

## **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 and CAVER are complex or highly specific to a specific visualization feature (e.g. tunnel or channels within protein structures). Thus, these programs have a steep learning curve and are challenging to use 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 3D from PDB files through a user-friendly graphical user interface (GUI). Here, users can visualize the PDB file of interest as either: 1) 3D atom point cloud or 2) 3D backbone graph. The user is then able to highlight, rotate and view specific amino acid residues and atom coordinates. Ultimately, 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 3D visualization of proteins 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 using a GUI to perform visualizations. No other Python skills should be required to utilize this package.

### **3. Use Cases**

- a) The user would load a PDB file into the GUI which will then parse the protein data into a Pandas DataFrame object and further processed to produce an object suitable for use with the Graphein visualization package.
- b) The user would choose to view the protein's atom point cloud graph which will then display the 3D atom point cloud graph in the user's default browser.
- c) The user would choose to view the protein's 3D backbone graph will then display the 3D backbone graph in the user's default browser.