

QAMP Checkpoint 2

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This project has been a difficult learning curve for me since I originally had no experience with the protein folding problem. As a result, I have spent a significant amount of time learning about protein folding in general, familiarizing myself with the IBM scientist's paper describing their algorithm, understanding the Qiskit Nature implementation, and going through with the existing demonstration code. I originally focused on getting the demonstration code working since it is the basis of the tasks that I will be working on during this project. This was helpful in understanding what the initial goal is by showing examples of real output for the "xyz" file generation task. My visual is actually an example output of what the xyz file data would look like once it is plotted on a three dimensional axis. The protein shown in the example is a 7 amino acid main chain with no side chain. I am still working on extracting the main chain of the protein from the code in Qiskit Nature. Once I have that, I will be able to use the predict structure encoded in the result to compute a set of x, y, and z coordinates of each amino acid. The next step will be to generate a three dimensional visualization like the one attached but more sophisticated.