

Functional Specifications

1. Background

Proteins are essential to biological functions, interacting with other proteins, nucleic acids, and organic molecules. Understanding and visualizing protein structures and interactions facilitates a mechanistic understanding of their roles and has applications across fields such as protein engineering and disease treatment. However, current platforms used to achieve this such as PyMOL are complex and require a steep learning curve, making them challenging for students and scientists new to structural biology.

This project aims to develop a Python package for straightforward protein structure visualization. The primary goal of this package is to enable users to load and visualize protein structures in 2D and 3D from PDB files in a user-friendly manner. It will focus on basic visualization and capabilities for highlighting and viewing specific features (e.g. amino acid residues). This package will provide an accessible foundation for protein structure visualization, serving as a stepping stone for more advanced tools such as PyMOL.

2. User Profile

This package is designed for users with a foundational understanding of protein structures and molecular features who are interested in basic 2D and 3D visualization but have minimal programming experience and prefer to avoid complex software. The tool is aimed at those who do not require extensive analysis features but want a simple and accessible visualization solution.

Users will need to be able to follow instructions to download the package via the terminal using pip install. They should also have access to PDB files and be comfortable calling basic Python functions provided in the package to perform visualizations.

3. Use Cases

- a) The user would load a PDB file which will then parse the protein data into a data object.
- b) The user would choose to view the protein's primary structure which will then display the linear sequence of amino acids in a 2D diagram.
- c) The user would choose to view the protein's 3D structure which will then render the full 3D structure, displaying all atoms and bonds in 3D space.