Université Libre de Bruxelles

Biophysics II

BIOL-F-459

Task 1 - Analysis of the proteins

Authors:
Hélène Libion
Charlotte Nachtegael

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1 Structure quality of 3MQ1

The PDB structure was obtained by X-Ray crystallography. Its R-value, which is a measure of the quality of the model, is within the usual range with a value of 0.226. The R-value free, calculated by qualifying how well the 10% of experimental data excluded during the refinement of the model is predicted, is also quite close to the R-value at 0.279. The overall quality of the structure is good.

According to the Electronic Density Server, the best structure of all the chains of the proteins is the Chain A. Firstly, the Chain A present no outlier value for the electronic density of its amino acids, whereas all the other chains have at least one outlier (Fig 1). Secondly, despite the fact that Chain D and E have no outlier for the ψ and ϕ angle values of their amino acids, Chain A only has one amino acid with unusual values for its ϕ and ψ angle (Fig 2). This is why we consider Chain A as the chain with the best structure.

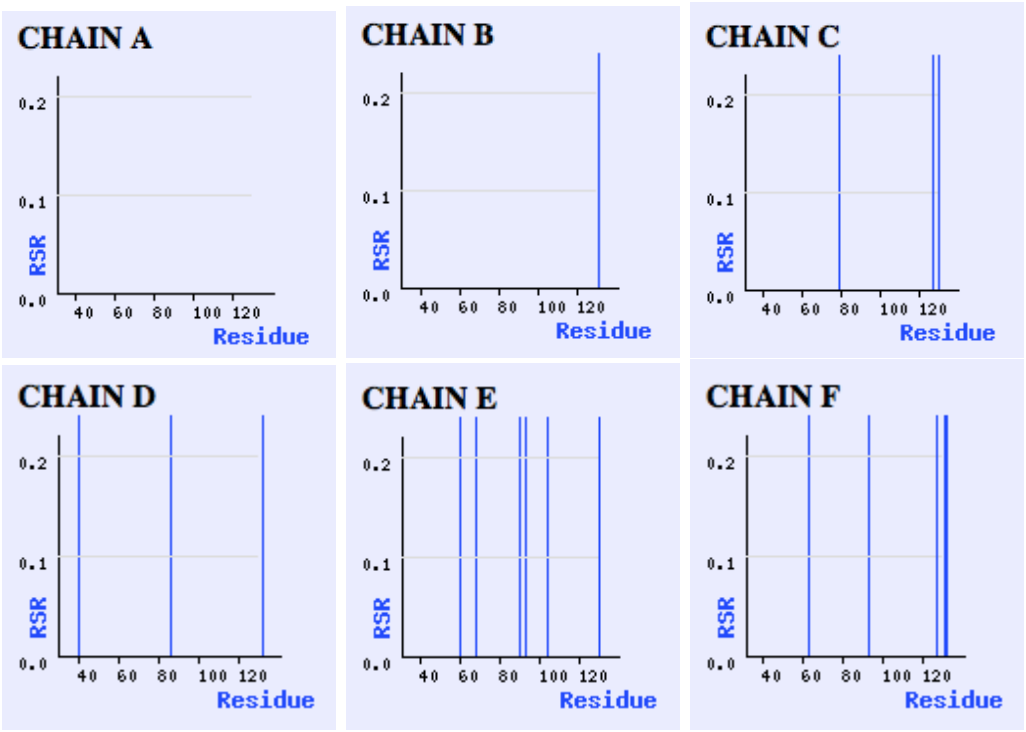

Figure 1: Representation of the amino acids with electronic density outside of the usual range of values.

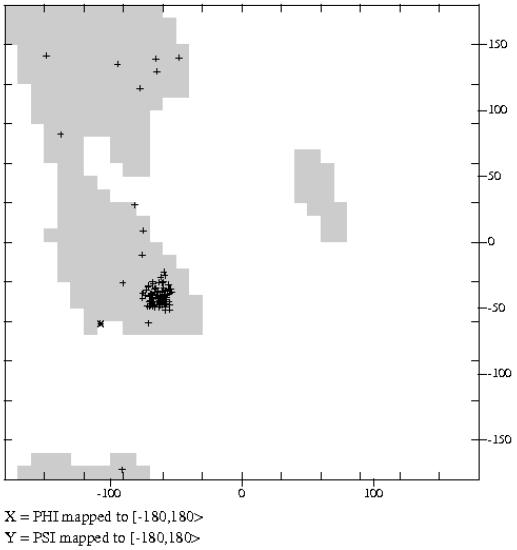

Figure 2: Ramachandran Plot for the chain A

2 Structural difference between a homodimer (Der p 5) and a monomer (Blo t 5)

The main structural difference observed here with *Pymol* is the position of one helix (see red in Fig 3). This helix in the homodimer is slightly crooked.

The position of the helix in Der p 5 could have stabilizing properties when Der p 5 binds with another Der p 5 protein. For example, it could favour specific interactions between amino acids contributing to the stabilization of the dimerization.

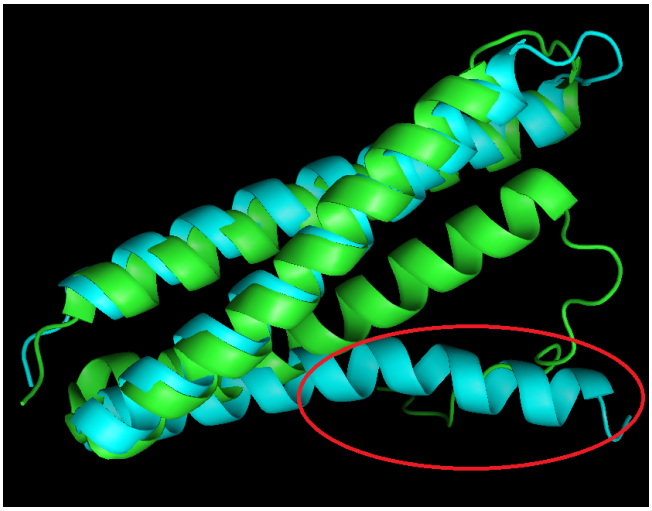

Figure 3: Superimposition of Der p 5 (blue) and Blo t 5 (green) by using *Pymol*

3 Residues of importance for the dimerization

The article underlines the hydrophobic interactions as stabilizing the dimerization in Der p 5 : $Met^{35} - Phe^{50}, Leu^{34} - Ile^{115}, Val^{84} - Gly^{88}$. These three interactions are found all across the protein (Fig 4). However, only one of these reactions ($Leu^{34} - Ile^{115}$) is found in the monomer Blo t 5, implying that the potential homodimer formed with Blo t 5 would not be stable due to the lack of these hydrophobic interactions.

We thought we would find these interactions mainly in the helix structurally different found in the previous point. Surprisingly, only three of six residues involved in these hydrophobic interactions are found in this specific helix.

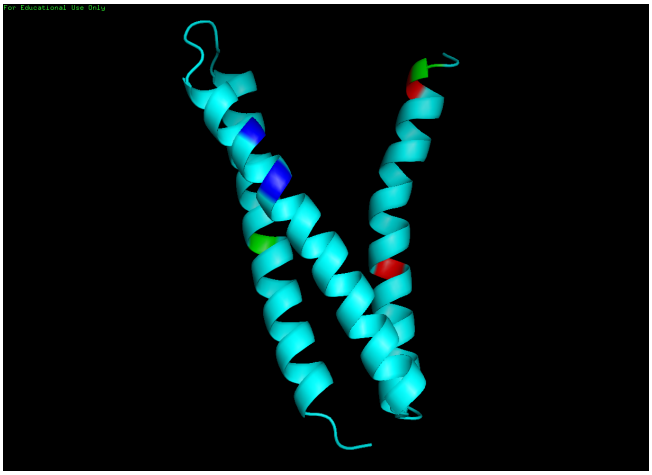

Figure 4: 3D representation of Der p 5 (light blue) on *Pymol*, with the three pairs of residues involved in the hydrophobic interactions highlighted in colors (red, dark blue and green)