RESULT ANALYSIS

Here we will test to build several macro-complexes using our program. We propose a set of macro-complexes which differ in structure and function. All the files can be found in the Examples folder (github)

We will follow the next schema of colors when showing pdb images:

Original PDB: **Light Brown** Modelled Macrocomplex: **Light Blue**

Example Structure

The complexes were delivered from the python professor. We found that a very similar macro-complex is found in the PDB 1EZM.

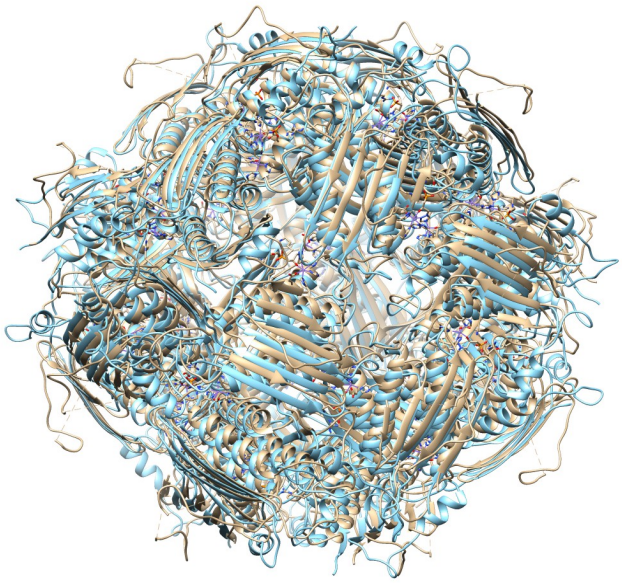


Image 1. PDB 1EZM (light brown) superposed with the Model output (light blue)

We saw that all the chains were placed correctly, acording to the existing model.

The output model was submitted into a minimization process. A minimized PDB was obtained.

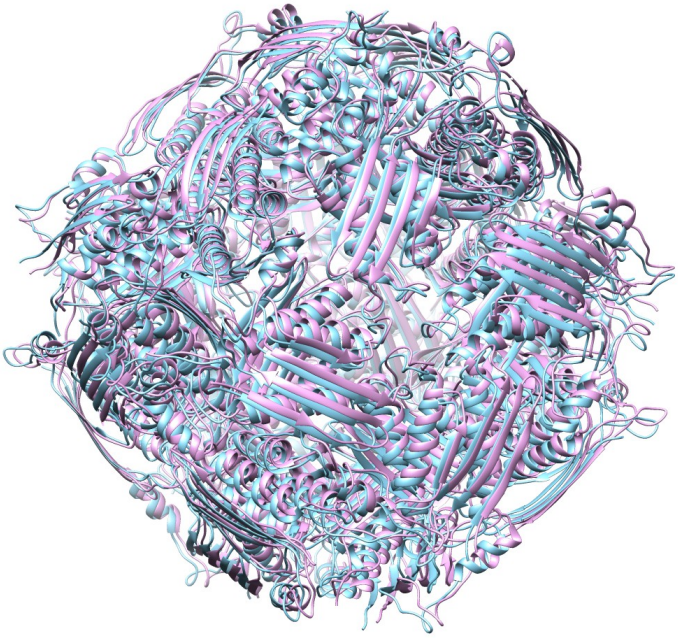


Image 2. Model output (light blue) superposed with the minimized its minimized structure (light purple)

In the image we can see that there are minor changes looking at the ribbon structure. However there are changes in the side chains of both models. As an example, here you will see an image win which we can see how two residues are interacting through a H bond in the minimized structure, whereas in the non-minimized structure, the residues are further.

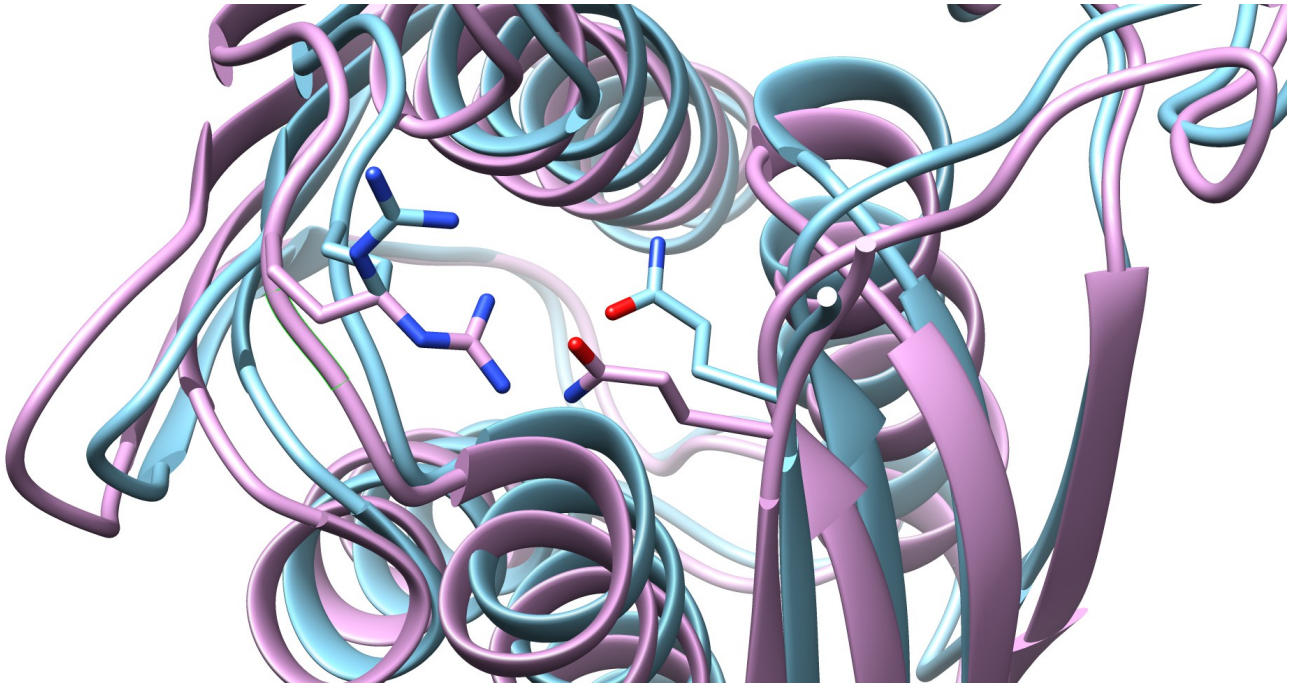
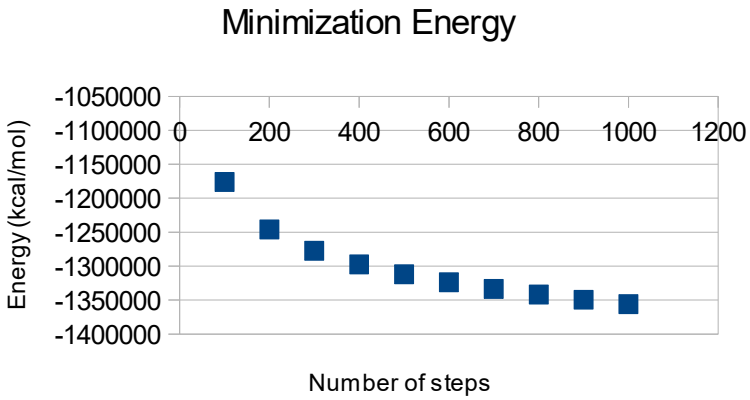


Image 3. In the minimized structure (light purple) we can see a H bond between GLN and ARG which can not be found in the non minimized structure.

Here we plot a graph, which shows how the total energy of the macrocomplex is getting lower through the minimization process (reaching stability). We could see a huge change in energy between the firsts steps. Those are not represented in the graph.

We will not perform the minimization procedure in the other examples.



ATP synthase

The macromolecular comples is a little bit more complicated to generate, due to the fact that the chains are not all identical. The PDB code for the template is 5ara.
Here we show 2 images of the template PDB structure and the model created.

Image 4. 5ara ATP synthase structure

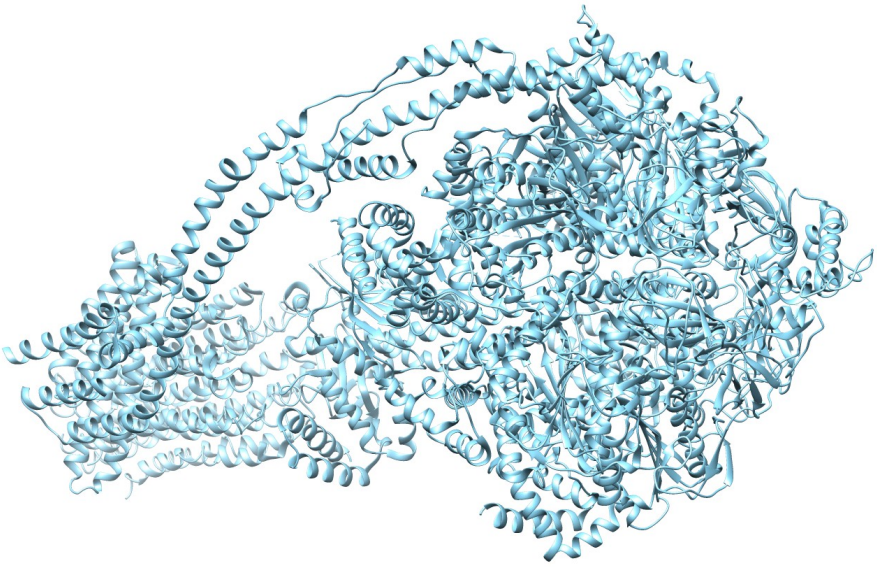


Image 5. Model generated by the program.

Both structures are identical. RMSD: 0.00 Angstroms

Nucleosome – PDB ID 3kuy

Here we find a DNA-Protein interaction. The programs models correctly the DNA-Protein system.

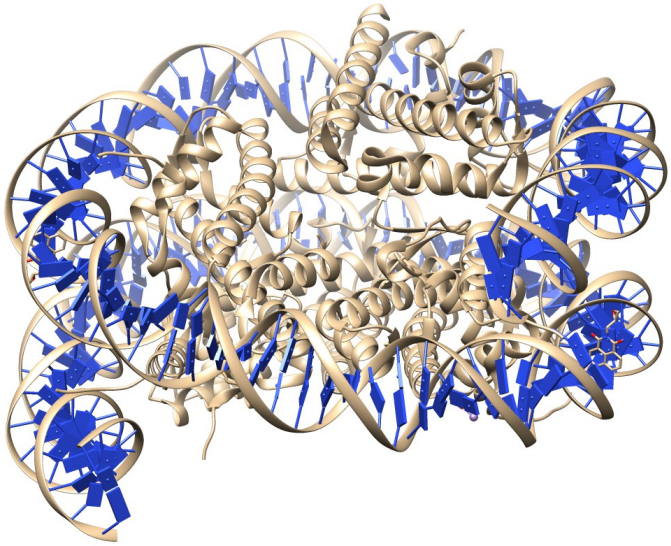


Image 6. Nucleosome PDB structure

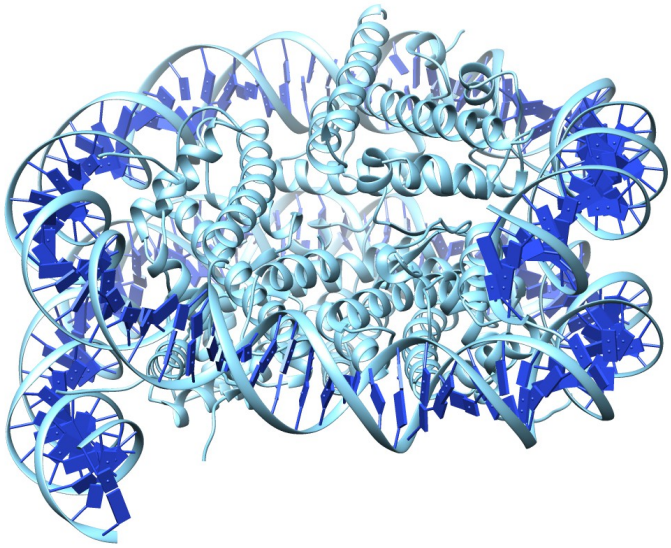


Image 7. Nucleosome modelled by the program

Ribosome – PDB code 1FJG

Here we test if the program is able to predict the macro-structure from a RNA-Prot system.
We had some problems defining this structure, and the number of possible clashes / chain was implemented in order to fully model this structure. There were atoms ina distance lower than 1.1 angstroms, and that is why we decided to add the number of possible clashes / chain threshole to 10.

Here we show the complete macro-complex modelled by our program, in which all the chains were correctly added.

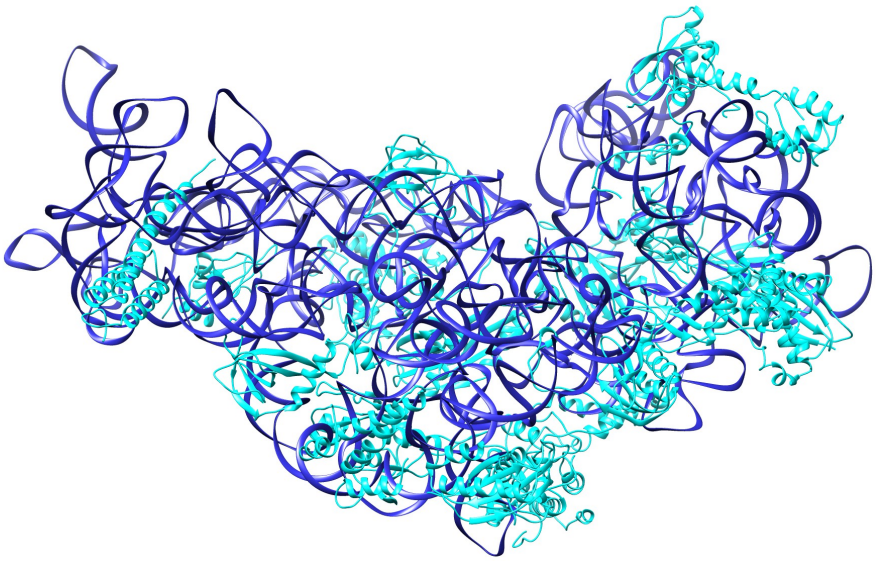


Image 8. Ribosome macro-complex. Models RNA-Prot interactions.

Virus capsid – PDB ID: 1JS9

The program can generate a big macro-complex from a few input complex delivered (if all the minimum interactions are defined). To show an example, here you can see all the inpus chains needed to create the capsid.

Image 9. Few viric chains required to build the macrocomplex

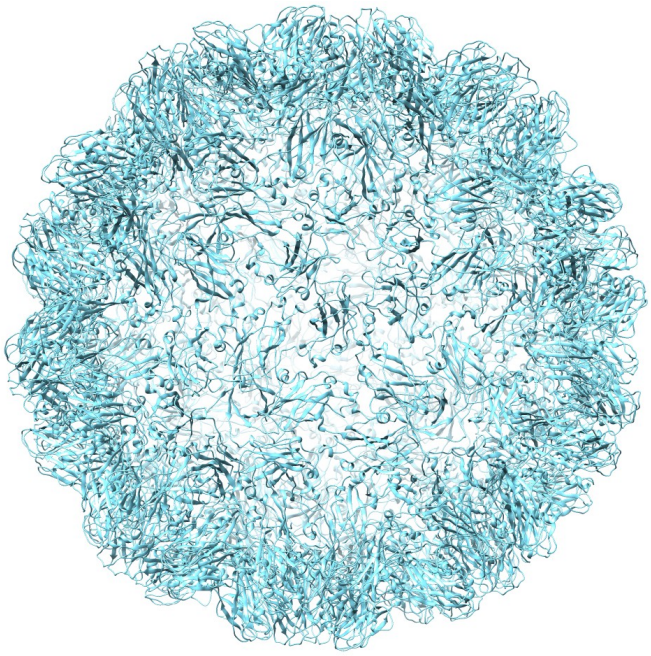


Image 10. Completed virus capsid (Output of the program)

The program is able to predict the full macro-complex structure. The user do not have to specify the needed numbers of chains in order to complete the macro-complex.

Virus capsid (Not well defined by user) – PDB ID 1QJZ

Here we show an example of a set of input chains which do not have all the minimum interactions to create the full complex. We will see how the program is not able to create the full structure.

Image 11. Bad defined input chains (do not define all the minimum interactions)

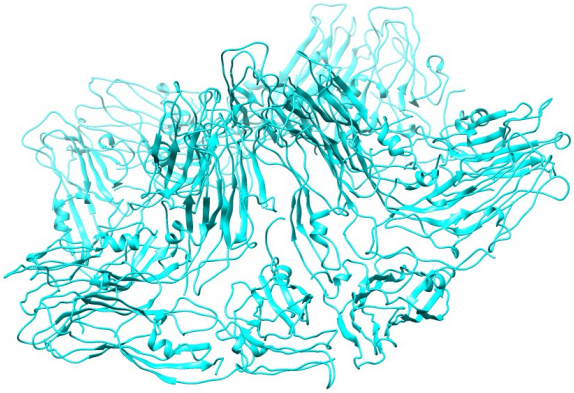


Image 12. Not fully finished structure. The input interactions were not enough to generate the full complex

Microtubule

We are dealing with an infinite macro-complex. The program default option is to only model 200 chains in order to stop loop sometime (the user can change that option).

We find out that the clash cut off distance for the creation of this especific macro-complex needed to be lower than 1.1 angstroms. The model was created successfully with a cut off of 0.8 angstroms. However we decided not to change the cut off distance to lower values becasue maybe other macro-complex may not be build properly.

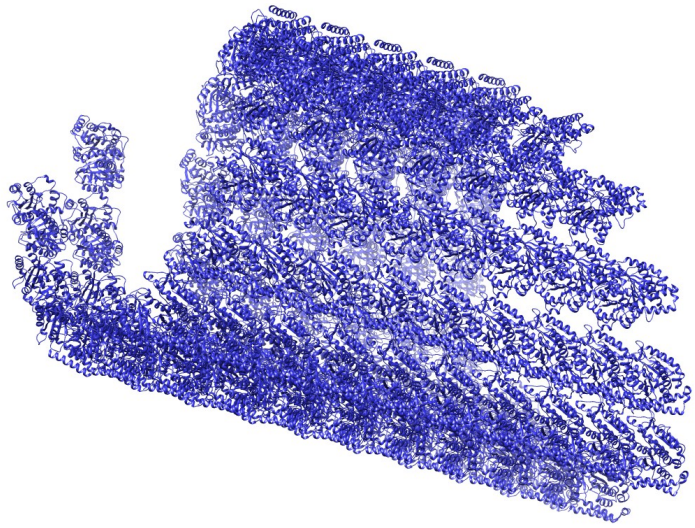


Image 13, Correct microtubule structure, perfromed with a clash cut off of 0,8 angstroms