* ***Now you have an idea of what a protein is. You know it has primary structure, secondary structure, tertiary structure and quaternary structure.***
* ***As we render the 3D structure of the protein, what information can we obtain?***

Remarks:

* No more than 100 words per answer!!!
* Use your own words or drawings to answer the questions
* Insert picture(s) in the space provided for hand-drawn figures (either pictures of pencil-and-paper drawings or digital drawings are ok)
* Submit the e-copy of your answer via electronic means

**2. From 2D to 3D: interpretation of 3D molecular models**

**2.1. 3D representations of protein structure**

*Recommend readings:*

<https://bio.libretexts.org/Bookshelves/Biochemistry/Fundamentals_of_Biochemistry_(LibreTexts)/01%3A_Unit_I-_Structure_and_Catalysis/04%3A_The_Three-Dimensional_Structure_of_Proteins/4.11%3A_Biomolecular_Visualization_-_Conceptions_and_Misconceptions>

Refer to the following figure to answer Q2.1.1-2.1.2:

|  |  |
| --- | --- |
|  |  |

|  |  |
| --- | --- |
| Q2.1.1 | What is the type of interaction represented by the dashed lines? Count the number of that interaction between the ligand’s adenine ring and the protein.  (hint: what is the structure of an adenine? Refer to the previous handout!) |
| Ans |  |
| Q2.1.2 | Name the four amino acid residues colored in green (ignore the repeated one). (hint: refer to amino acid structures from the previous material) |
| Ans |  |

**2.2. Protein-ligand binding**

Recommended readings:

<https://en.wikipedia.org/wiki/Protein%E2%80%93ligand_complex>

For questions 2.2.1-2.2.2, open this link <https://durrantlab.pitt.edu/binana/> in browser and click “use example files”.

|  |  |
| --- | --- |
| Q2.2.1 | Referring to the legend below the molecular viewer, give one example of each of the detected protein-ligand interactions. Hover your mouse onto the residue to see their name if you need. The pi-pi interaction is used as an example. |
| Ans | |  |  | | --- | --- | | **pi-pi stacking** | between the protein’s Phe209 and the ligand’s adenine ring | | **Hydrogen bond** |  | | **Salt bridge** |  | |
| Q2.2.2 | In the molecular viewer, click “surface”. Can you see how the ligand’s shape complementary to the binding site? Put a screenshot of this representation in the answer here. |
| Ans |  |