Acta Scientific Biotechnology

Volume 2 Issue 6 September 2021

Review Article

The Structure of Globular Proteins with Accompanied Spiral Structures Parallel and Antiparallel Amino Acid Residues

Gennadiy Vladimirovich Zhizhin*

Russian Academy of Natural Sciences, St. Petersburg, Russia

***Corresponding Author:** Gennadiy Vladimirovich Zhizhin, Russian Academy of Natural Sciences, St. Petersburg, Russia.

Received: August 07, 2021

Published: August 10, 2021

Abstract

Using the theory of polytopic prismahedrons [1-4], the structure of complete filling (partitioning) of the space of globular proteins with residues of amino acid molecules, accompanied by the formation of various conformations of fibrillar proteins: spirals of structures with parallel and antiparallel amino acid residues, is investigated. Since the residue of an amino acid is geometrically an object of dimension 4 (a tetrahedron with a center), the structure of a globular protein is modeled by a set of connected tetrahedrons with a center, which form a space of the highest dimension. Examples of the thus obtained native structures of the highest dimension that simulate the structure of globular proteins are given.

Keywords: Amino Acid; Polytopic Prismahedrons; Enzymes, Hemoglobin

Introduction

Globular proteins are compact globules that include chains, helices, sheets, and individual amino acid molecules. Globular proteins include the most important biological formations necessary for the functioning of living organisms (enzymes, hemoglobin, immunoglobulin, etc.). They are extremely complex so that until now their detailed structure remains unknown, although data on the presence of various conformations of amino acid compounds [5-8] in them has been accumulated about many proteins. However, a description of the entire set of residues of amino acid molecules entering the globule meets significant difficulties. At the same time, it became known that any disturbances in the dense packing of amino acid molecules lead to the loss of functionality of the globular protein and even to its destruction [5,8].

It should be noted that when describing the structure of globular proteins, they are traditionally considered three-dimensional. However, as shown, for example, in [1,3], the molecules of almost all chemical compounds have the highest dimension. This certainly applies to the residues of amino acid molecules and their compounds. Therefore, in this work, the native structure of globular proteins is considered in the space of the highest dimension. The appeal to the space of the highest dimension reflects the nature of matter and allows you to establish a hidden order in the nanoworld. This was the case when establishing translational symmetry in quasicrystals [9,10] and establishing the order of interaction of nucleic acids [11,12].

Native structure of globular proteins with parallel and antiparallel arrangement of amino acid residues, and α - spirals

When analyzing the structure of globular proteins, the task is to continuously fill a certain finite volume (globules) with amino acid molecules. To solve this problem, one should turn to the theory of normal decomposition of n-dimensional spaces [1-4]. This theory

is based on the concept of polytopic prismahedron, that is, prisms, the bases of which are some polytopes of the highest dimension. It is proved that it is precisely the polytopic prismahedrons that provide the possibility of solving the 18th problem of Hilbert [13] on the construction of n-dimensional spaces using congruent figures, which was introduced 120 years ago. A polytopic prismahedron is the product of an arbitrary polytope by geometric elements of various dimensions (one-dimensional segment, triangle, tetrahedron, etc.). The basis for applying the theory of polytopic prismahedrons to the analysis of the native structure of globular proteins is the idea that the amino acid molecule of which the globule mainly consists, from a geometric point of view, is a tetrahedron with a center (Figure 1). At the vertices of the tetrahedron are located an amino group -NH_2, a hydrogen atom, a carboxyl group -OH and a functional group R having a different composition depending on the amino acid in question. In the center of the tetrahedron is a carbon atom (denoted as α-carbon). The carbon atom in the center of the tetrahedron is bonded to the vertices by a covalent chemical bond. These links are indicated by red dashed lines.

Figure 1: Molecules of amino acid.

The black solid lines in figure 1, connecting the vertices, are the edges of the tetrahedron, they define the geometric shape of the tetrahedron. Amino acid molecules can be linked to each other by a covalent bond, whereby the hydrogen atom H of the amino group of one amino acid molecule combines with a hydroxyl group OH from the carboxyl group of another amino acid molecule, with the elimination of a water molecule. The dimension of such a polyhedron can be determined by the Euler-Poincaré [14]:

$$\sum_{i=0}^{n-1}(-1)^i f_i(n) = N = 1+(-1)^{n-1}, \text{ --------(1)}$$

In (1) $f_i(n)$ is the number of elements of a polytope P of dimension n having dimension i.

From figure 1 it follows that the number of vertices of the tetrahedron with center is 5, the number of edges is 10, the number of two-dimensional faces is 10, the number of three-dimensional faces is 5. In this case $f_0 = 5, f_1 = 10, f_2 = 10, f_3 = 5.$

Substituting the obtained values $f_i, i = 0 \div 3$ into equation (1), we obtain,

5 - 10 + 10 - 5 = 0.

Thus, Euler-Poincaré's equation for a tetrahedron with a center holds for n = 4. This proves that a tetrahedron with a center (amino acid molecule) has dimension 4.

It is known that the residues of amino acid molecules (after the cleavage of water molecules) can be located in a protein in a parallel position. Two such residues, considered together, form a polytopic prismahedron with dimension 5 [6-8]. Two tetrahedrons centered in the antiparallel position form a cross-polytope of dimensions 5 [2,11]. In order to describe the **α** -helices existing in the native structure of proteins with the help of tetrahedra with a center, in addition to parallel and antiparallel tetrahedra with a center, it is necessary to have an intermediate state of a tetrahedron with a center between the two indicated states. It can be obtained by rotating each edge of the tetrahedron centered at 90 degrees, since the antiparallel state to this state is obtained by rotating each edge of the tetrahedron centered at 180 degrees.

Each of the polytopes, consisting of two tetrahedra with a center, rotated relative to each other by 90 degrees, have dimension 5. Indeed, let us denote by integers the vertices of any of these polytopes (Figure 2).

The polytope in figure 2 is not a prismahedron, since the lines connecting the vertices of the two tetrahedra in it are not parallel to each other. This polytope can be called a self-orthogonal polytope. Its dimension can be determined by equation (1). In this polytope the number of vertices is 10, the number of edges is 22: 1 - 2, 1 - 4,

Figure 2: Polytope, consisting of two tetrahedra with the center, rotated relative to each other by 90 degrees.

1 - 3, 1 - 5, 2 - 5, 2 - 4, 2 - 3, 3 - 4, 3 - 5, 3 - 10, 4 - 5, 5 - 6, 6 - 10, 6 - 9, 6 - 8, 6 - 7, 7 - 8, 7 - 9, 7 - 10, 8 - 9, 8 - 10, 10 - 9; the number of two-dimensional faces is 22: 1 - 5 - 3, 1 - 2 - 3, 1 - 2 - 5, 1 - 4 - 5, 1 - 2 - 4, 1 - 3 - 5, 2 - 4 - 5, 2 - 3 - 5, 2 - 3 - 4, 3 - 4 - 5, 3 - 5 - 10 - 6, 2 - 3 - 9 - 10, 7 - 9 - 10, 7 - 10 - 8, 7 - 6 - 8, 7 - 6 - 10, 7 - 9 - 6, 6 - 8 - 10, 6 - 8 - 9, 8 - 9 - 10, 6 - 9 - 10, 2 - 5 - 9 - 6; the number of three-dimensional faces is 11: 1 - 2 - 3 - 5, 1 - 4 - 3 - 5, 1 - 2 - 4 - 3, 1 - 2 - 4 - 5, 2 - 4 - 3 - 5, 6 - 8 - 9 - 10, 7 - 9 - 8 - 6, 7 - 8 - 9 - 10, 7 - 8 - 6 - 10, 7 - 9 - 6 - 10, 1 - 2 - 3 - 5 - 6 - 8 - 9 - 10 (polyhedron bounded by the outer surface of the polytope); the number of four -dimensional faces is 3: 1 - 2 - 3 - 4 - 5, 6 - 7 - 8 - 9 - 10, 2 - 4 - 3 - 5 - 10 - 9 - 7 - 6. In this case $f_0 = 10, f_1 = 22, f_2 = 22, f_3 = 11, f_4 = 3.$

Substituting the obtained values $f_i, i = 0 \div 4$ into equation (1), we obtain,

10 - 22 + 22 - 11 + 3 = 2.

Thus, Euler-Poincaré's equation in this case holds for n = 5. This proves that a polytope on figure 1 has dimension 5. The four-dimensional polytopes include two tetrahedra with a center and a polytope 2 - 4 - 3 - 5 - 10 - 9 - 7 - 6. Let us prove that this polytope has dimension 4. In this polytope the number of vertices is 8, the number of edges is 15: 2 - 4, 2 - 5, 2 - 3, 4 - 3, 5 - 3, 3 - 10, 4 - 7, 5 - 6, 2 - 9, 10 - 9, 10 - 7, 10 - 6, 7 - 6, 7 - 9, 9 - 6; the number of two-dimensional faces is 13: 2 - 4 - 5, 2 - 4 - 3, 5 - 4 - 3, 2 - 3 - 5, 10 - 7 - 9, 7 - 9 - 6, 10 - 7 - 6, 10 - 9 - 6, 2 - 3 - 10 - 9, 2 - 4 - 7 - 9, 2 - 5 - 9 - 6, 5 - 4 - 7 - 6, 5 - 3 - 10 - 6; the number of three-dimensional faces is 6: 2 - 3 - 5 - 10 - 9 - 6, 2 - 3 - 4 - 5, 7 - 9 - 10 - 6, 2 - 4 - 5 - 7 - 9 - 6, 5 - 4 - 3 - 10 - 7 - 6, 2 - 3 - 4 - 10 - 7 - 9. In this case $f_0 = 8, f_1 = 15, f_2 = 13, f_3 = 6.$

Substituting the obtained values $f_i, i = 0 \div 3$ into equation (1), we obtain,

8 - 15 + 13 - 6 = 0.

Thus, Euler-Poincaré's equation in this case holds for n = 4. This proves that a polytope 2 - 4 - 3 - 5 - 10 - 9 - 7 - 6 has dimension 4.

Consequently, all possible polytopes that can be created from two tetrahedrons with a center somehow, polytopic prisms, cross-polytopes and self-orthogonal polytopes, have dimension 5. Each such polytope leads to polytopic prismahedrons, with the smallest dimension 6, with the help of which, in accordance with the theory of polytopic prismahedrons, it is possible to construct a space of the highest dimension.

When this intermediate state and the state antiparallel to it are included in the set of possible states of a tetrahedron with a center, a picture is obtained that describes all the variety of states observed in the native structure of the protein (Figure 3).

Figure 3: Native structure of globular proteins.

Consequently, all possible polytopes that can be created from two tetrahedrons with a center somehow, polytopic prisms, cross-polytopes and self-orthogonal polytopes, have dimension 5. Each such polytope leads to polytopic prismahedrons, with the smallest dimension 6, with the help of which, in accordance with the theory of polytopic prismahedrons, it is possible to construct a space of the highest dimension. This, in particular, is realized in the native structure of globular proteins.

If we multiply the picture in figure 3 by geometric elements of different dimensions (segment, triangle, tetrahedron, etc.), we can see how different spatial β-sheets are formed in the native protein structure with parallel and antiparallel arrangement of residues of acid amine molecules, and various α-helices. The presence or absence of certain secondary conformations of protein molecules will be limited by the presence or absence of certain chemical bonds between tetrahedrons centered on a common structure.

Conclusion

Using the theory of polytopic prismahedrons [2], which made it possible to solve the 18th problem of Hilbert [13] about constructing an n-dimensional space using congruent figures [4], the problem of constructing the native structure of globular proteins in the entire volume of a globule is considered. For the first time, a mathematical model of the tertiary structure of a protein was obtained with an indication of the distribution of residues of amino acid molecules throughout the volume of a globule with the formation of all known conformations of protein molecules. It is shown that polytopic prismahedrons consisting of four amino acid residues in both the case of parallel and antiparallel and self-orthogonal arrangement of amino acid residues have dimension 6. An increase in the number of amino acid residues in the polytopic prismahedrons leads to an increase in the dimension of the polytopic prismahedrons and to increase the flow of information necessary for the effective functioning of active centers in enzymes. Geometric images of the native structure of globular proteins with the participation of various conformations of protein molecules are presented.

Bibliography

1. Zhizhin GV. "Chemical Compound Structures and the Higher Dimension of Molecules: Emerging Research and Opportunities". IGI Global (2018).
2. Zhizhin GV. "The Geometry of Higher-Dimensional Polytopes". IGI Global (2019a).
3. Zhizhin GV. "Attractors and Higher Dimensions in Population and Molecular Biology". IGI Global (2019b).
4. Zhizhin GV. "Normal Partitions and Hierarchical Fillings of N-Dimensional Spaces". IGI Global (2021a).
5. Dixon M and Webb EC. "Enzymes". Longman Group Ltd (1979).
6. Metzler DE. "Biochemistry. The Chemical Reactions of Living Cells". Academic Press, United States (1980).
7. Lehninger AL. "Principles of Biochemistry". Worth Publishers, United States (1982).
8. Koolman J and Roehm KH. "Color Atlas of Biochemistry". Thime, Stuttgart, New York (2013).
9. Zhizhin GV. "World - 4D". Polytechnic Service, Russia (2014).
10. Zhizhin GV and Diudea MV. "Space of Nanoworld". In MV Put, MC Mirica (Eds), Sustainable Nanosystems, Development, Properties, and Applications, IGI Global (2016).
11. Zhizhin GV. "The Polytope of Hereditary Information: Structure, Location, Signification". *Biochemistry and Modern Applications* 2 (2019c): 56-62.
12. Zhizhin GV. "Hidden Nucleic Order Bond?" *Acta Scientific Biotechnology* 1.4 (2020): 34-36.
13. Hilbert D. "Gesammelte Abhandlangen". *Archive Mathematics and Physics* 3.1 (1901): 44-63, 213-237.
14. Poincaré A. "Analysis situs". *Journal of Polytechnic School* 1 (1895): 1 – 121.

Volume 2 Issue 6 September 2021