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# RMSD Calculations for Comparing Protein Three-Dimensional Structures

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**Abstract.** The root Mean Square Deviation (*RMSD*) is a popular measure of structural similarity between protein structures in the field of bioinformatics. The *RMSD* calculations involve alignment and optimal superposition between matched pairs of atoms, searching for the lowest *RMSD* result for both structures. Among the popular methods for calculating the optimal rotation matrix that minimizes the *RMSD* are the Kabsch algorithm and the Quaternion algorithm. The aim of this research is to present a simple tool for calculation of the *RMSD* between pairs of aligned three dimensional structures by applying the methods mentioned above. As an implementation language the object-oriented C# programming language has been chosen.

**Keywords:** computer modelling · Root Mean Square Deviation (*RMSD*) · Protein sequences · C # programming language

## 1 Introduction

In the field of bioinformatics, the molecular structure alignment is the matching between two or more macromolecular structures based on the optimal superposition of their shape and three-dimensional (3D) conformation. A protein is usually compared to other proteins. It is useful for better understanding of their properties. Proteins with similar amino acid sequences or 3D structures are found to be evolutionary related and have similar functions, see [1–4]. An important topic in structural bioinformatics and computational chemistry is the analysis of protein sequences and their biological functions. Also important is the assessment of the protein structural similarities. These studies find wide application in both protein structure prediction and drug design, homology modeling approaches and even more. The difference between two conformations of molecules is most commonly measured by calculating the Root Mean Square Deviation (*RMSD*) which is the sum of the squares of the distances between the equivalent atom pairs. It is important to find the minimal value of *RMSD*. The main problem

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