possible to go down in the object tree and see the title of all graphs that appeared in the **Chart of data analysis** window.



As we can observe in our case there are big differences between energy values and radius of gyration values, therefore the red plot is almost invisible. To analyse radius of gyration changes we need to hide the plot that describe energy changes. In order to hide the plot double click on the grey upper dot opposite the **Energy** name in the **Objects** window.

The blue plot disappear, while the values described in the **Chart for data analysis** window are recalculated for the red plot.

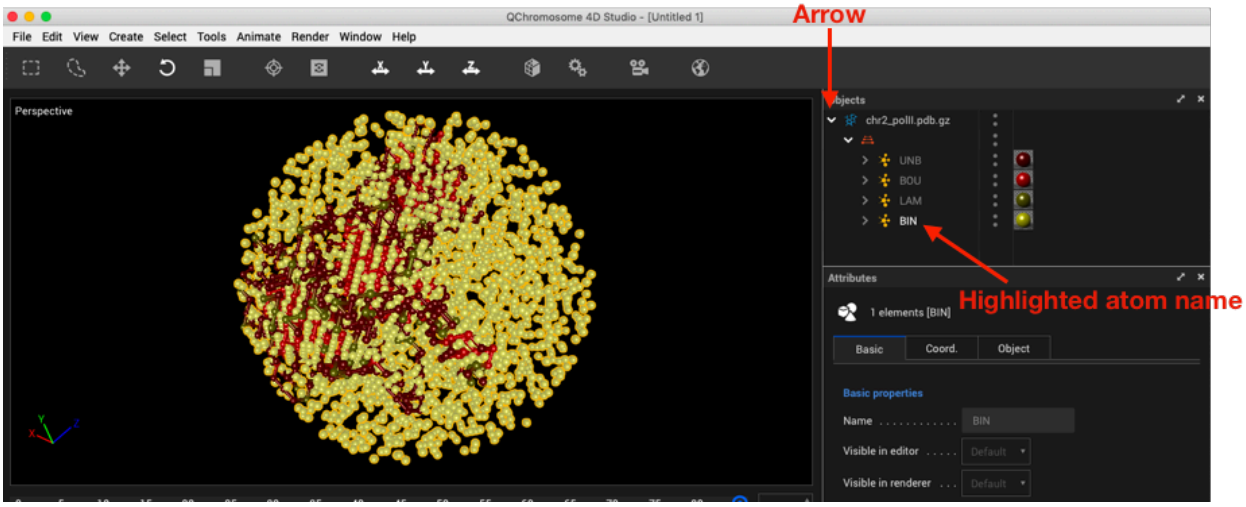


As you can see, the indicator of the structure that is displayed in the main window is not only on the line that describe loaded frames of trajectory, but also on the plot, what is very convenient for example to analyse changing of the structure in the place of a sudden drop/rise in energy/ radius of gyration/temperature etc.

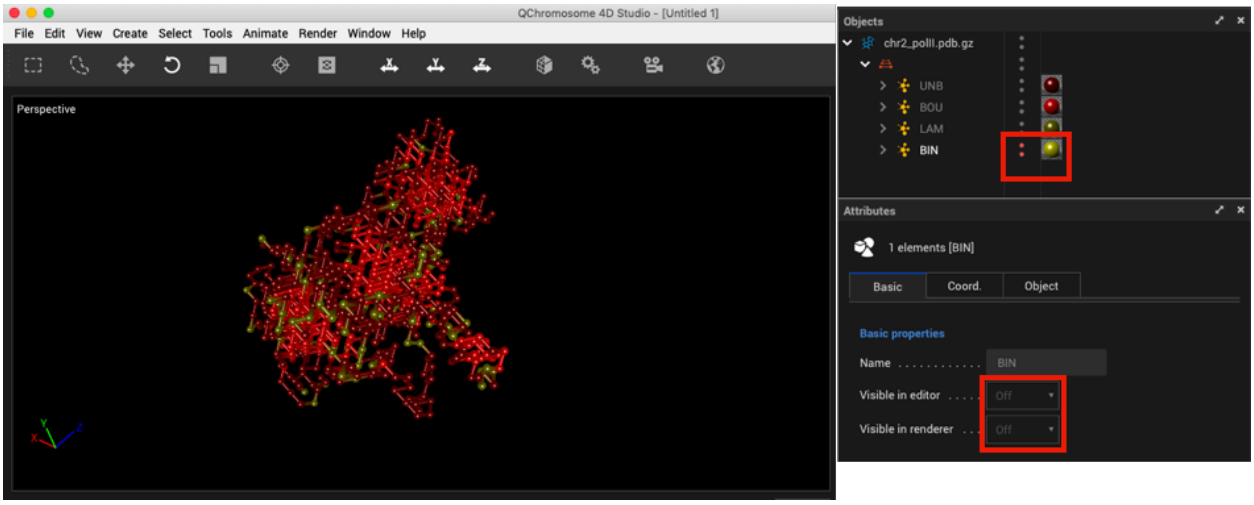
Changing the visualisation of the molecule

In the QCV program each object has a tree structure. In the **Object** window click on the arrow near the molecule to go down in the object tree. The arrow becomes white instead of grey and daughter objects appear.

Go down until atoms names (**UNB, BOU, LAM, BIN**) appear and click on the **BIN** atom name. It will be highlighted both in the **Object** window as well as in the main program window.

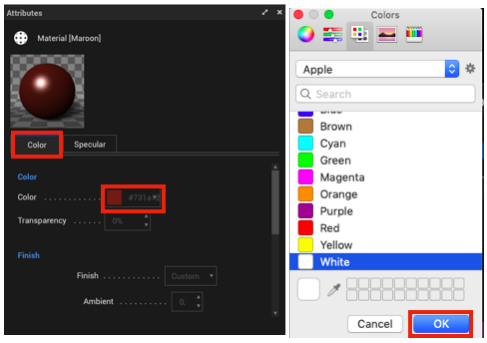


There is two ways to hide atoms in the QCV. First is to double click on the grey dots opposite the **BIN** name in the **Objects** window. The upper dot is responsible for hiding/visualising on the screen, while the lower one - for hiding/visualising during the rendering a picture. If atoms are hidden, the dot is marked red (see red square on the Figure below). Second - to chose **off** for the **Visible in editor** or/and **Visible in renderer** options in the **Attributes** window. Choose the most convenient way for you and hide BIN atoms.

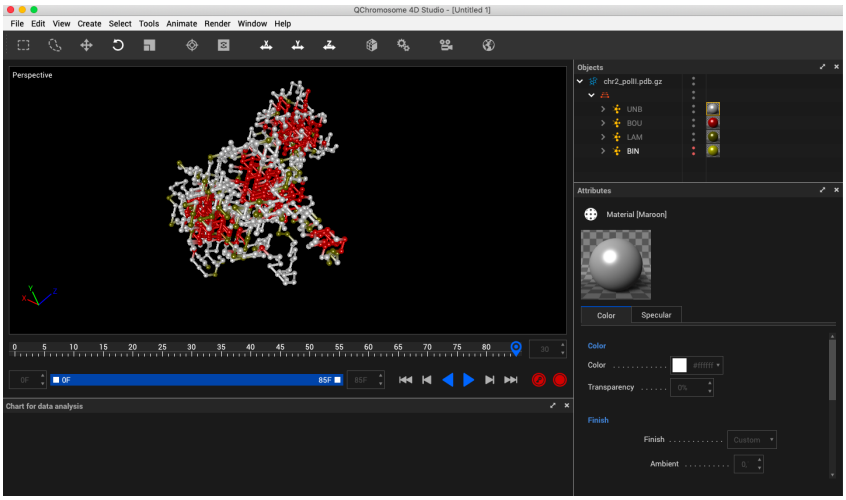


In order to change the atom colour and material click on the ball that represent atom in the **Object** window. The ball will be highlighted.

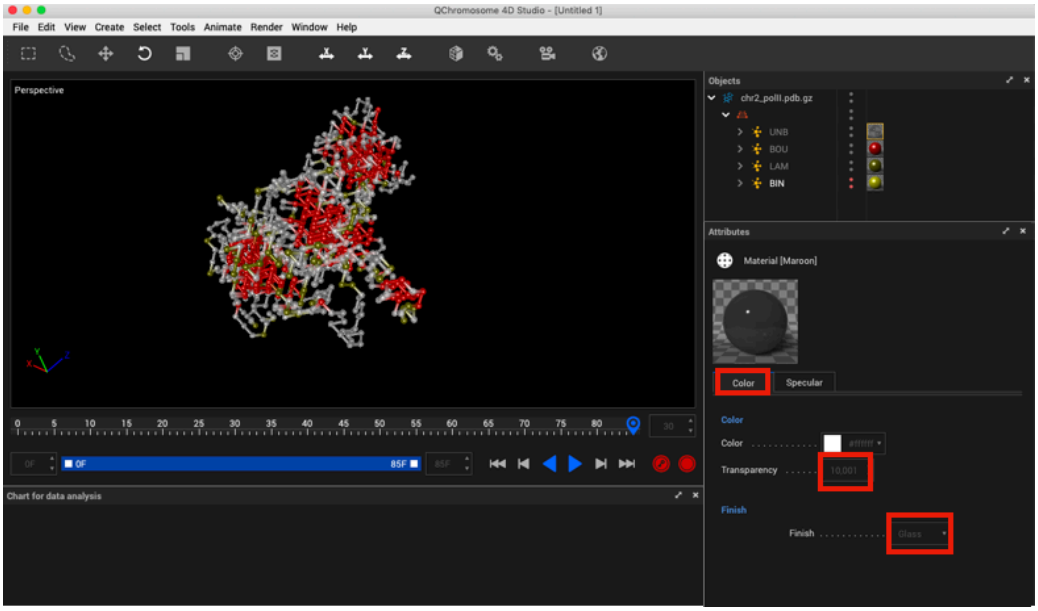
Simultaneously in the **Attributes** window appear attributes connected with atom representation. Click on the colour opposite **Color** option and choose any colour you want from the **Colors** window. I chose white. Click **Ok** button.



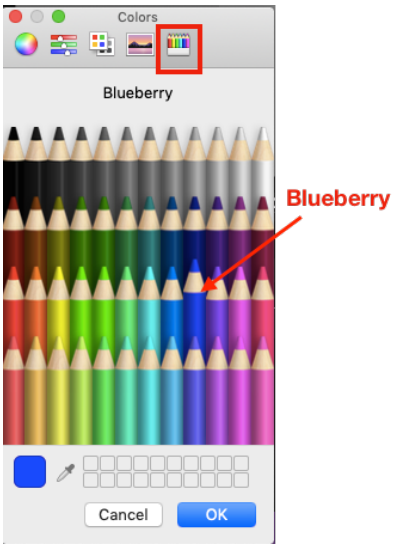
The representation of the atoms will change in all available windows.

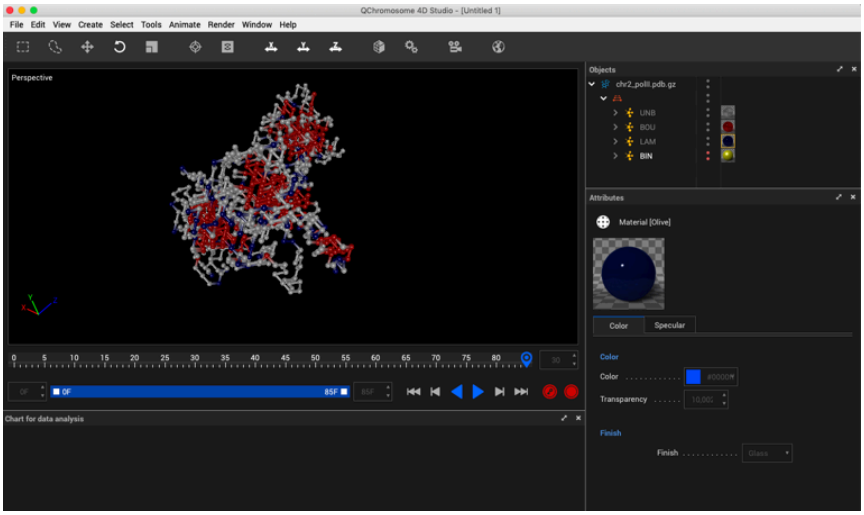


In the **Attributes** window choose **Color** tab and change **Transparency** parameter to 10% and **Finish** option to **Glass** (red squares). Representation of atoms will change.

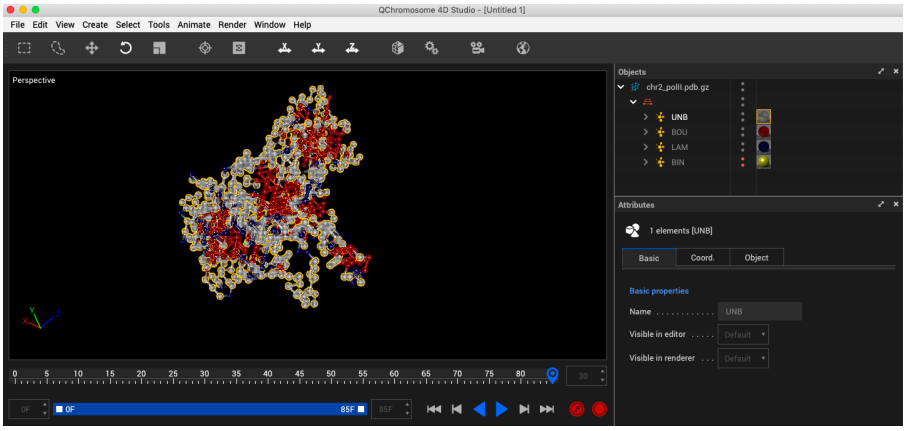


Repeat the same steps for all atom types. I leave red colour for **BOU** atoms and change **LAM** atom color to **Blueberry** (the colors dialog shown is different on different platforms, the one shown is from Mac OS X).

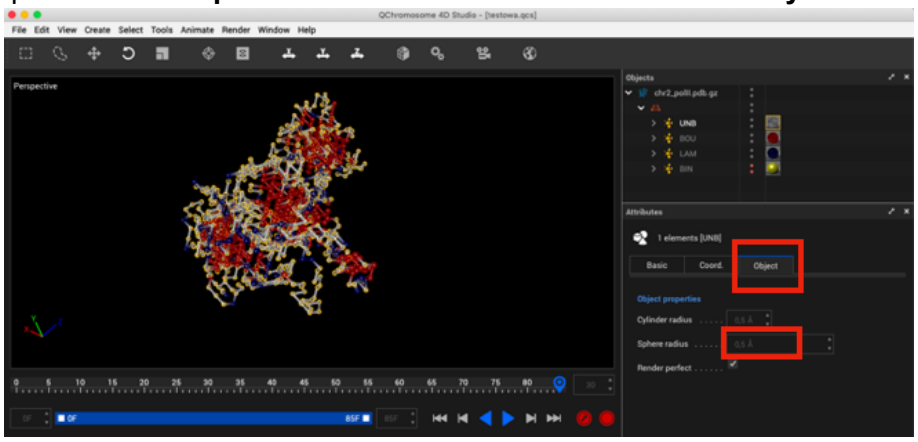




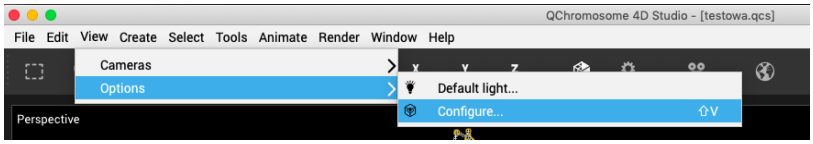
In our trajectory UNB atoms do not play an important role in the chromatin structure, therefore we will reduce their size. In order to change the size of UNB atoms click on the atom name **UNB** in the **Object** window and UNB name in the **Objects** window will be highlighted as well as appropriate atoms in the main window. In the **Attributes** window appear attributes of atoms.

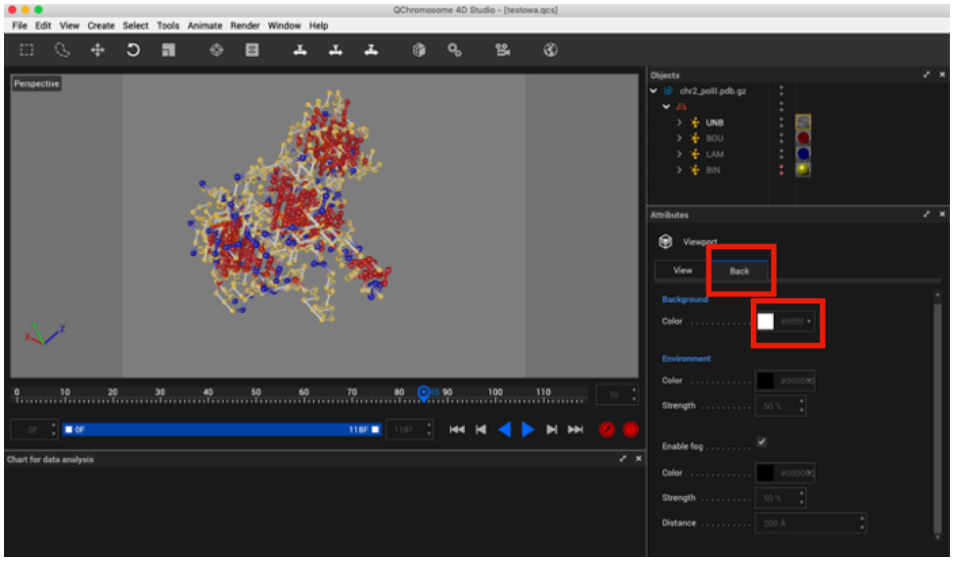


Click on the **Object** tab of the **Attributes** window and change **Sphere radius** to 0,5 values. It should be emphasized that **Sphere radius** value can not be lower than **Cylinder radius**.

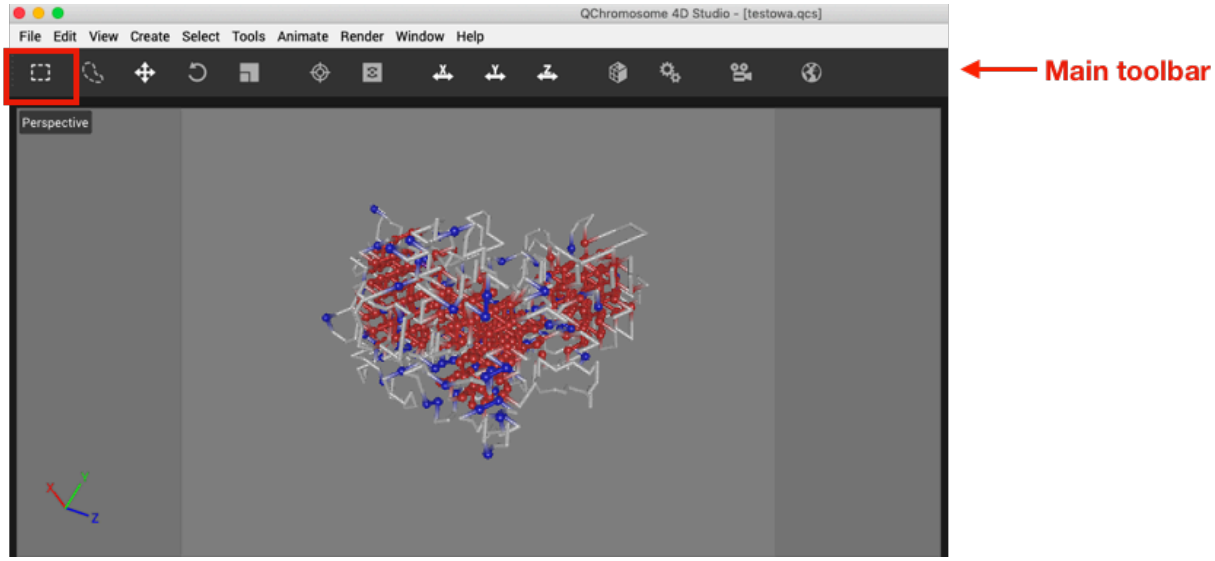


In order to change the background color choose **View** → **Options** → **Configure,** in the **Attributes** window, click on the **Back** tab and change the **Background** color to white or your favorite one. Due to the fog effect is on and the color of fog is black, the background is not white, but rather light grey. However we do not recommend to turn the fog off.



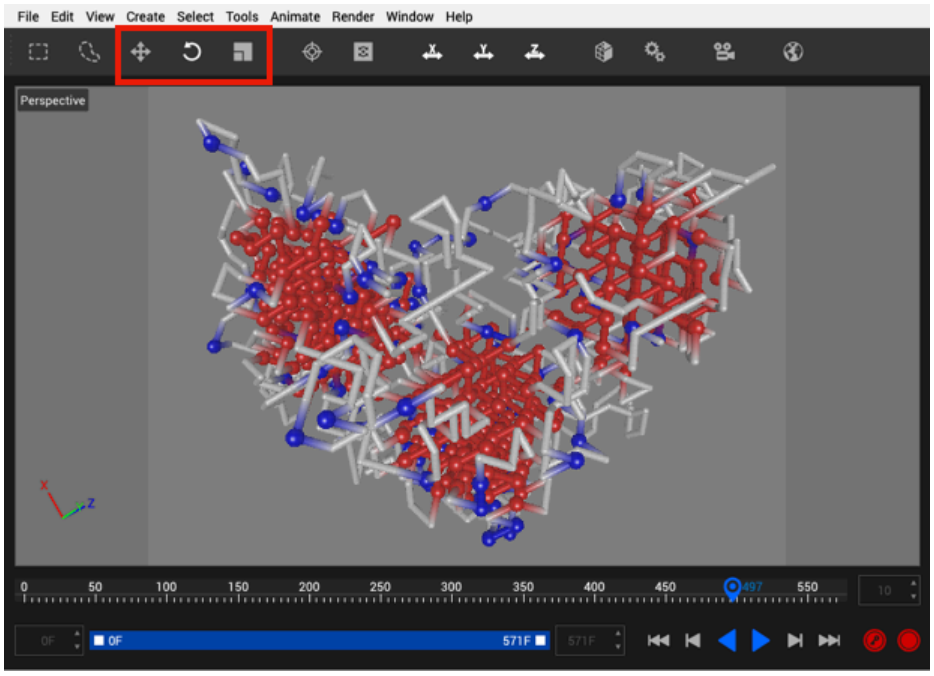


In order to turn off highlighting of atoms in the main window, click on the **Rectangle selection** icon on the **Main toolbar** or choose Select → Rectangle selection, and next click on the background of the main window.

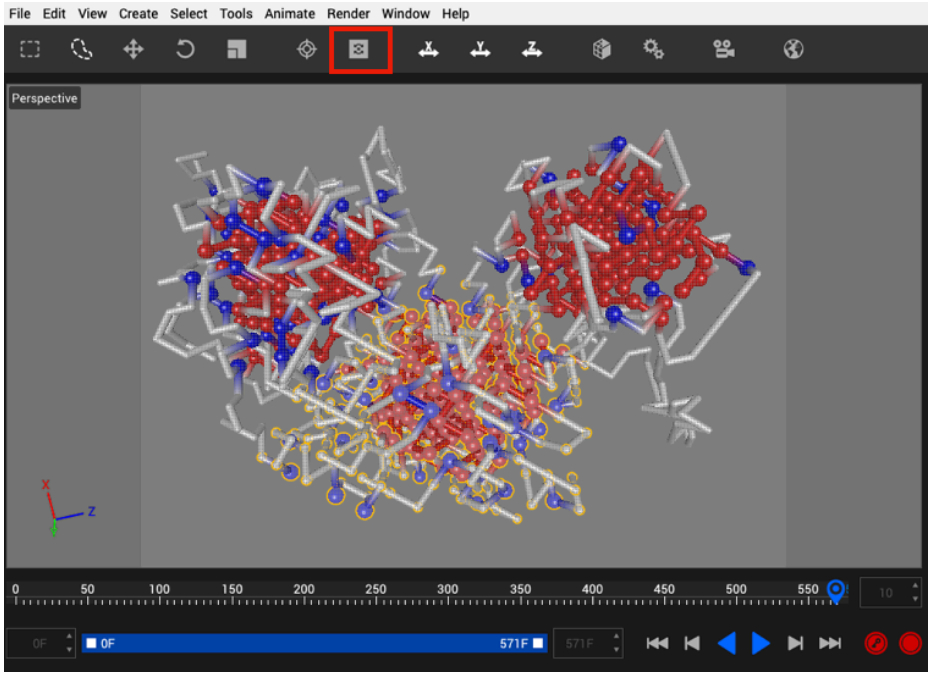


Save high quality pictures

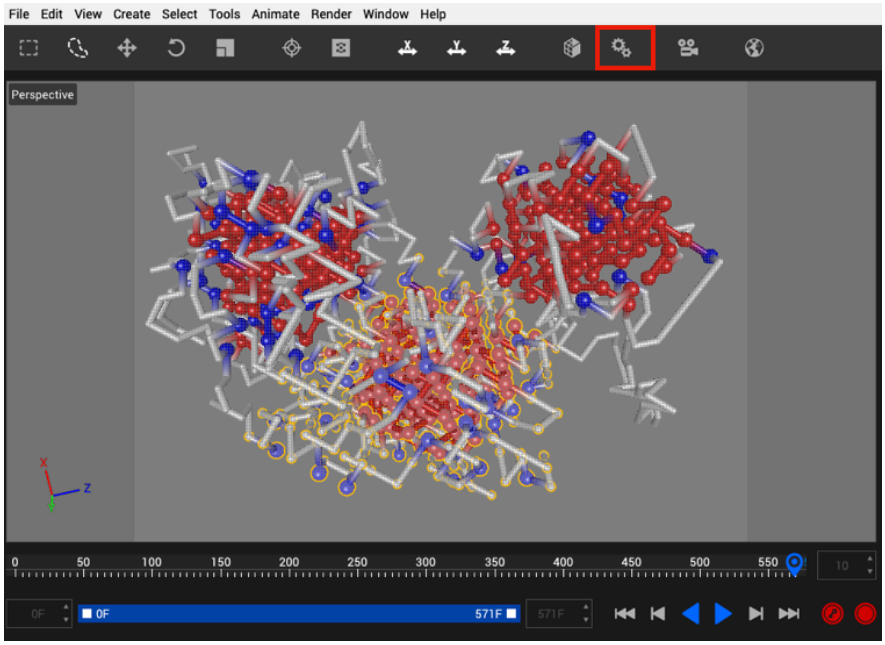
Click on the **Play** button and load the rest of trajectory, next find your favorite frame. Manipulate of molecule by using **Move, Rotate** or **Scale** buttons on the **Main toolbar**, or in the **Menu Tools,** to see it from the most interesting perspective.



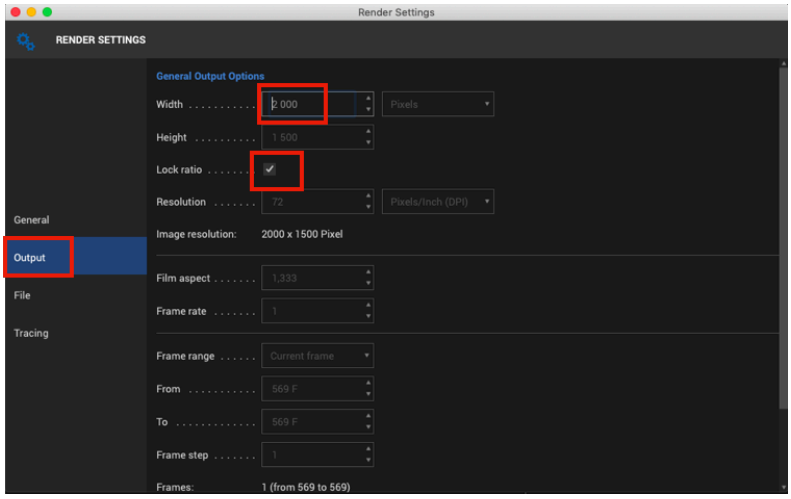
QCV program rotates the molecule around its center of mass. If you want to change the rotation center, select the group of atoms or one particular atom and click on the **Pivot point** button on the **Main toolbar**.



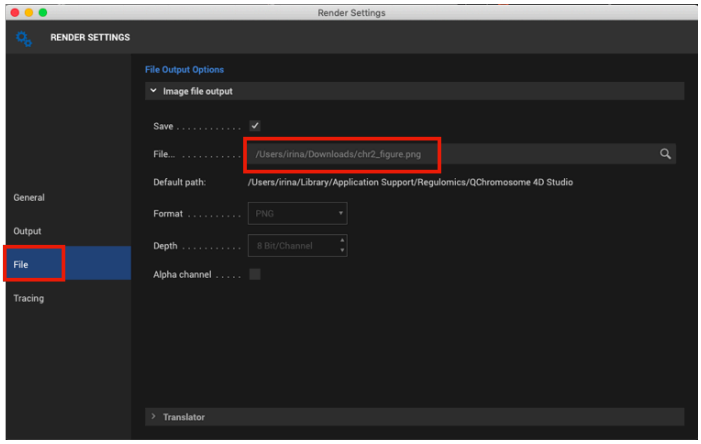
To set appropriate options of rendering, click on the **Render setting** bottom in the **Main toolbar** or choose **Render** → **Render setting**.



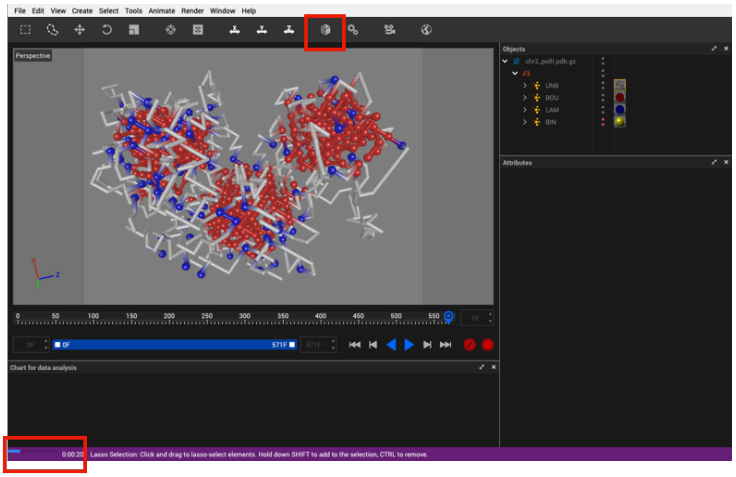
Choose **Output** tab in the opened **Render Settings** window and make sure that **Lock ratio** is selected. If not, select it. Change **Width** value to 2000 and press **Enter**. The **Height** value will change automatically.



Choose **File** tab in the **Render Settings** window and write the file name in the **File** option.

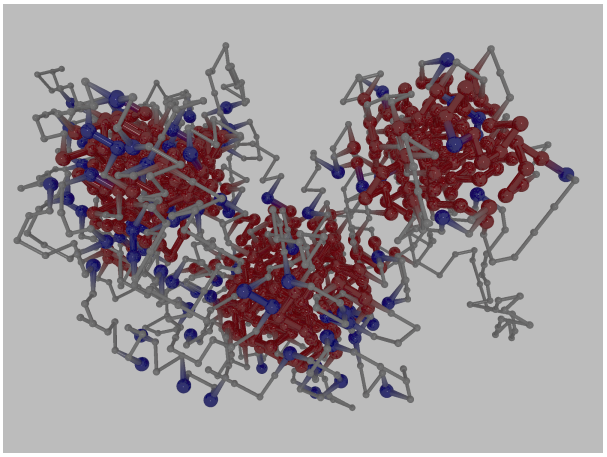


Close **Render Settings** window and click on the **Render** button in the **Main toolbar** or choose **Render → Render to Picture Viewer** and the process bar will appear on the bottom of the program windows.



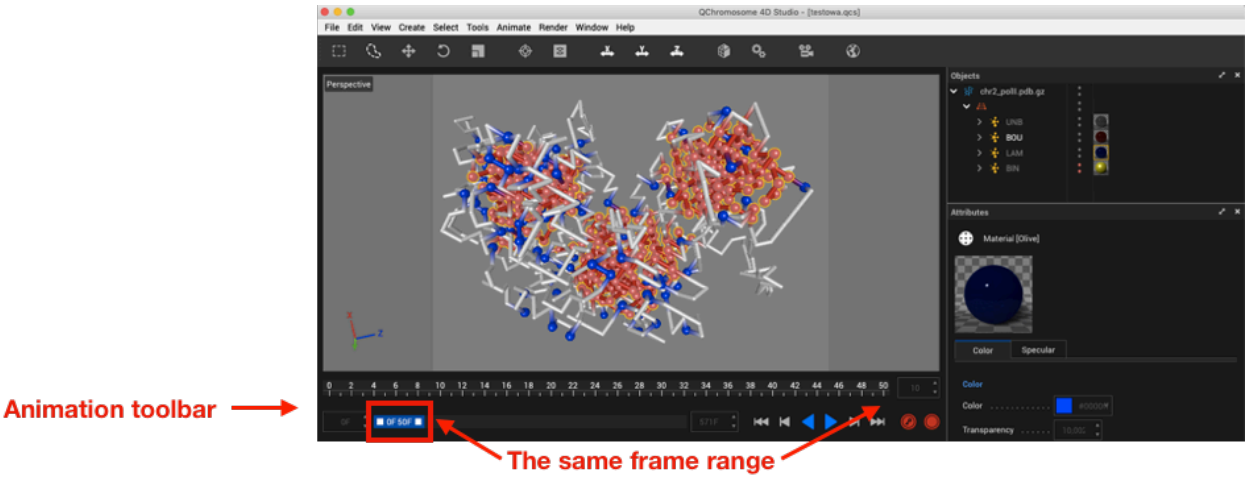
When the process of rendering the image is finished, the figure will appear in the selected fold-

er. Below is the picture we obtained after finishing the render process. You can find it in the Tutorial folder called chr2_polII_figure.png.

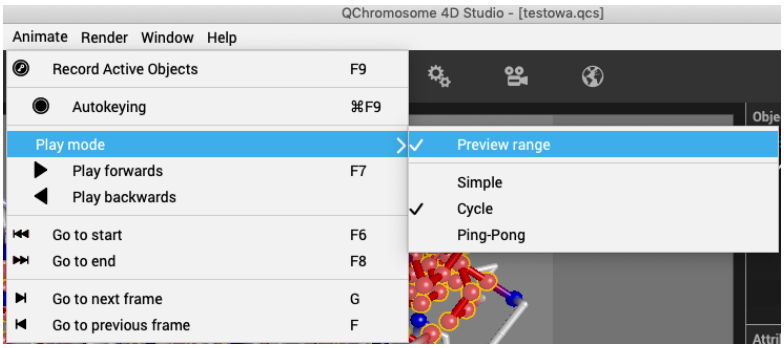


Movie Making

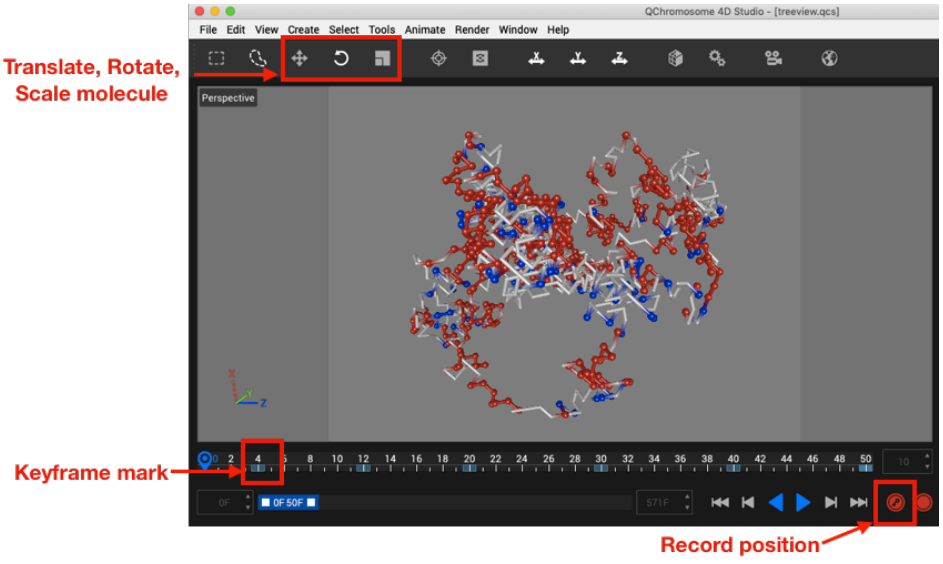
If you do not want to record all trajectory, choose any part of loaded frames by moving the end points of the blue slider in the **Animation Toolbar**. I chose first fifty frames. In the same time the range of loaded frames is limited to the one set by you by moving the blue slider.



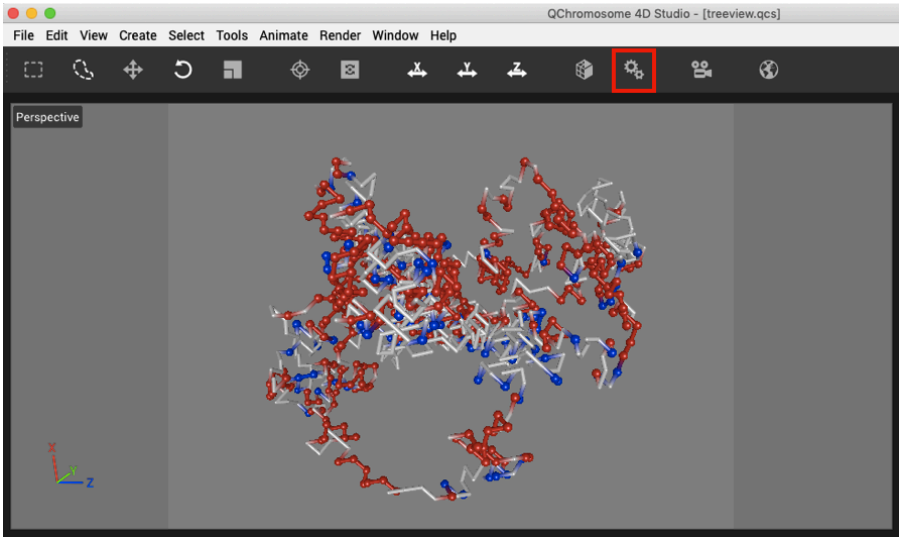
Now, when you press the **Play** button, the animation will continue to play outside the range of selected frames. To limit the playback of the animation to the selected by the user by moving the blue slider, choose **Animate** → **Play mode** → **Preview range**.



Now click on the **Play** button and change the position of the molecule (rotate, translate, scale) so that it is clearly visible on the monitor during the entire playback process.
In order to add addition movement to the animation (rotations, translations, or scale) we need to add keyframes. Click on the forth frame of animation and rotate slightly molecule. Next press **Record position** button on the **Animiation Toolbar**. The mark of the saving keyframe will appear. Each keyframe can be deleted by selecting the keyframe mark and next pressing **Del** button on the keyboard.
During the rotation of the molecule using mouse or touchpad, the program moves the camera around the molecule. While during the play/render the simulation with keyframes, where molecule was rotated, the program interpolates the path between the nearest keyframes. Please remember that if the rotation is interpolated over large angles (i.e. two consecutive keyframes showing the chromosome from the opposite sides), the movement between keyframes during the animation may become difficult to predict (e.g. there can be moments when camera is not facing the molecule or there might be sudden changes of perspective). In order to avoid this, rotation movement between keyframes should not to cover large angles. This can be achieved by adding additional keyframes to give more point to the interpolating process. If during playback of the simulation the movement of the molecule between two frames with rotation is unexpected, simply go to the affected frame, scale/move the molecule to the place you want it to be and add a new keyframe.

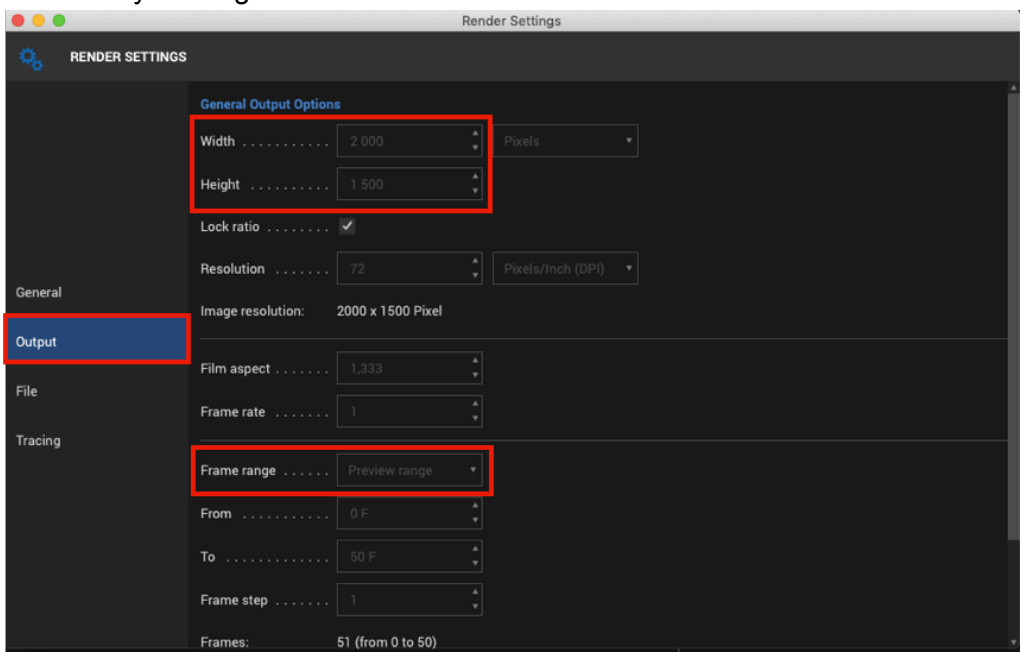


Now open render settings, by clicking on the **Edit render settings** button in the **Main toolbar.**

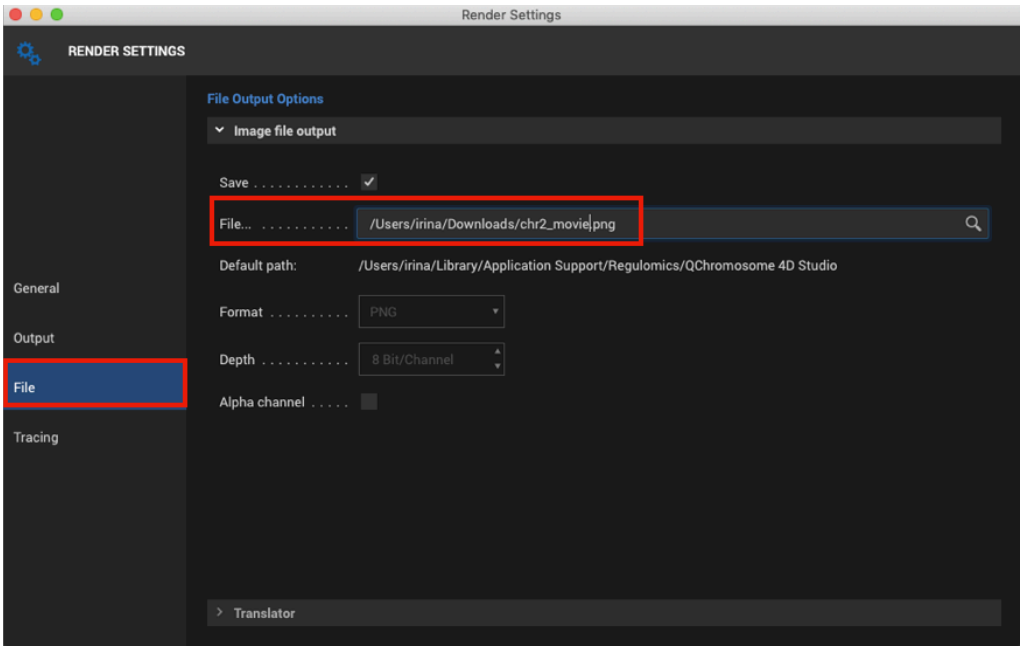


The **Render settings** window will open. Choose **Output** tab and check if the resolution is appropriate. We have already changed it, when rendering the picture. It should be at least as high as your screen resolution (usually 1920x1090 for high definition displays), however if you want to obtain really good movies, we recommend generation of higher resolution images e.g. in 4K resolution, as higher resolution movies downsampled to the native resolution tend to look better.

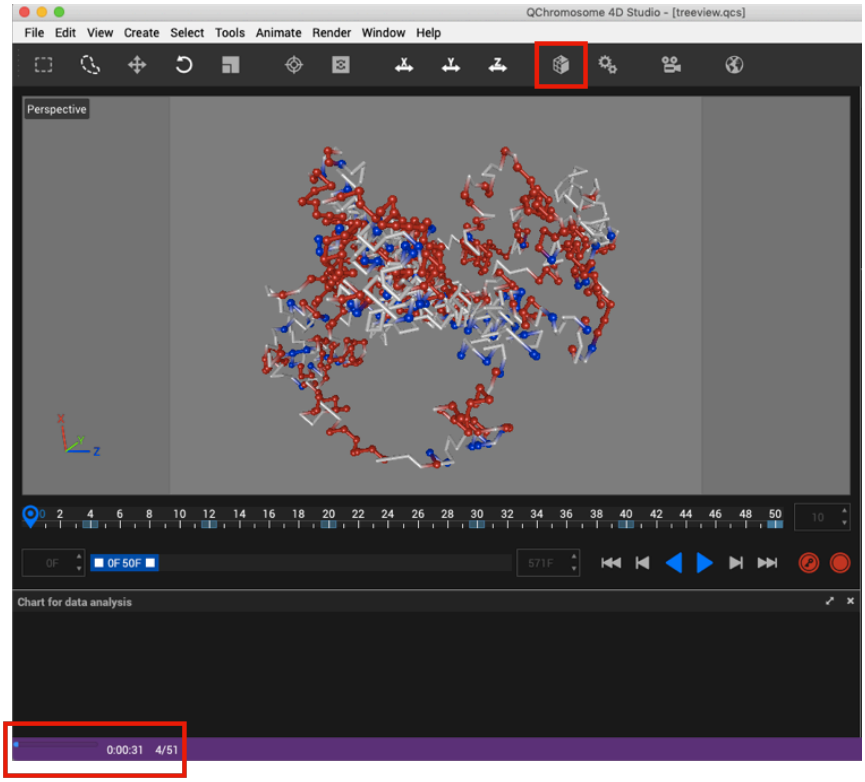
Change the **Frame range** options to **Preview range**, so your movie will have only those frames, you have chosen by moving the blue slider in the main window.



Now choose **File** tab and change the filename in the **File** gap. Next close **Render settings** window.

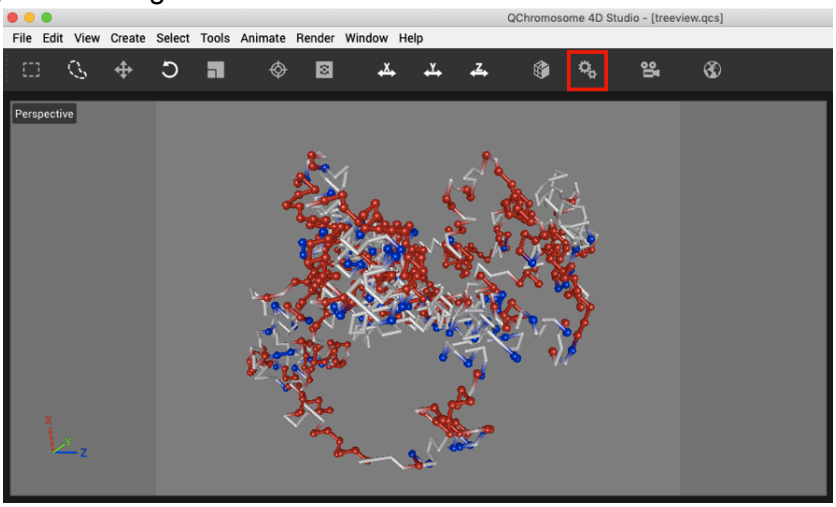


Now click on the **Render** button in the **Main toolbar** or choose **Render** → **Render to Picture Viewer** and the process bar will appear on the bottom of the program windows.

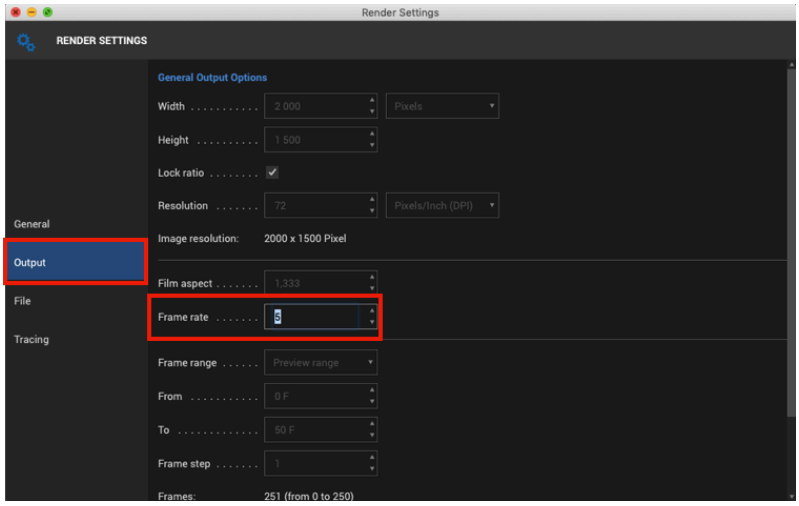


When rendering process is finished open the movie and playback the simulation. My movie file is called chr2_movie.avi and it is available in the **Tutorial** folder.

If your simulation frames are far apart (many pseudoatoms move at the same time) the movement of molecule might be quite rapid and “jerky”. We can smooth the animation movement by adding interpolated frames in between the simulation frames. For that, we need to open the **Render Settings** window again.

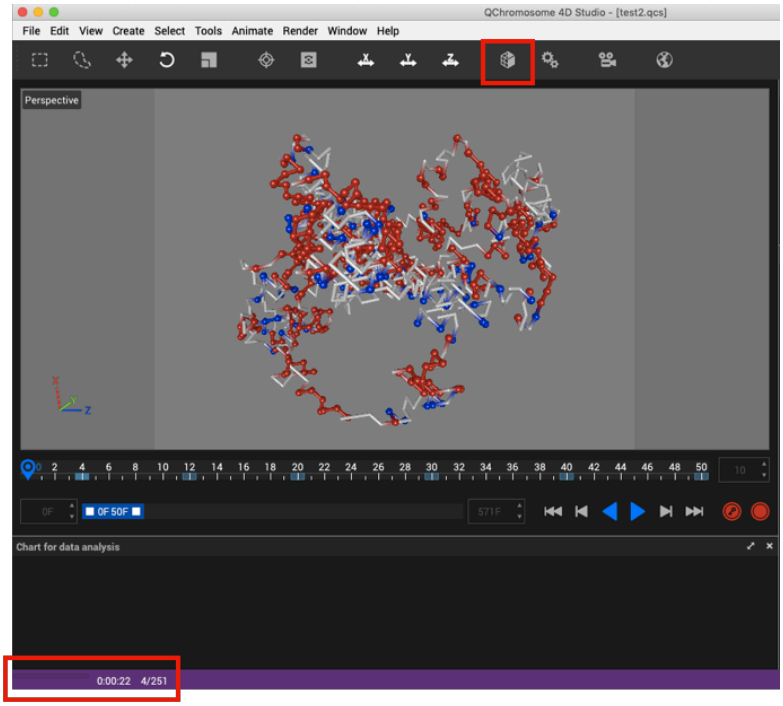


Choose **Output** tab and change **Frame rate** parameter to a value higher than 1 (e.g. 5), that makes QCV we will putt addition four virtual frames between each pair of consecutive frames with positions of all pseudoatoms and the camera smoothly interpolated in beetween. That should smooth the movement between the actual simulation frames. Naturally, we should remember that while this greatly improves the visual appearance, it should not be misinterpreted as the direct representation of the simulation states.

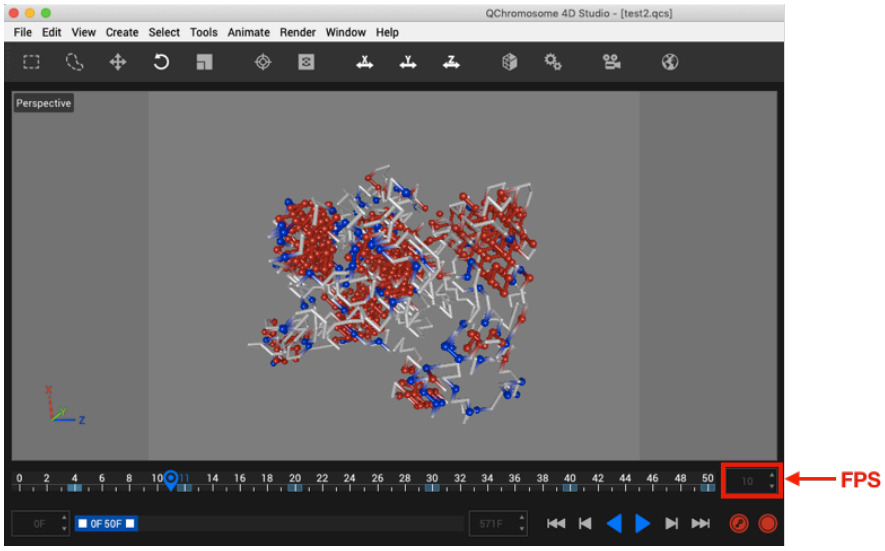


Change the file name in the **FIle** tab of the **Render Settings** window and close **Render Settings** window. Click on the **Render** button in the **Main toolbar** or choose **Render → Render to Picture Viewer** and the process bar will appear on the bottom of the program windows. You can

notice that now there is five time more frames than before.



After finishing the render process, you could compare movies. My movie with additional virtual frames is called chr2_movie_smooth.avi and you could find it in the Tutorial folder. You can change **Frame rate** parameter in the **Render Settings** window to smooth the animation and **FPS** (Frames Per Second) parameter to slowing down/speeding up the simulation.



Generating 360 stereoscopic video

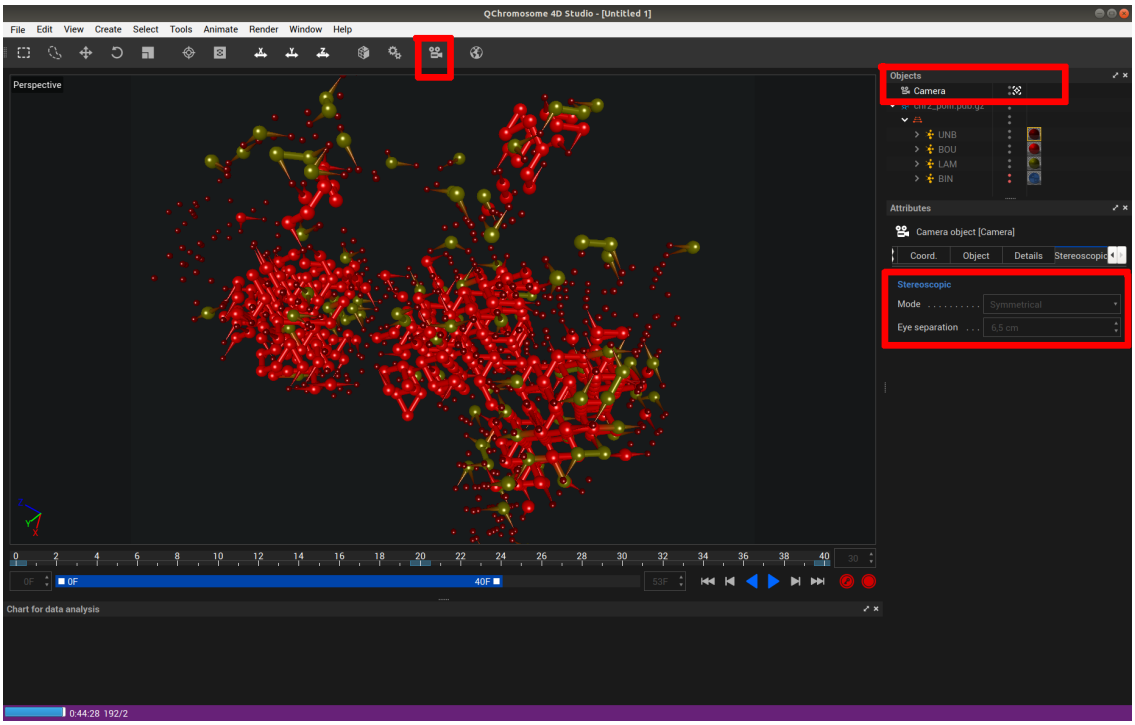
Since the advent of the new technologies for immersive visualization, commonly called VR, there are multiple technologies allowing visualisations including the full sphere of vision and allowing the viewer to “look around” in the scene as the animation/movie progresses. Since chro-

mosomes are very complex 3d objects, we think that using these new tools should allow us to better understand the processes occuring in our simulations.

QCV allows us to generate such spherical (360) movies that are compatible with the popular youtube platform. When the user decides to generate such a visualization, it can be uploaded to youtube and viewed either on a regular computer (allowing to move the viewport by dragging with the mouse) or on a VR headset such as Google VR, Google cardboard or any other platform supporting google 360 videos.

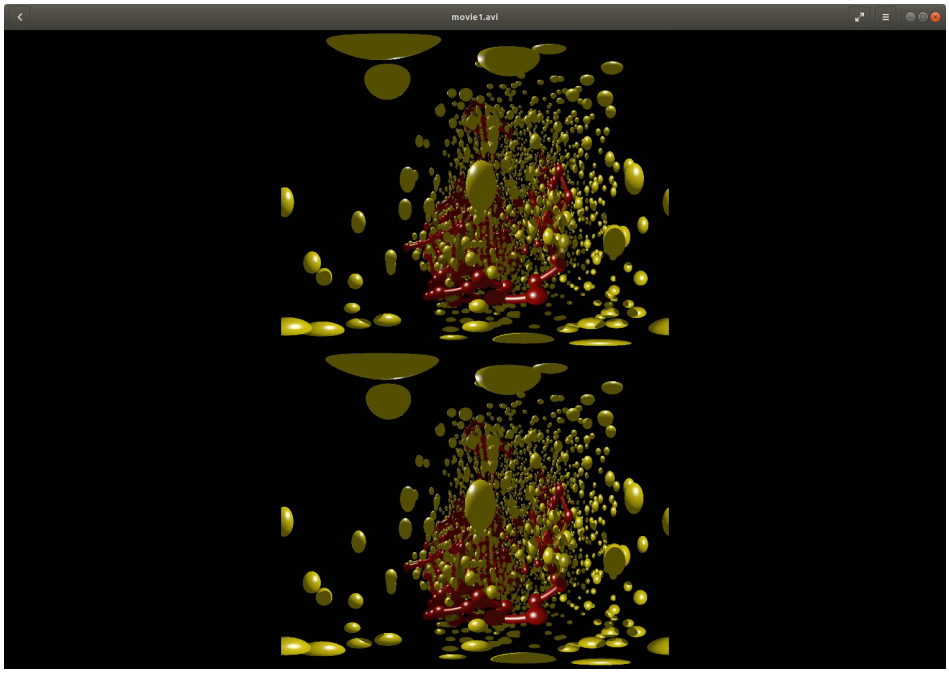
In order to record 360 videos, you need to create a new camera object, by selecting the **Add camera object** option from the **Main toolbar**. Then you can see a new camera appears in the objects browser on the right panel and you can activate it by clicking the icon beside it. If you activate it, you will see that this camera has its own set of attributes in the **Attributes** window, and you can change many of its features, such as the viewing angle. However the most important option for us is now in the **Stereoscopic attributes** tab on the far right. If you switch the mode of the camera to the **Symmetrical** options as it is shown in the figure below, you will generate the video for two-eye 360 videos. You can also choose to generate video sequences for the left and right eye separately, if you want to use other techniques for visualization.

Please note, that you can have more than one camera object, and that the keyframes for each camera object can be different, so please remember to make sure that you have activated the right camera object and that it has all the necessary keyframes set before rendering.



Once you have everything set up, you can click on the **Render** button in the **Main toolbar** and after a little while, you should see your 360 movie playing in a system video player. The movie

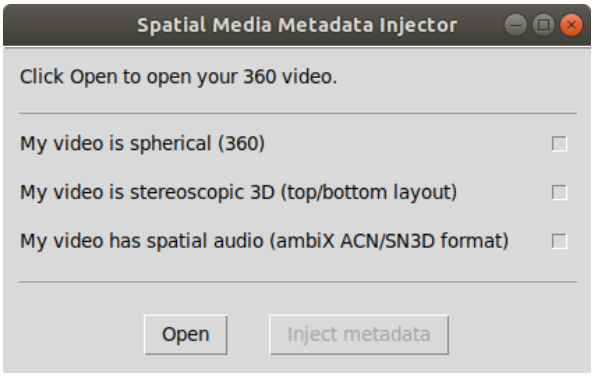
will look strange in the standard video player, as the images for both eyes are placed above one another and the perspective is highly distorted because of the cylindrical projection as in the screenshot below:



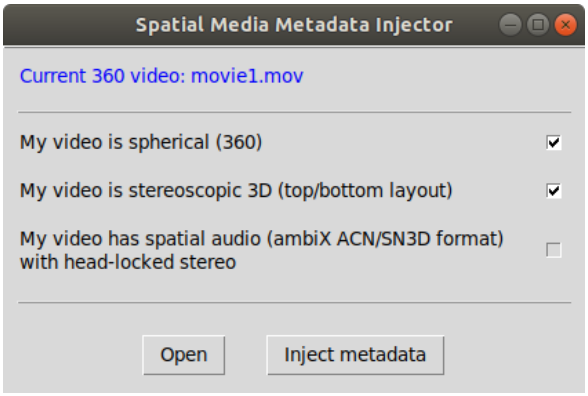
My movie file is called movie1.avi and it is available in the Tutorial folder.
Now that you have generated the .avi file and verified that it is viewable on your system (even though it does look different) you can prepare it for upload to youtube. Currently it involves two steps: preparation of the file and upload.
In order for youtube software to recognize the movie as a 360 spherical video, we need to use their metadata editor, distributed freely through their github account: https://github.com/google/spatial-media/releases/tag/v2.1
There are versions available for windows and Mac and the source code version can be run on linux systems.
Since their application only works on Mpe4 files, we need to start by converting our movie to the mpeg format by issuing the ffmpeg command:

```
ffmpeg -i movie1.avi -acodec libmp3lame movie1.mov
```

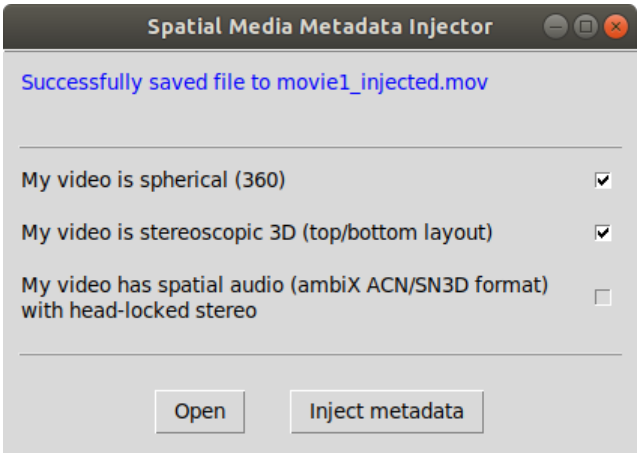
Assuming that we have named our output file movie1.avi, we should obtain a new file called movie2.mov in this way. Now we are ready to inject the metadata by starting the GUI version of the spatial media tool from google. We should see a dialog box like the following:



Once we click on the **Open** button it will allow us to select our mpeg4 encoded video:

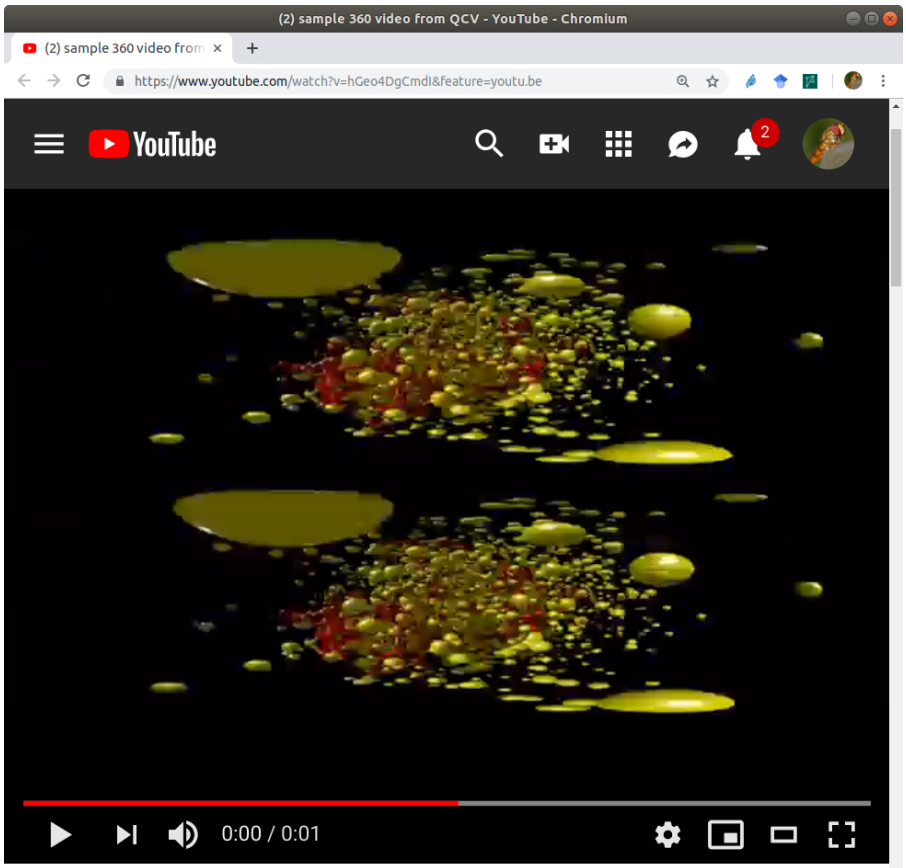


After selecting the video, we should be able to select both options for the stereoscopic 360 video and click on the **Inject metadata** button creating a new file (in this case movie1_injected.mov).



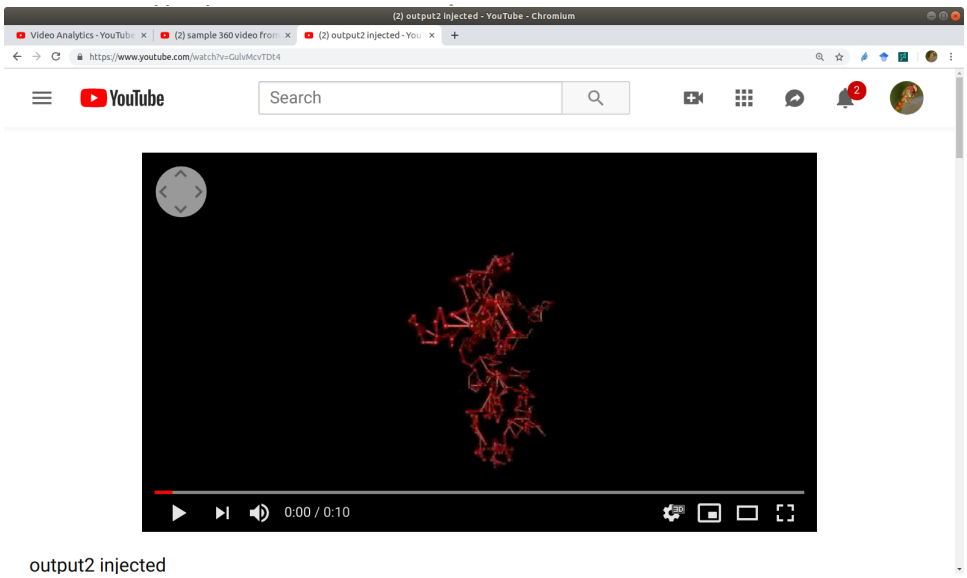
After this process is done, we can head to the upload screen on youtube and upload the video. After uploading the video will be viewable in the 360 mode. It should be noted that it may take a few moments before the movie is fully processed by youtube, and during that time the video may not be properly recognized as spherical, as shown in the screenshot below:

Once the processing is over, the video will be visible in the 360 version of youtube browser allowing for tilting the view and other “3D” options as shown below:



sample 360 video from QCV

Unlisted

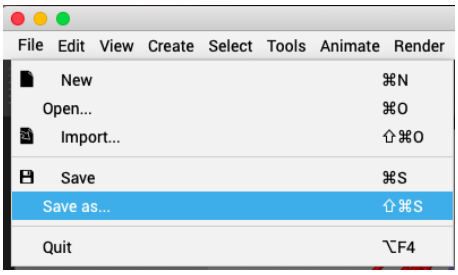


output2 injected

The same video viewed in the VR capable browser, such as a cellphone with a gyro sensor or a VR headset will be automatically presented in the stereoscopic view.

Saving the project

QCV program allows you to save and later open all settings and changes applied by you. In order to save session, choose **File → Save as…**, next choose appropriate path and filename and enter **OK**. My project is called chr2_polII.qcs and is available in the **Tutorial** folder. You should remember that if you download my chr2_polII.qcs file, you should change paths to chr2_polII.pdb.gz, chr2_movie.png and chr2_polII.xvg files.



In order to open saved session choose **File → Open**, choose file with QCV session and enter **OK**.