| *Name* | *Surname* | *ID* |
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## Midterm test No. 1

### 28 / 03 / 2022

Please answer all questions below and submit this document in **PDF format** by **12:30 - 11 April 2022** (two weeks after) to **damiano.piovesan@unipd.it**.

Each student is assigned a different **protein structure (PDB ID)**. The entire exercise is based on the analysis of that structure. Please add your **name**, **surname**, **university ID** and **email** in the **assignment file** here which contains a list of PDB IDs. **Assignment file** [**here**](https://docs.google.com/spreadsheets/d/1JexKhGl-g_UV3n0gkncbXQwkc-C4sAUCeXMZTIUXo2E/edit?usp=sharing)

## Questions

Answer the following questions concisely (**max 500 words in total**).

1. What is the difference between an ionic bond and a covalent bond?
2. What is the difference between a weak and strong acid?
3. What is the isoelectric point of a protein?
4. What is the “native conformation” of a protein?
5. What is the difference between the asymmetric unit and the biological entity of a PDB structure?
6. What are “missing residues” in a PDB structure?

Download the assigned PDB structure and create a new file removing non relevant chains (if it is a complex), solvent molecules and cofactors. For each question **concisely explain all passages** **(max 5 rows)** necessary to reproduce the results (e.g. parameters, database queries, algorithms, etc.). Optionally, if relevant, you can provide source code (not necessary).

1. Plot a heatmap representing distances between beta-carbons (CB), consider alpha-carbons when the CB is missing, i.e. for proline. Provide residue indexes along the axes.
2. Plot the contacts map from the matrix above considering a distance threshold of 5 Å.
3. Report the number of residues in contacts for different ranges of sequence separation. Consider the following intervals [0,6], [7,12] and [13,24] and [25,∞].
4. Generate the Ramachandran plot of your protein.
5. How many residues are Ramachandran outliers? Consider the Ramachandran regions as shown during the practicals.