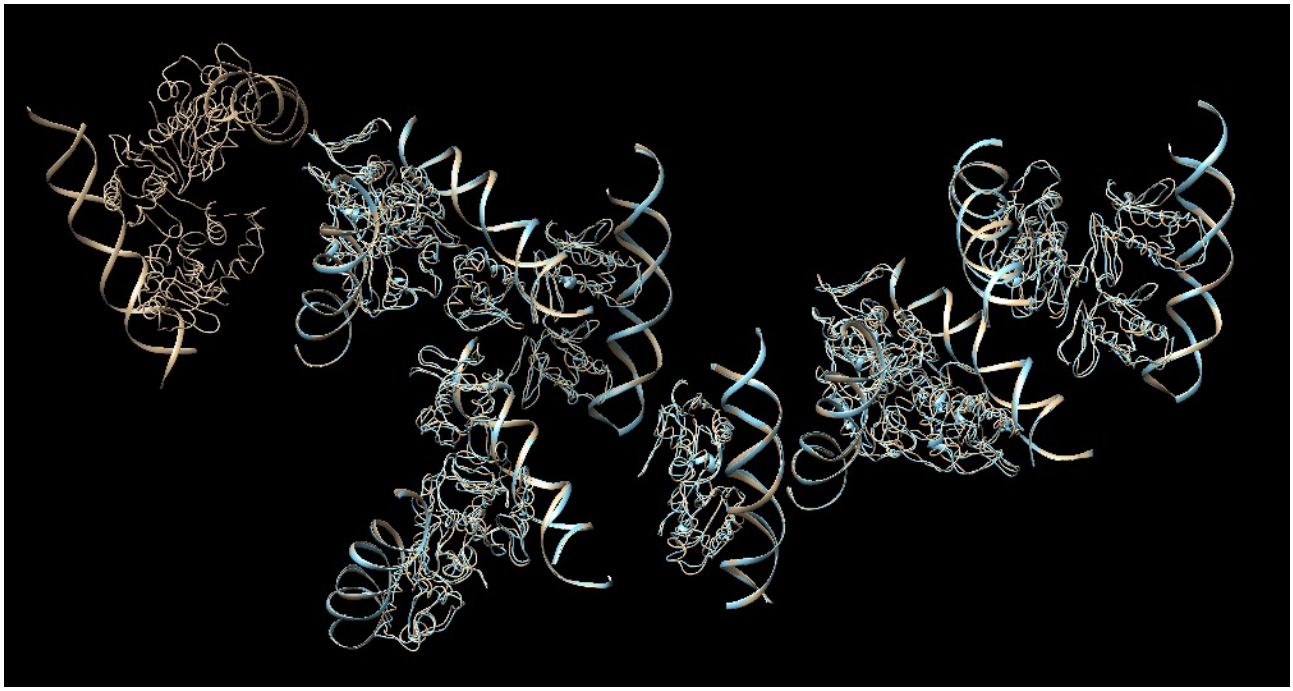
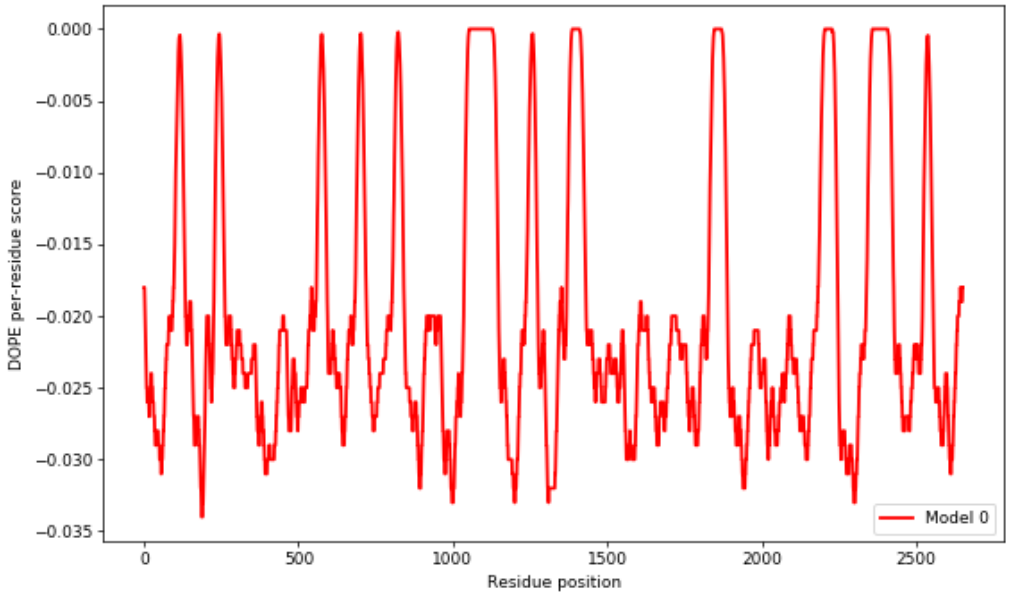
3t72



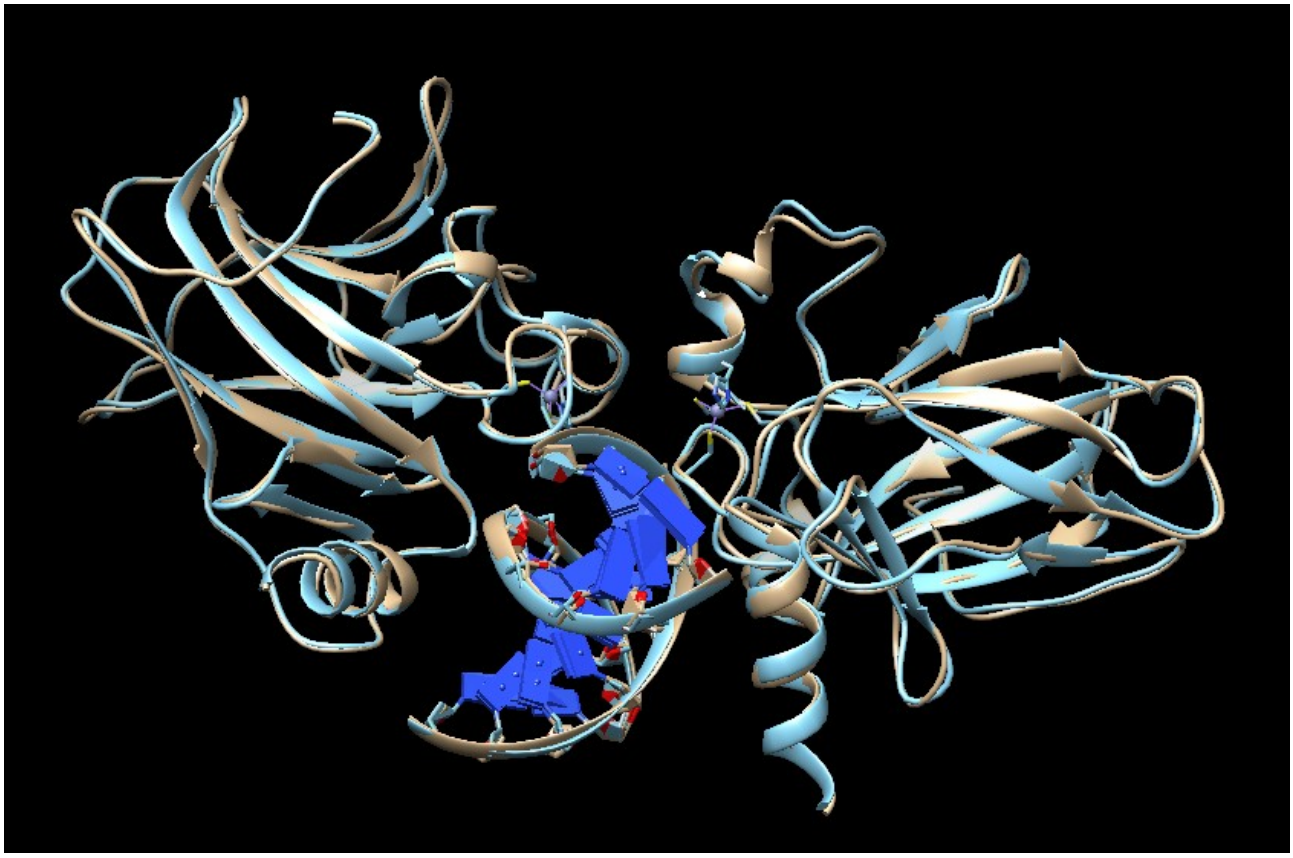
Single model obtained: Blue.
Using the pairs found in Examples/3t72, ComplexAssembler is capable of building the hole complex in 3t72 except for a small part with no clear connection with the rest of the complex.

After optimizing the final model, it computed the following energies using Modeller:



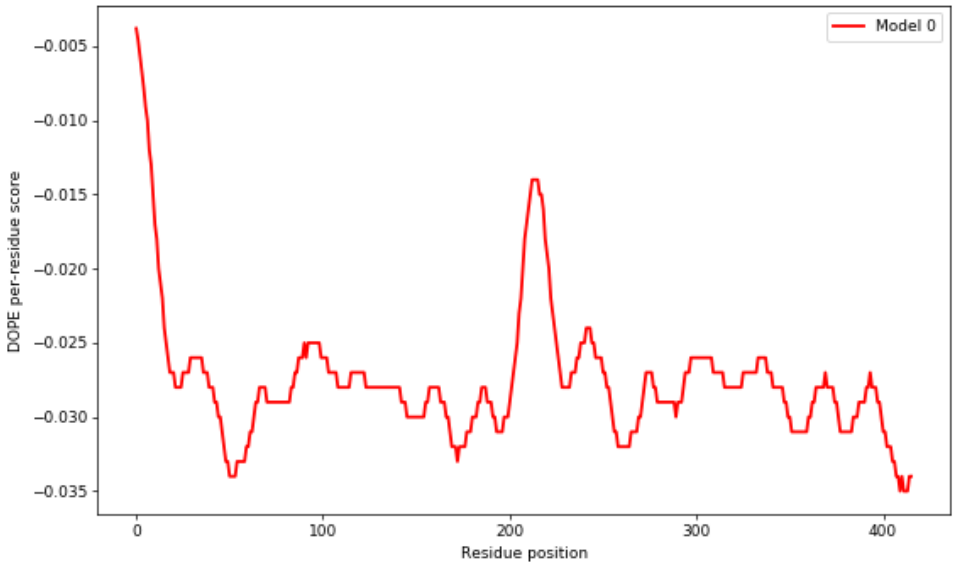
It is difficult to conclude anything from this results because some parts of the real complex are obviously missing (the double strands of DNA are not really that short).

4g83



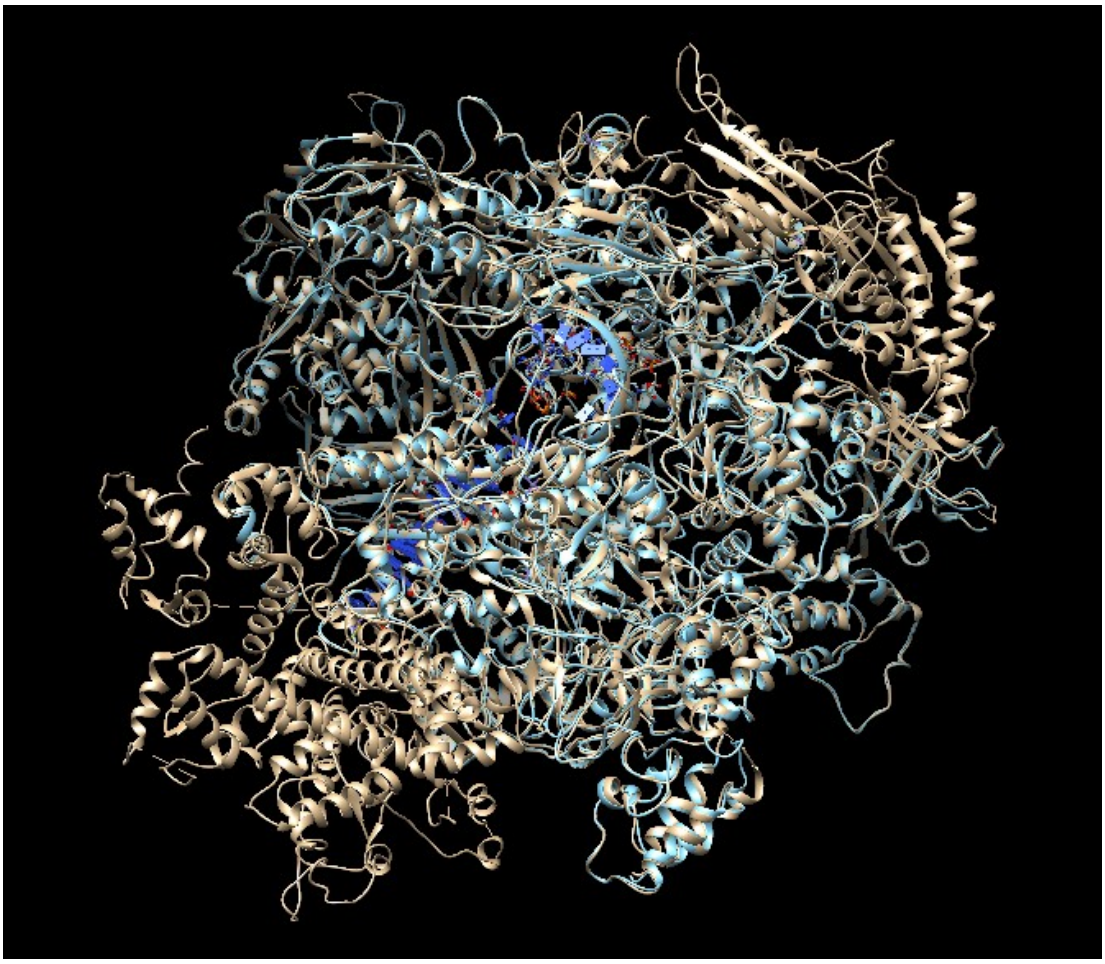
Single model obtained: Light blue

Using the pairs in Examples/4g83, the whole complex was perfectly reconstructed. Modeler optimization produced slight changes to the protein structure, most notably on the loops.



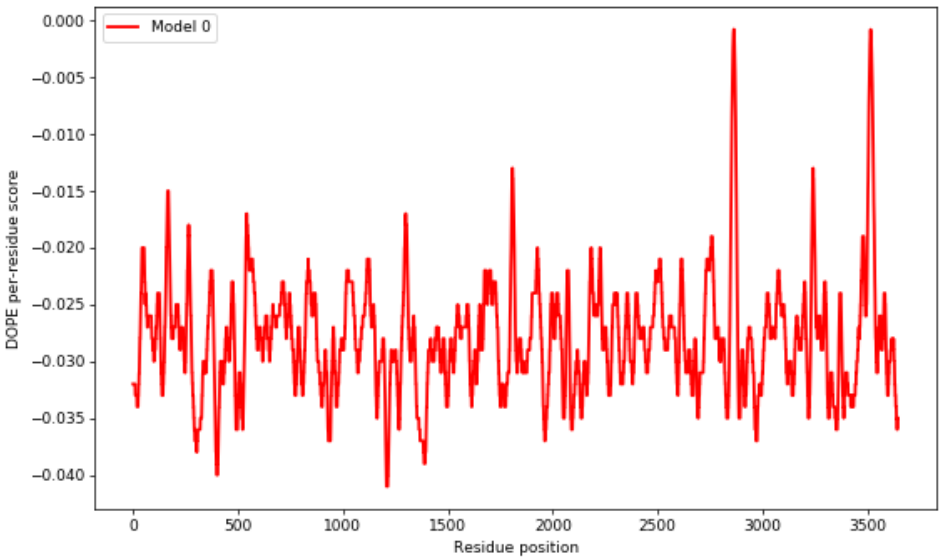
Overall the computed energy seems good, never getting to positive values.

5fj8



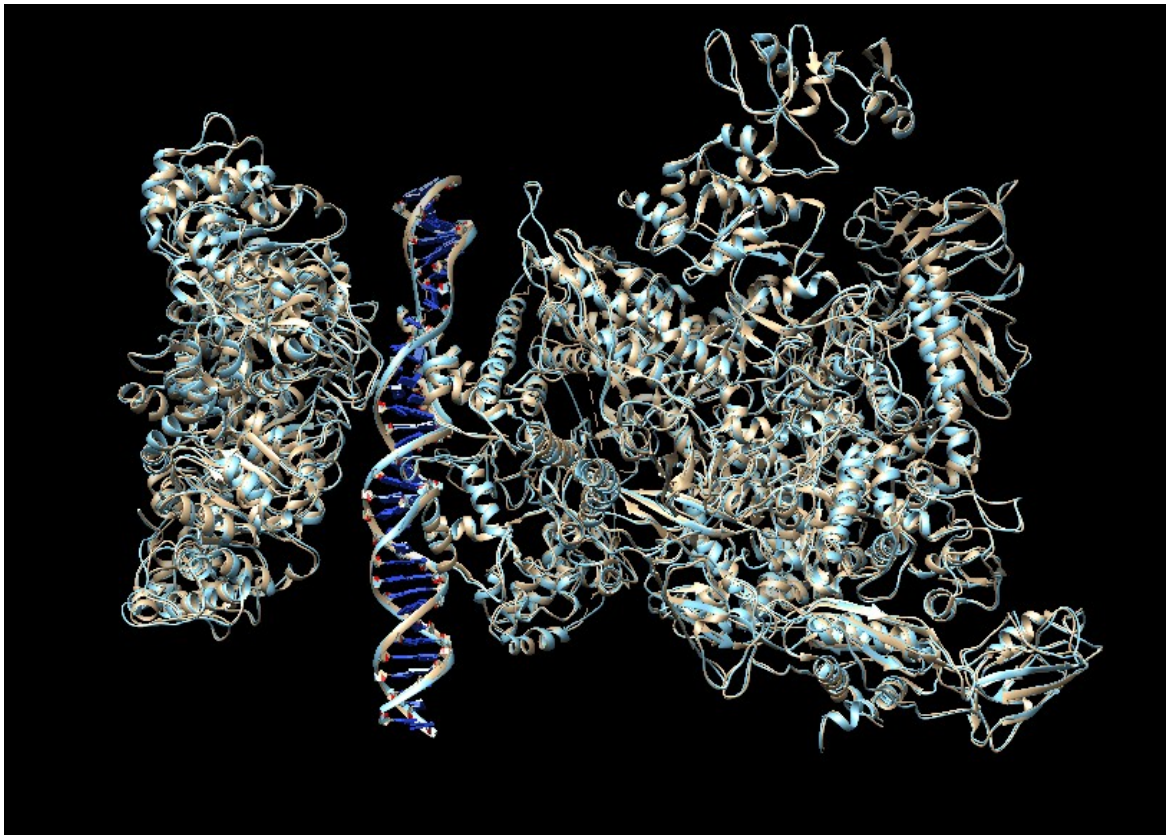
Single model obtained: Light blue

Using the pairs in Examples/5fj8, most of the complex was perfectly reconstructed.



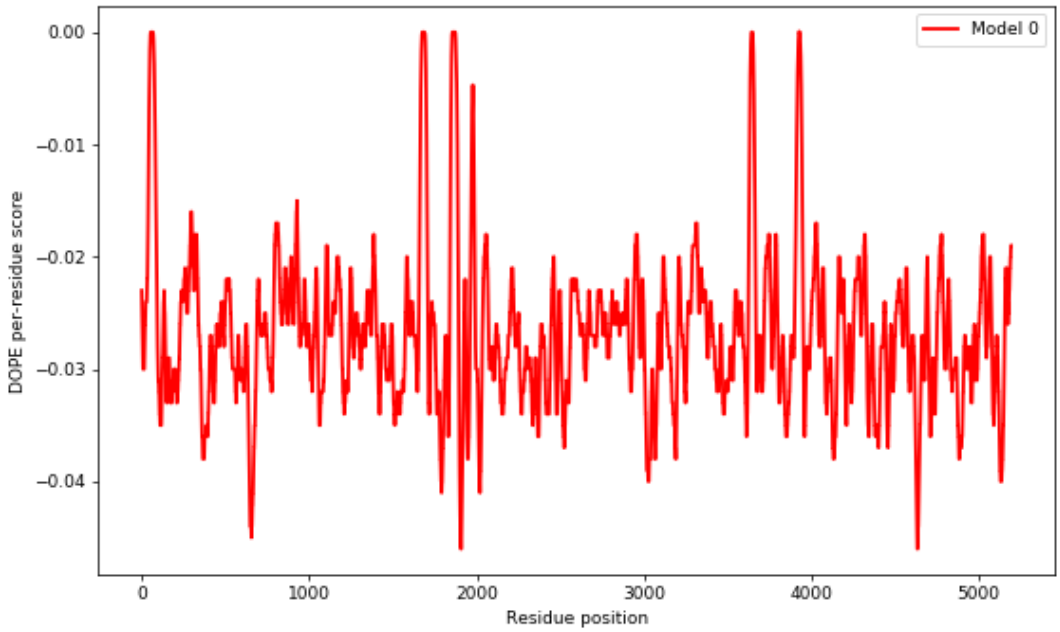
After optimization the energy obtained has 2 relatively highly energetic, maybe due to the missing parts.

5nss



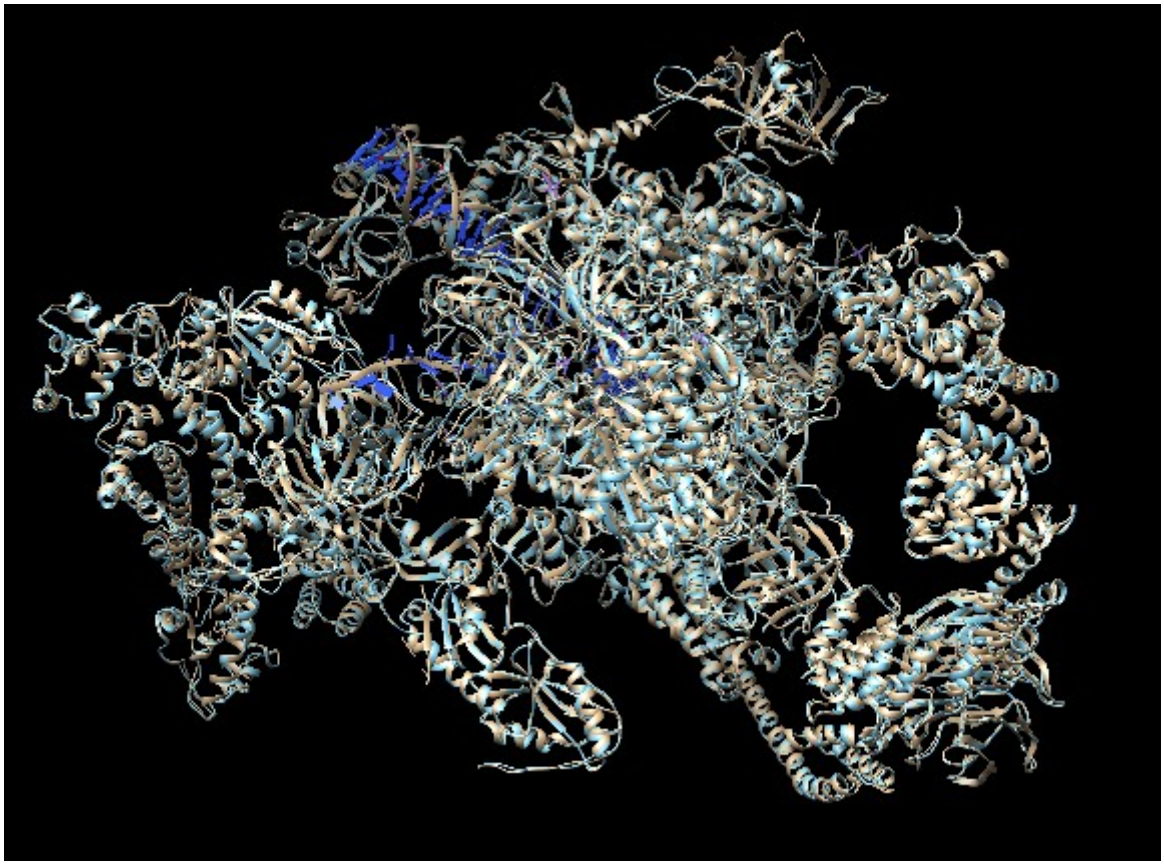
Single model obtained: Light blue

Using the pairs in Examples/5nns, the whole complex was perfectly reconstructed. Modeler optimization produced slight changes to the protein structure, most notably on the loops.



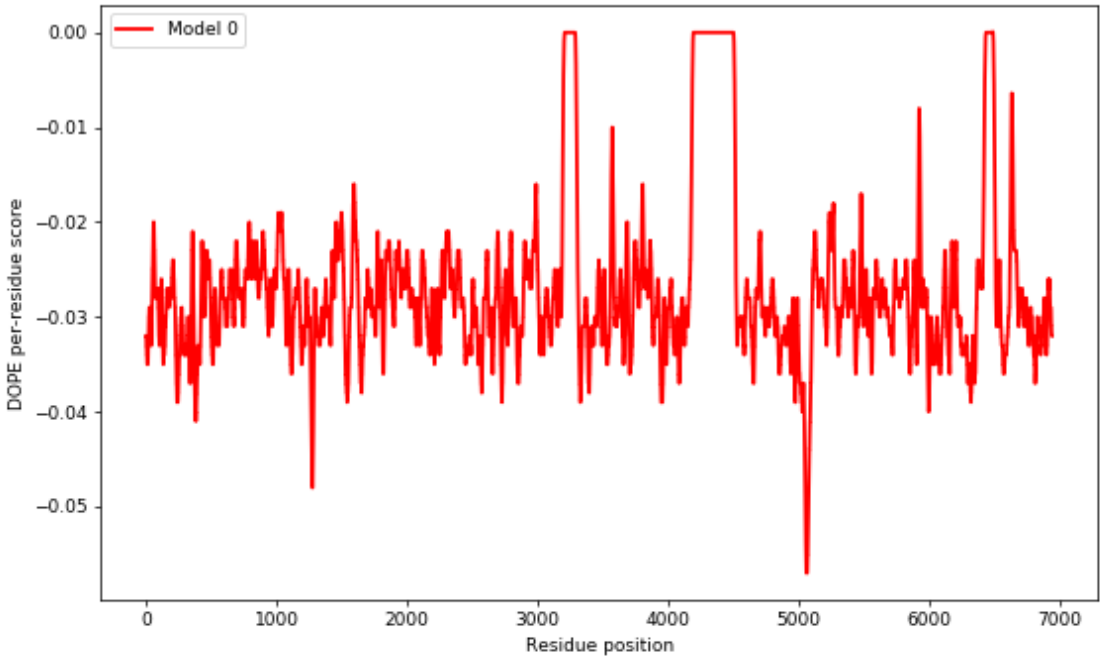
Surprisingly enough, after optimization this model still has relatively high energy regions.

6gmh



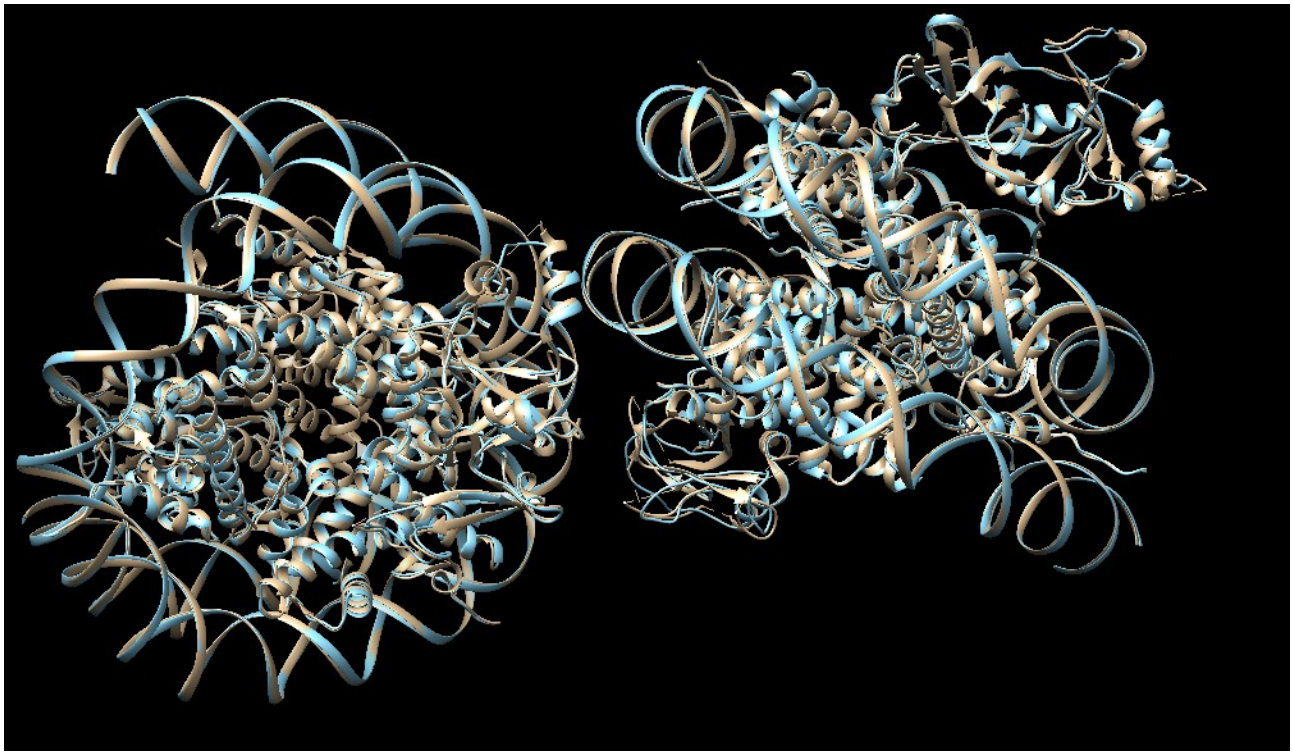
Single model obtained: Light blue

Using the pairs in Examples/6gmh, the whole complex was perfectly reconstructed except for one chain of DNA(because of missing interactions, possible in the real laboratory scenario). Modeler optimization produced slight changes to the protein structure, most notably on the loops.



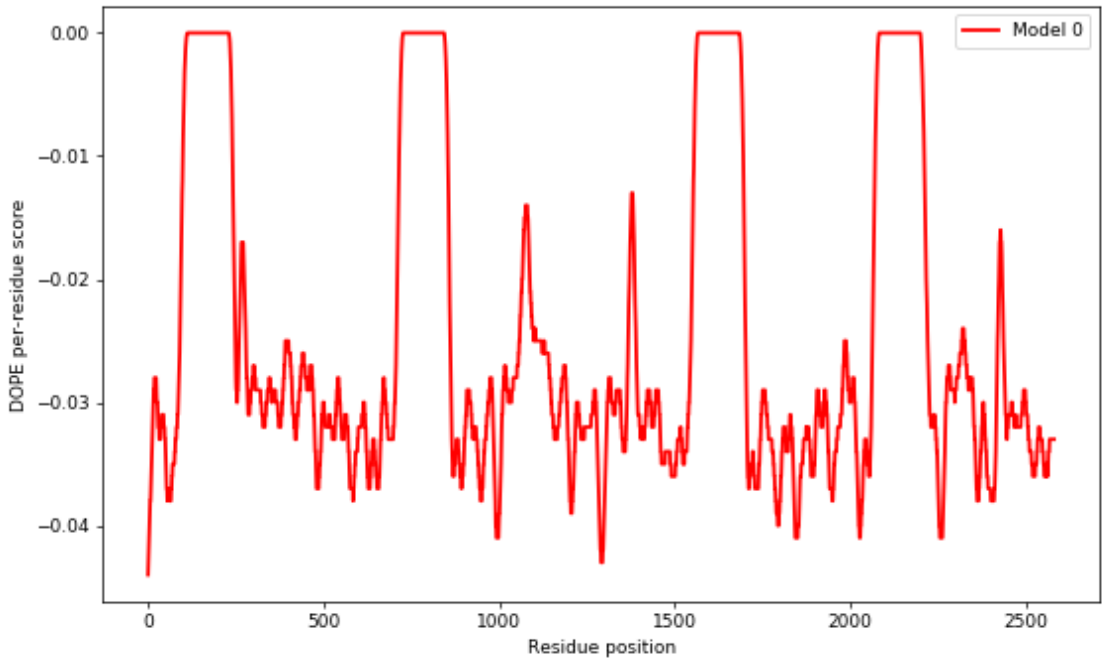
After optimization, we see a highly energetic region probably corresponding to the DNA, that is single-stranded.

6om3



Single model obtained: Light blue

Using the pairs in Examples/6om3, the whole complex was perfectly reconstructed. Modeler optimization produced slight changes to the protein structure, most notably on the loops.



After optimization some regions show a pour energy, maybe some conditions of the complex were not taken into account for the computation but important for this specific case. (as ph on the nucleolus being different.)

Remark: None of these examples generate more than a single model. In fact, when coding, we tried to take into account all the possible scenarios that could make our program give pour results, but none of those scenarios are given when splinting a PDB and reconstructing it. Probably on real live scenarios some of those cases would arise and our work on that aspect would shine brighter. Some of that work includes the possibility to generate multiple models if clashes found, the possibility of the same interaction to be given more than once on a complex and the rule of never assuming the first decision was right and using it to discard other possibilities (leading us to not use stoichiometry.).