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Research Article

Higher Dimensions in Linear, Helicoidal and Folded Structures of Protein Molecules

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Abstract

It was shown that the widespread quasi-plane models of the Pauling protein structure do not reflect and even contradict the spatial structures of the protein in various conformations. It was found that the linear structures and β - structures of the protein in space of the highest dimension have translational symmetry. The elementary elements of the protein translational symmetry were determined, and their dimensions were calculated (9 for the linear structures and 23 for β - structures).

Keywords: Molecule; Protein; Chain; Spiral; Dimension; Polytope; Translational Symmetry

Introduction

Back in the middle of the last century, the diffraction patterns of crystals of amino acids and simple di- and tri- peptides were studied [1-5]. The characteristic lengths of valence bonds and the values of bond angles were determined. Based on the results of these studies, three-dimensional models in linear, helicoidal and folder structures of protein molecules were built. They have found widespread use up to the present time [6-8]. However, it has recently been found that amino acid molecules are of the highest dimension [9,10]. In this paper linear, helicoidal and folder structures of protein molecules are considered taking into account the highest dimension of amino acid molecules using the metric data obtained in the previous period. It is shown that quasi-plane models of the Pauling protein structure contradict the results of the analysis of the spatial structures of protein molecules. Rejection of simplifying assumptions leads to fundamentally different structures of the conformations of protein molecules.

Dimensions of protein molecules

Amino acids are chemical compounds that simultaneously include a carboxyl group COO^- and an amine group H_3N^+. These groups are covalently linked to a carbon atom (α - carbon), to which a hydrogen atom H and a side chain R are also covalently attached [8]. Amino acids have two enantiomorphic forms L and D, which are Fischer planar views shown in figure 1. From Figure 1 it can be seen that the two enantiomorphic forms are related by mirror image relative to the line passing through the amine and carboxyl groups.

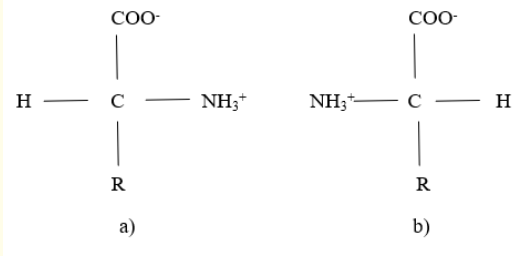

Figure 1: Enantiomorphic forms of the amino acid molecule.

a) L - amino acid, b) D - amino acid

The side chains in Figure 1 have 20 variants in classic amino acids [8]. They determine the properties of the corresponding amino acids. Fisher's projections do not reflect the spatial structure of amino acids, although it is clear that these are spatial objects. Spatial images of enantiomorphic amino acids [9] are presented in figure 2.

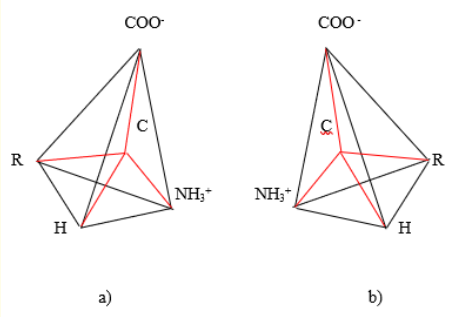

Figure 2: Spatial images of amino acids.

a) L - amino acid, b) D - amino acid

In figure 2, covalent bonds are indicated in red. The rest of the segments define the spatial shape of the molecule, they are marked in black.

From figure 2 it follows that the amino acid molecule is a tetrahedron with a center. The dimension of such a polyhedron can be determined by the Euler-Poincaré equation [11]

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

There n is dimension of a polytope P, f_i is the number of elements with dimension i in the polytope P.

From Figure 2 it follows that in any of the two enantiomorphic forms of the amino acid molecule, the number of vertices 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.

i.e. 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.

Linear polypeptide chain structure

The study of diffraction patterns of crystals of amino acids [1-4] made it possible to establish some values of bond bonds and bond angles in an amino acid. However, the interpretation of the spatial arrangement of atoms in an amino acid requires additional instructions. An example of the possibility of ambiguous interpretation of diffraction patterns can be found in numerous works on the description of quasicrystals. In particular, the apparent icosahedral symmetry of the diffraction patterns of quasicrystals was proposed to be explained [12] by multiple twinning of cubic crystals. Pauling based his arguments on the radial arrangement of the spots in the diffractograms. However, high-resolution photomicrographs refuted this assumption [13]. The statement about the absence of translational symmetry in quasicrystals [14] was constructed using the representations of the three-dimensional geometry of Euclid. Later this statement was refuted [15-18]. It was proved that translational symmetry in the diffractograms of quasicrystals appears if the diffractograms are considered as projections of structures from the space of higher dimensions. When studying diffraction patterns of amino acid crystals in the works of Pauling joint authors the values of a number of parameters were not determined, for example, bond lengths R - C depending on the species R, bond angles between carbon atoms and nitrogen atoms, between hydrogen atoms and R, etc.

To compensate for these disadvantages, it was proposed to use a simplifying assumption about the arrangement of a group of atoms of a peptide bond and centers of tetrahedrons in a plane

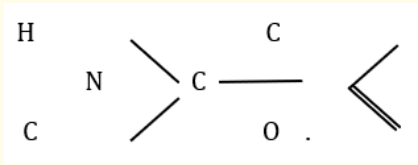

Figure a

Under this assumption, knowledge of the indicated quantities was not required. It should be noted that in subsequent publications by other authors [6-8] with a reference to Pauling's work, it was argued that the arrangement of these atoms in the plane was proved in Pauling's works. But this is not so, to be convinced of this it is enough to refer to these works. This unproven statement became the basis for the construction of three-dimensional models of protein molecules of various conformations in Pauling's works. Let us consider this issue in detail when constructing spatial struc-

tures of a linear polypeptide chain. In this case, the atoms of amino acid molecules must be located on a set of parallel lines. Then the polypeptide chain of two molecules of L- amino acids, taking into account the four-dimensionality of amino acid molecules, has the form shown in figure 3.

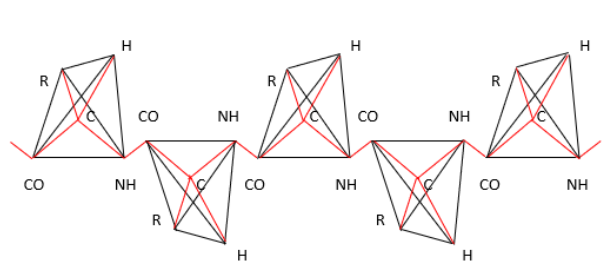

Figure 3: Linear polypeptide chain of L - molecules amino acids.

In the case of a D - amino acid, such a polypeptide chain is shown in figure 4.

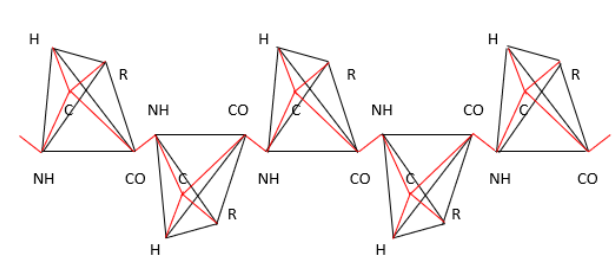

Figure 4: Linear polypeptide chain of D - molecules amino acids.

From Figure 3 and Figure 4 it can be seen that in order for the corresponding vertices of tetrahedrons with the center (i.e., specific atoms or functional groups) could lie on a system of parallel lines (i.e., form a linear polypeptide chain), it is necessary that the amino acid molecules in the chain alternate with their mirror image relative to the edge in the tetrahedron connecting the bond centers of the polypeptide chain (i.e., relative to the segment CO - NH). The chains in Figure 3 and Figure 4 differ by the mirror reflection of the molecules relative to the perpendicular to the segment CO - NH (L- and D - molecules).

In figures 3 and 4, you can see the translational symmetry of the circuits. Moreover, the elementary translational element in this case is a group of two linked amino acid molecules, one of which is a mirror image of another amino acid molecule relative to the segment. From these two linked amino acid molecules, you can create a convex polytope by connecting edges of each vertex of any of the molecules with all other vertices in the group. This is how a simplex polytope of dimension 9 is formed, since the dimension of a simplex polytope is one less than the number of vertices in a simplex [19], and the number of vertices in two tetrahedrons with a center is 10. Therefore, a polypeptide linear amino acid chain has translation symmetry, in which an elementary translation element is a simplex polytope of dimension 9. In Figures 3 and 4, as well as in Fischer's projections (Figure 1) and in spatial images of molecules (Figure 2), in accordance with the definition of functional dimension, functional groups R, CO, NH were used. If we open the images of functional groups CO, NH and accept Pauling's assumption about their arrangement in the plane, then we will have a sequence of their alternation as shown in figure 5 in the case of D-molecules of amino acids.

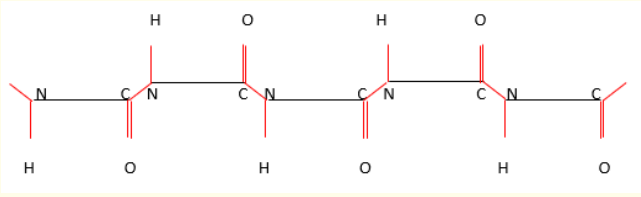

Figure 5: The location of the edges of peptide bonds in the chain of D-molecules of amino acids.

However, it is essential (see Figure 5) that the α-carbon atoms do not lie in the same plane with the peptide bond atoms. From a comparison of Figures 3 - 5 it follows that α-carbon atoms lie either above the plane in which the atoms of the peptide bond are located, or below this plane, and can never lie on this plane. Therefore, Pauling's idea that α-carbon atoms lie in the same plane with functional groups CO, NH is erroneous. Therefore, Pauling's approximation cannot be used both in the construction of linear polypeptide chains and in the construction of more complex conformations of amino acid molecules.

Spiral polypeptide chains

In the previous section, it was proved that the centers of tetrahedrons cannot lie on a flat sheet in which the peptide bond is located. Therefore, Pauling's idea of the connection of such flat

leaves at the centers of tetrahedrons to form a helical peptide chain, as Pauling did, cannot be used. There is a relatively simple way of forming a helical polypeptide chain based on the concept of the four-dimensionality of amino acid molecules. This method was proposed in 2016 [9]. Suppose another amino acid molecule (not in a mirror image) is attached to an amino acid molecule (tetrahedron with a center) by a peptide bond C - N (Figure 6) so that in the general case between the valence bond C - C of the first molecule and the peptide bond C - N there is a certain angle less than 180 degrees (since there is no reason to assert that one of these connections is an exact continuation of the other).

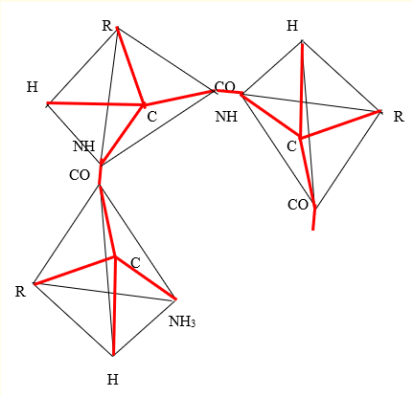

Figure 6: Spiral polypeptide chains.

Therefore, the second amino acid molecule is rotated by some angle relative to the first amino acid molecule. At the same time, while maintaining the shape of the second amino acid molecule, the second peptide bond, with the help of which the third amino acid molecule can be attached, turns out to be significantly (almost 90 degrees) rotated with respect to the first peptide bond. The third peptide bond is thus almost antiparallel to the first peptide bond. There is a rotation of the attached amino acid molecules relative to some center O [9,10]. If we designate the length of the peptide bond "*a*", the length of the edge of the tetrahedron between the atoms C and N "*b*", then in the projection onto the plane perpendicular to the axis of rotation, we get a polygon (Figure 7), which corresponds to the particular with the period of rotation of the molecules equal to 4.

If we continue the nearest sides of the polygon *b* until they intersect with each other, we find the angle between these extensions. This is the angle $\theta = 180 - 2(180 - \alpha), \alpha$ is the angle between sides *a* and *b*. From here we find the connection between the period *n* and the angle α

$$n\theta = 360, \alpha = \frac{1}{2}(\frac{360}{n} + 180).$$

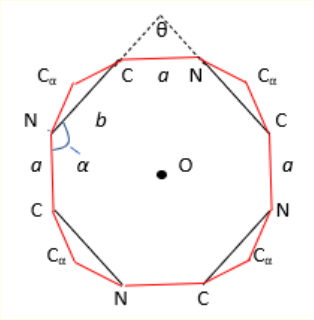

Figure 7: Rotation of peptide bonds.

If the period *n* = 4 so α = 135^0. Pauling had a minimum period of 3.6, but it should be noted that the rotation period of an amino acid molecule can only be an integer. If we now assume that the lines connecting the centers of the tetrahedrons do not lie in the plane of rotation, but have a certain angle with respect to this plane, then we get a helicoid of rotation of the amino acid molecule (i.e., α - helix, since α -carbon atoms are located at the centers of the tetrahedrons). It can be shown that if we use the values of the valence bond lengths and the bond angle determined in Pauling's works, then to achieve the distance between the turns of 0.54 nm in the spiral (adopted in Pauling's works), the required value of the angle between the line connecting the centers of the tetrahedra and the plane of rotation, is equal to 1.5 degrees. It should be noted that when constructing a helix, a fundamentally different method of connecting amino acid molecules is used in comparison with a linear peptide chain. This method is more natural since it does not require the use of mirror-opposite amino acid molecules. Between adjacent turns of the spiral of amino acid molecules there is a stabilizing hydrogen bond between the *H* atoms of the peptide bond and the *O* atoms of the peptide bond with a double bond.

β - structures of the amino acids

One of the important principles of protein structure formation is the formation of as many hydrogen bonds between groups as possible. This is especially pronounced in the so-called β - structures (folder structures) in which elongated chains of amino acid

molecules are hydrogen bonded to each other to form a continuous layer. In these structures, the hydrogen bond plays a decisive role, and when calculating the dimensions of the compounds, it must be taken into account on an equal footing with the covalent bond. The repeating element in these β - structures is a polyhedron composed of two amino acid molecules. Figure 8 shows one of two variants of such polyhedrons.

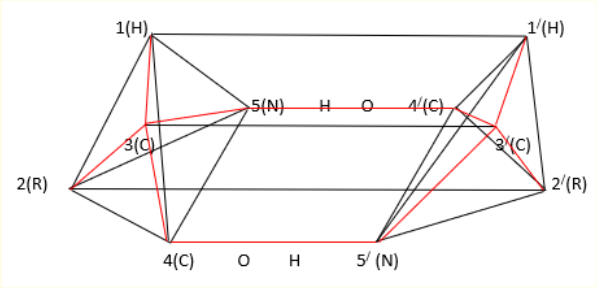

Figure 8: Polyhedron composed of two amino acid molecules.

The ribs of the CN in Figure 8 are in an antiparallel position. It should be noted that the H and O atoms are not the tops of the figure. Therefore, the polyhedron in Figure 8 has 10 vertices ($f_0 = 10$), 24 edges ($f_1 = 24$), 29 two-dimensional faces ($f_2 = 29$), 20 three-dimensional faces ($f_3 = 20$), 7 four-dimensional faces ($f_4 = 7$). Four-dimensional faces are faces 12345, $1/2/3/4/5/$, like tetrahedrons with a center. In addition, tetrahedrons are four-dimensional faces located on four triangular faces of tetrahedra with centers $13451/3/4/5/$, $13251/3/2/5/$, $12341/2/3/4/$, $32543/2/5/4/$. These figures are topologically equivalent to the products of tetrahedrons and a one-dimensional segment [19]. The difference between these figures and the products of tetrahedra and a one-dimensional segment is only that in this case the one-dimensional segment as a factor in these figures discretely changes its length. But this does not change the number of elements of different dimensions included in the figure. Therefore, as well as the product of a tetrahedron and a one-dimensional segment, these figures include 8 vertices ($f_0 = 8$), 16 edges each ($f_1 = 16$), 14 flat faces ($f_2 = 14$), 6 three-dimensional faces ($f_3 = 6$). Substituting these numbers into the Euler-Poincaré equation (1), we obtain

8 - 16 + 14 - 6 = 0.

This proves that for all the listed figures with vertices 3 and $3/$ the Euler-Poincaré equation is fulfilled for n = 4, i.e. all of them have dimension 4. Another four-dimensional figure is formed by two tetrahedrons 1254 and $1/2/5/4/$ connected by parallel lines. They are also topologically equivalent to the product of a tetrahedron and a one-dimensional segment. Thus, the total number of four-dimensional figures included in Figure 8 is 7. Substituting the values obtained for Figure 8 into the Euler Poincaré equation (1), we find 10 - 24 + 29 - 20 + 7 = 2.

This proves that in this case the Euler-Poincaré equation is fulfilled for n = 5, i.e. figure 8 has dimension 5.

In a continuous layer of amino acid molecules, the polyhedron in Figure 8 alternates with another polyhedron formed by two tetrahedrons with center at other positions (Figure 9).

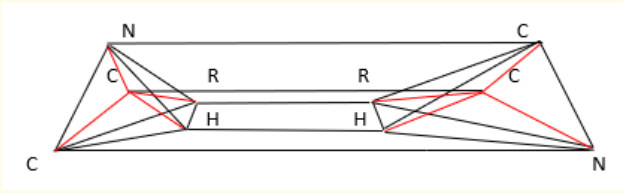

Figure 9: Second polyhedron formed by two tetrahedrons with center.

It can be seen that Figure 9 is also topologically equivalent to the product of a tetrahedron with center on a one-dimensional segment and therefore has dimension 5. The polyhedrons in Figure 8 and Figure 9 cannot directly adjoin each other. Between them are other polyhedron formed from two three-dimensional pyramids attached to each other along flat faces. One of these topologically equivalent polyhedrons is shown in figure 10.

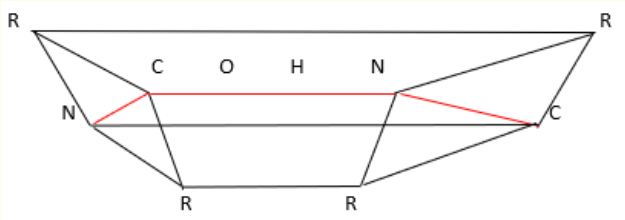

Figure 10: Polyhedron of two three-dimension pyramids.

You can see that it has 8 vertices ($f_0 = 8$), 14 edges ($f_1 = 14$), 9 two-dimensional faces ($f_2 = 9$), 3 three-dimensional faces ($f_3 = 3$

). Substituting these numbers into the Euler - Poincaré equation (1), we find

8 - 14 + 9 - 3 = 0.

Therefore, figure 10 satisfies the Euler - Poincaré equations for n = 4, i.e. it has dimension 4. A topologically equivalent figure 11 also has dimension 4.

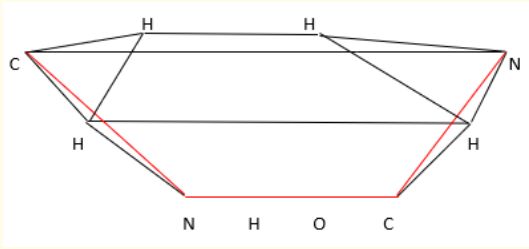

Figure 11: Polyhedron of two three-dimension pyramids equivalent Figure 10.

A part of the common layer composed of periodically repeating polyhedrons 8, 9, 10, 11 is shown in figure 12.

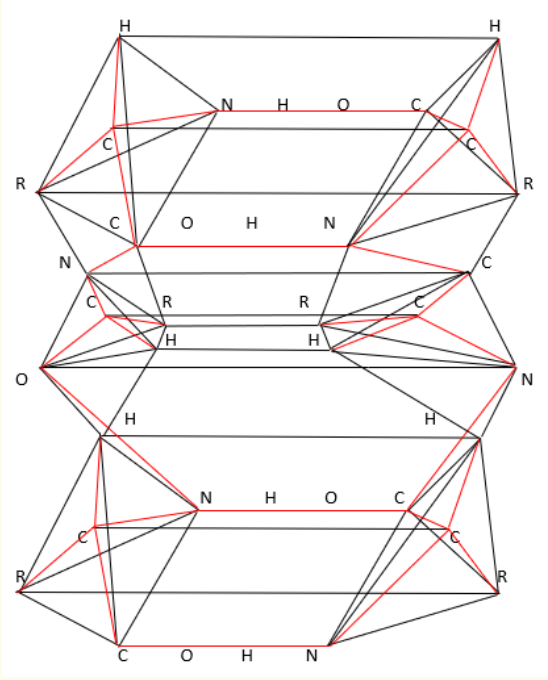

Figure 12: Layer composed of periodically repeating polyhedrons 8,9,10, 11.

Figure 12 shows that the β - structure has translational symmetry. An elementary element of translational symmetry is the sequence of polyhedrons shown in Figures 8 - 11. If we denote the polyhedron in Figure 8 by symbol 5 (1), the polyhedron in Figure 9 by symbol 5 (2), and the polyhedron in Figure 10 by symbol 4 (1), the polyhedron in figure 11 by the symbol 4 (2), then the translational element of the β - structure in Figure 12 is the polyhedron 5 (1)-4 (1)-5 (2)-4 (2). This polyhedron contains 24 vertices. If we connect each vertex of this polyhedron with all other vertices by edges, we get a single convex simplex polyhedron of dimension 23. Thus, the translational element of the β - structure in Figure 12 is a simplex of dimension 23.

In the literature, the β - structures traditionally described are called antiparallel and are depicted as alternating flat two-dimensional stripes (sheets).

However, it is clear that the name anti-parallel in this case does not reflect much of the essence of the structure in Figure 12. More precisely, this structure could be called non-parallel. In addition, and this is essential, the β - structures are fundamentally not flat and represent periodically repeating 5-dimensional and 4-dimensional regions, and each of these regions has two topologically equivalent images.

There are β - structures that include parallel 4-dimensional amino acid molecules with two different orientations. In these structures, alternation of 5-dimensional and 4-dimensional regions (polyhedrons) also occurs. In continuous form, it is presented in figure 13. Figure 13 shows that the β - structure has translational symmetry too.

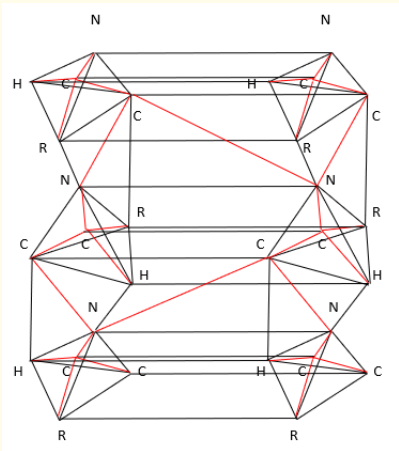

Figure 13: Parallel β - structure.

For this structure, you can conditionally save the name of the parallel structure.

Similar this the β - structure in Figure 12, it is also possible to define the sequence of polyhedrons of dimensions 5 and 4, which make up the translational element of the β - structure in Figure 13. Given the difference in the form of polyhedrons in Figures 12 and 13, the sequence of polyhedrons that make up the translational element of the structure in Figure 13 can be written as 5 (3)-4 (3)-5 (4)-4 (4). The particular type of polyhedrons of dimensions 5 and 4 is easy to determine from Figure 13. The translational element of β - structure in Figure 13 also includes 24 vertices and, therefore, is a simplex polyhedron of dimension 23.

Conclusion

It is shown that the widespread quasi - plane Pauling models do not reflect and even contradict the spatial structure of polypeptide amino acid molecules, taking into account their highest dimension. This applies to all types of polypeptide chain conformation. In this regard, new models of linear polypeptide chains were construct and it was found that these chains have translational symmetry in the space of higher dimensions. The elementary element of the translational symmetry of these chains is the 9-dimensional polyhedron, which consists of two mirror-opposite amino acid molecules. Helical conformations of polypeptide chains are also composed of higher-dimensional elements. The rotation of monomeric amino acid units in a helical conformation is determined only by the alternation of active centers in an asymmetric amino acid molecule. The study of the amino acid β - structures showed that they also have translational symmetry in the space of the highest dimension. Moreover, both the so-called "parallel" and "antiparallel" β - structures have elements of translation symmetry with dimension 23, consisting of two topologically equivalent polyhedrons of dimension 5 and two topologically equivalent polyhedrons of dimension 4. The resulting polyhedrons in high dimension, as translation elements of the construction of spaces protein molecules, should be further compared with the general theory of normal partitioning of n-dimensional spaces and corresponding high-dimensional parallelohedrons [20].

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