

The study of the torsion angles between helical axes in pairs of helices in protein molecules

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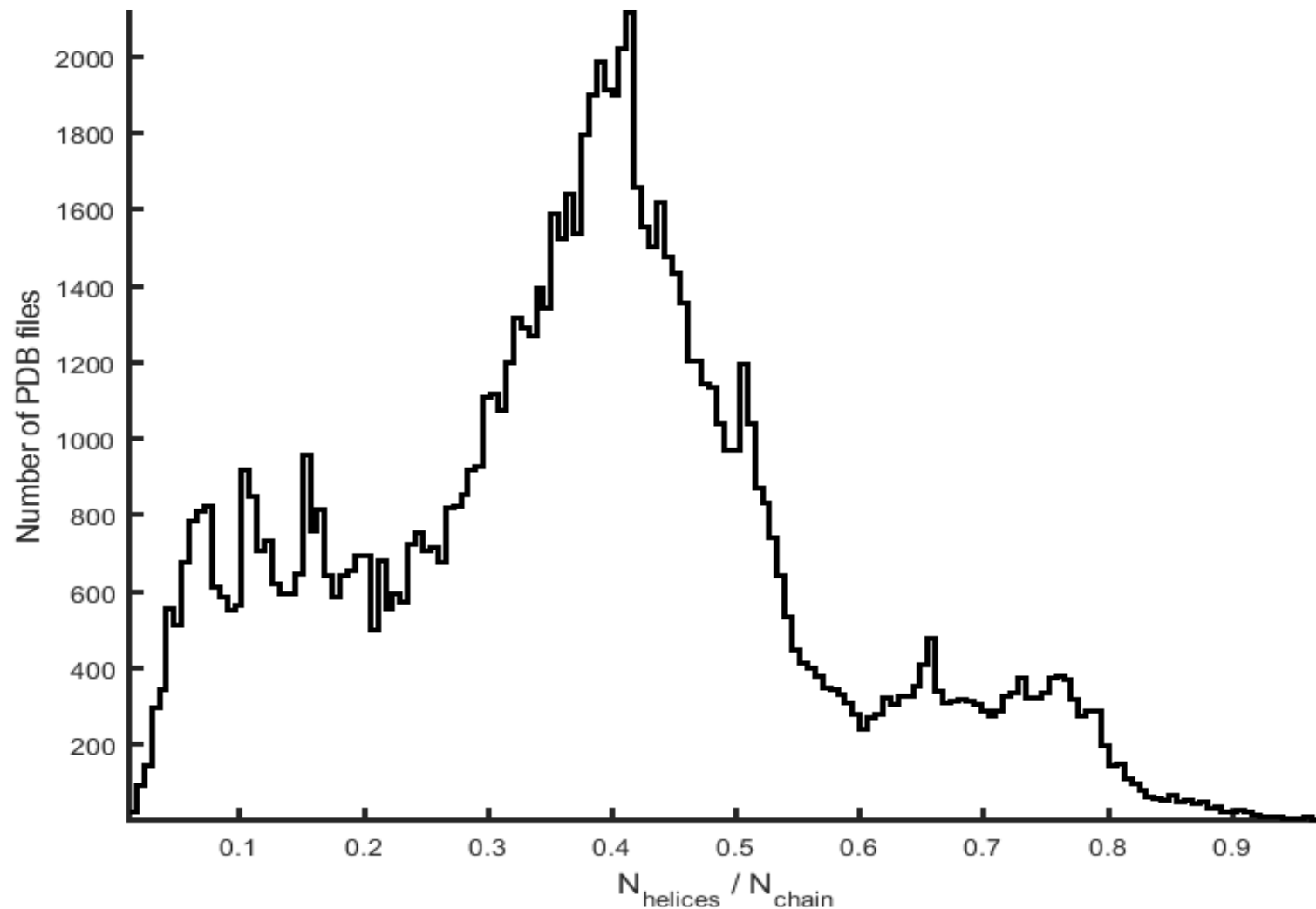
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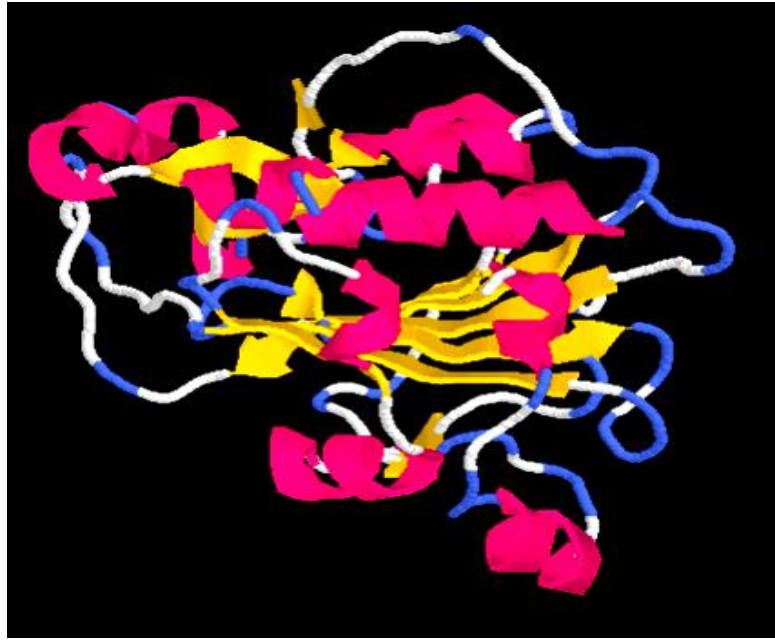
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**The study was made with the support from the RFBR:
project 16-01-00692-a,
project 18-07-01031-a.**

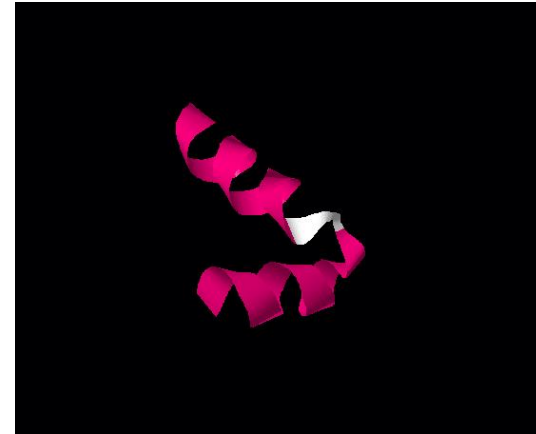
Distribution of the number of proteins in PDB depending on the ratio of amino acids in the helices to the total number of amino acids in the protein

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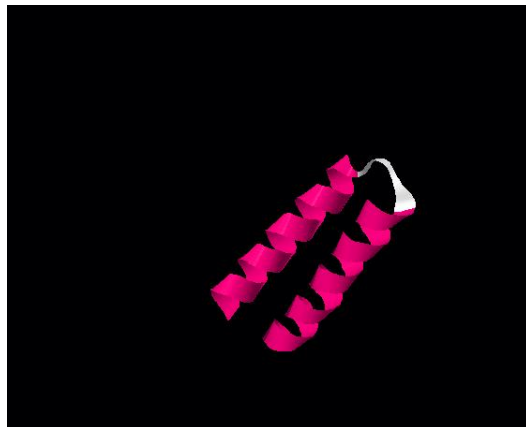




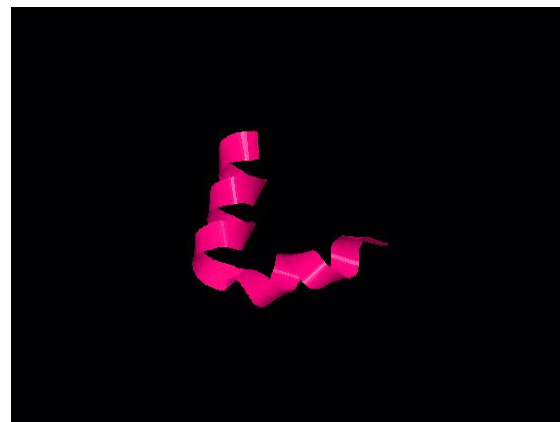
α - α -corner



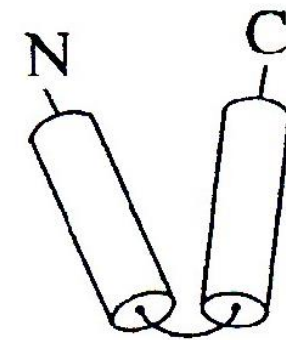
α - α -hairpins



L- shaped structure



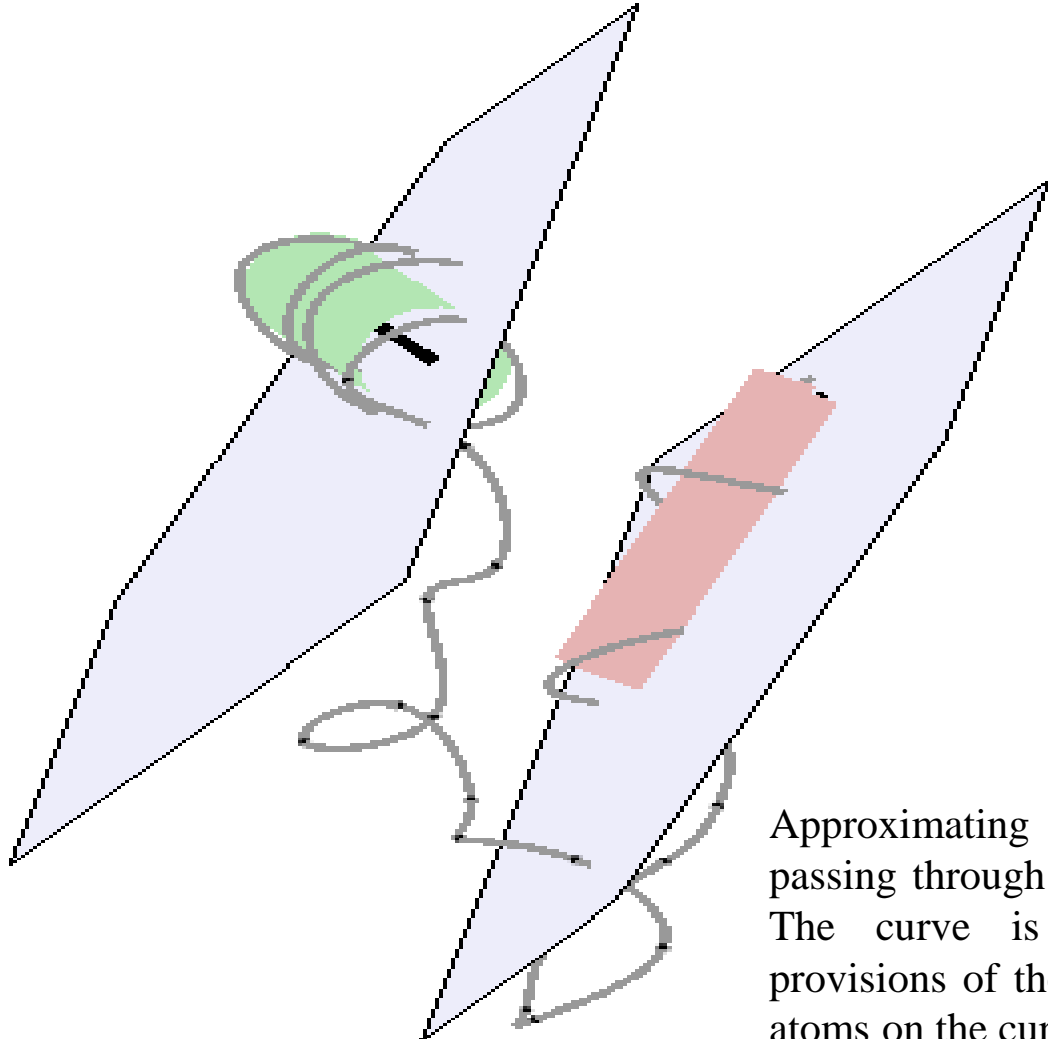
V- shaped structure



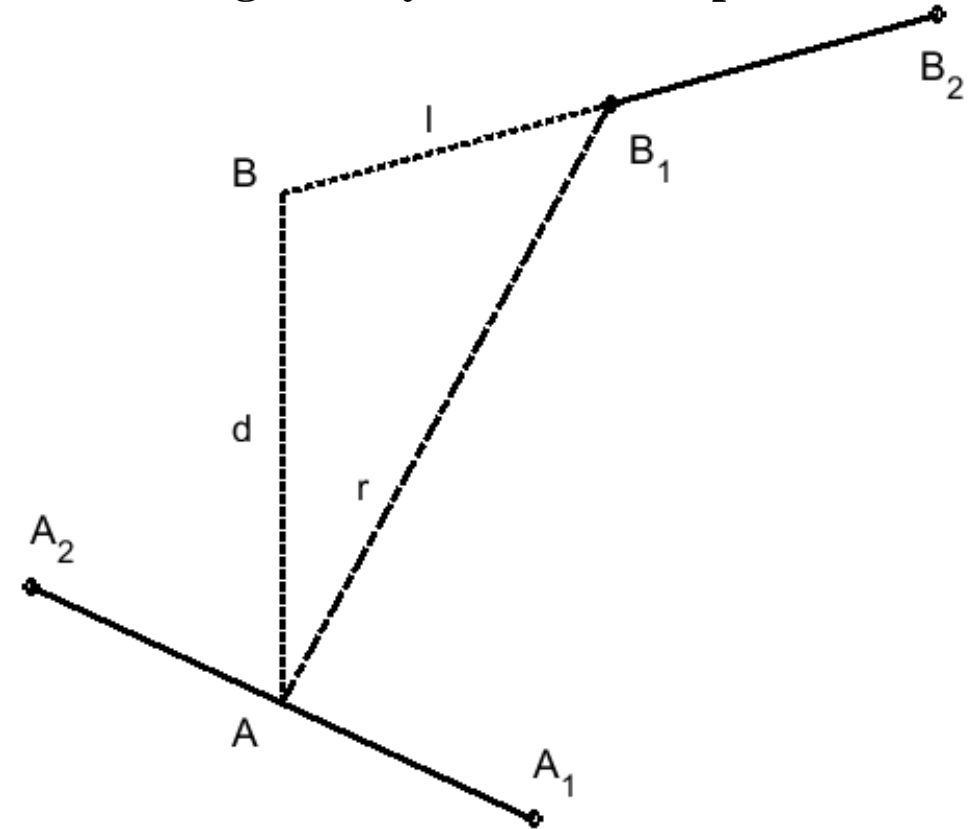
In the present study we delivered two basic tasks:

- select from the protein data bank PDB all structural motifs formed by two helices of any type located in the polypeptide chains one after another and connected by a by connections of varying length and conformation, and create a database for the further studies of such two-helical structures;
- the study of the torsion angles between axes of helices in helical pairs of protein molecules.

An example of the helical pair. A fragment of a protein chain from protein data Bank (PDB 3A0B ID, the coordinates of the site: 1000-1037).

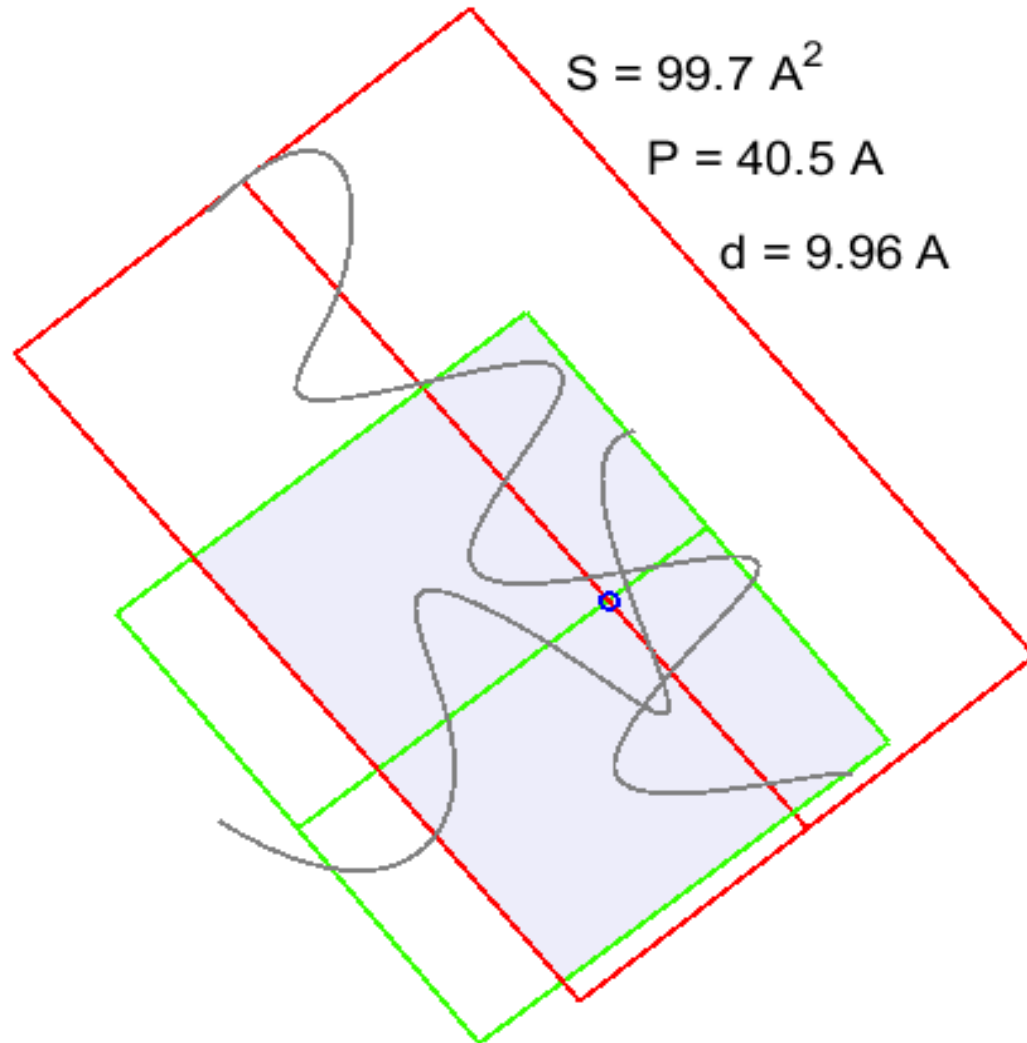


The geometry of the helical pair

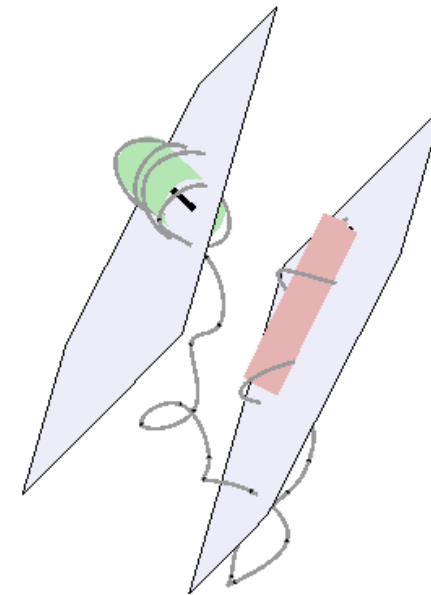


Approximating the helix cylinders and the plane passing through the axis of the cylinders are shown. The curve is approximated according to the provisions of the C α atoms of the protein chain, the atoms on the curve are indicated by dots.

**The intersection of the projections of the cylinder
of helices of the helical pair. Polygon of helices
projections intersection for the helical pair (PDB
ID 3A0B. the coordinates of the site: 1000-1037)**



An example of the helical pair. A fragment of a protein chain from protein data Bank (PDB 3A0B ID, the coordinates of the site: 1000-1037).



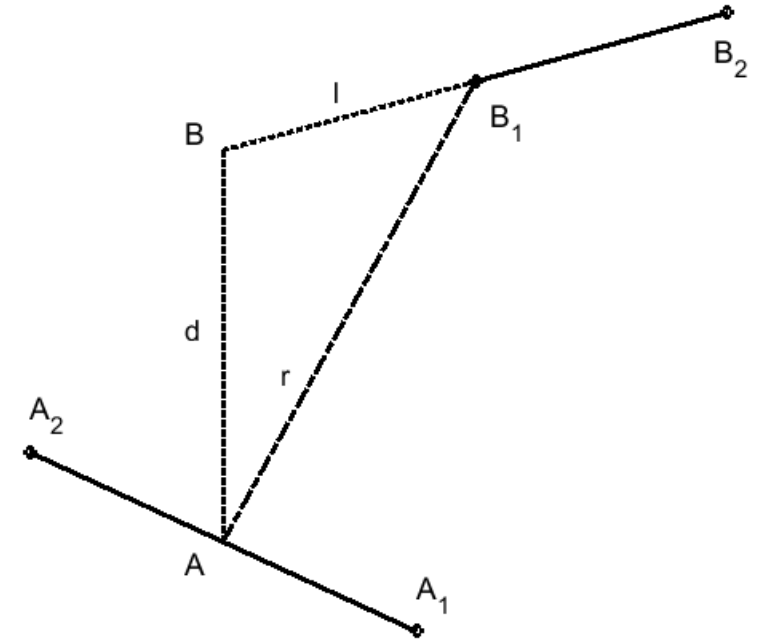
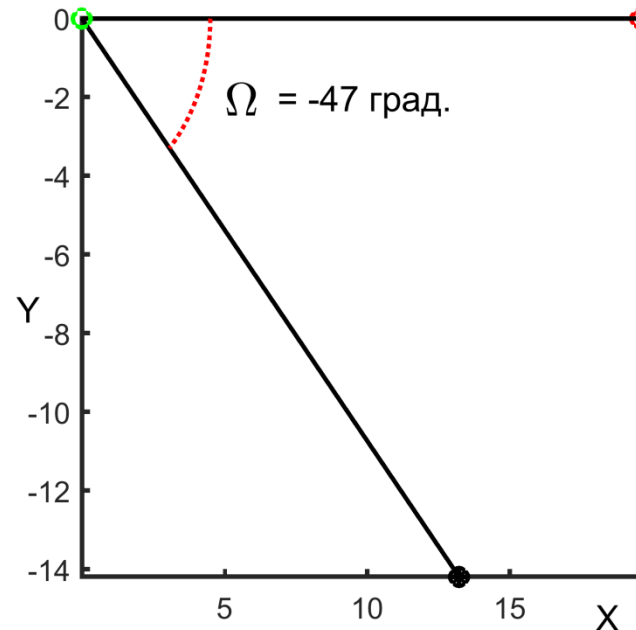
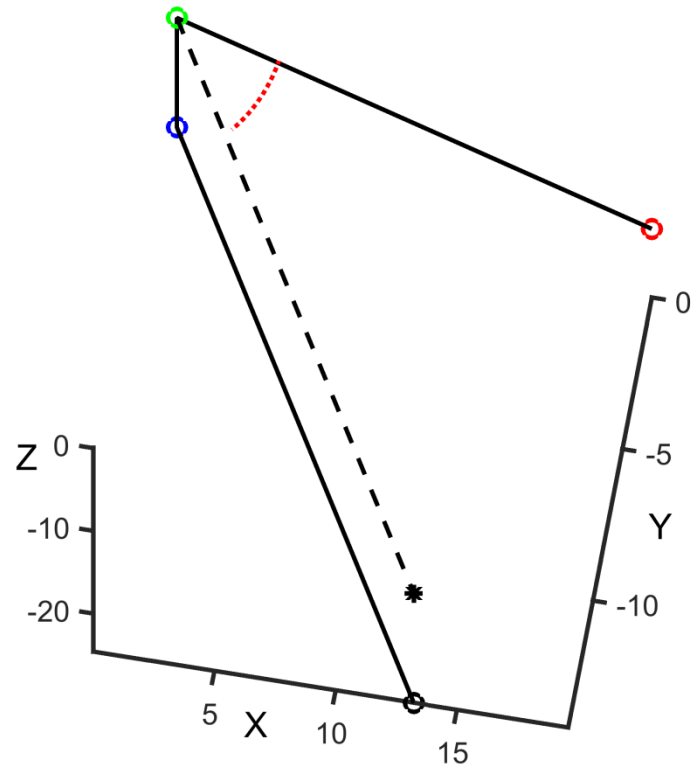
- 1) - {A}**
- 2) - {B}**
- 3) - {C}**

The number of processed protein structures PDB	The number of the processed of amino acid residues	The number of processed amino acid chains	Number of H-type helices	Number of G-type helices	Number of I-type helices
100397	66546491	384666	1952658 <i>(72.16%)</i>	750605 <i>(27.73%)</i>	2908 <i>(0.1%)</i>

The sets of helical pairs	Types of helical pairs						Number of sets of elements
	HH	HG	GG	HI	GI	II	
{A}	402912	441055	125766	1588	643	0	971964
{B}	570830	349024	45513	1677	244	1	967289
{C}	234000	31719	1598	26	9	0	267352
The total number of helical pairs by types	1207742 <i>(54.7%)</i>	821798	172877	3291	896	1	2206605

Determining the torsion angle Ω between the helical axes

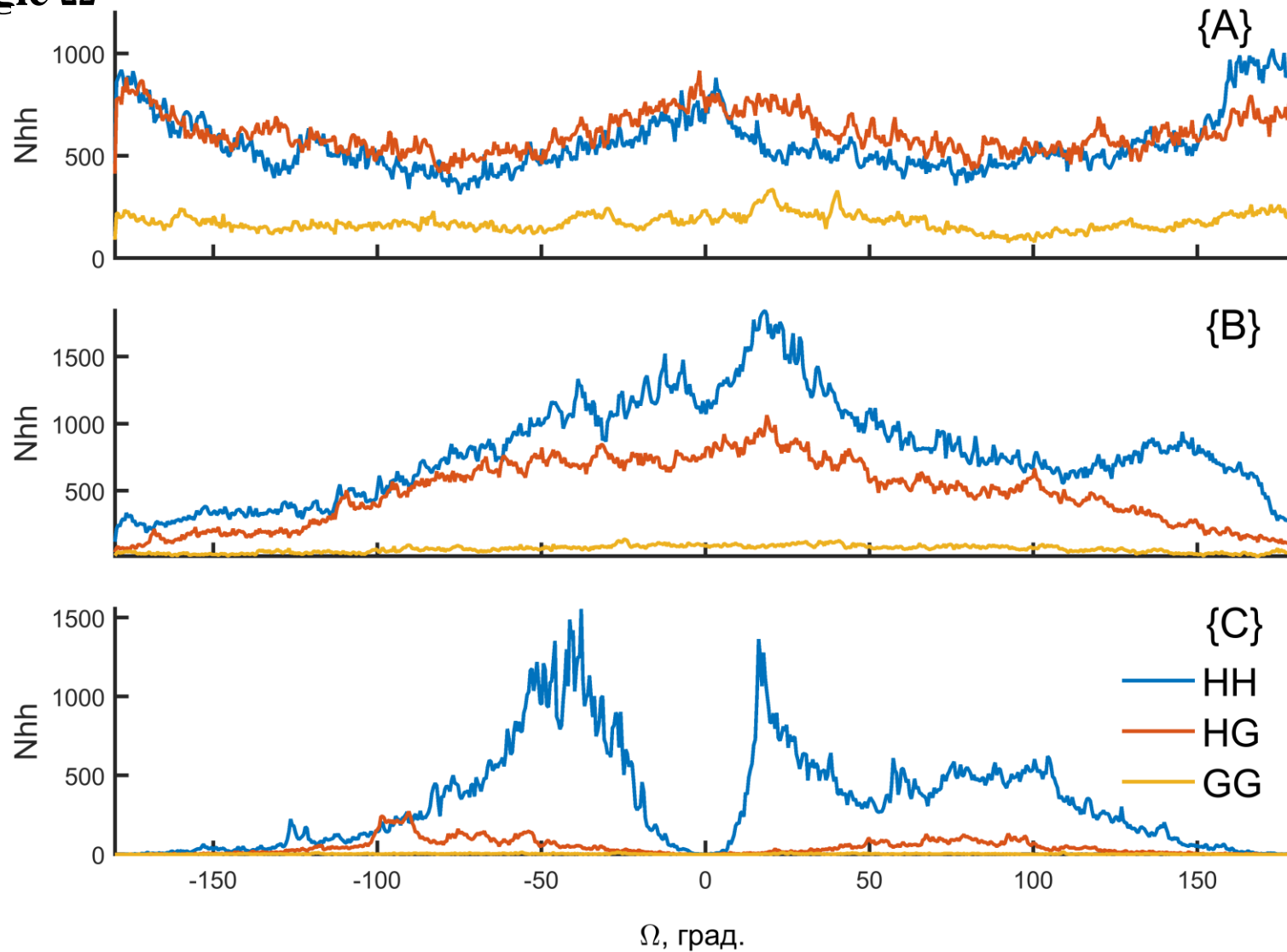
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The anticlockwise direction is considered to be a positive angle while the clockwise direction is believed to be a negative angle .

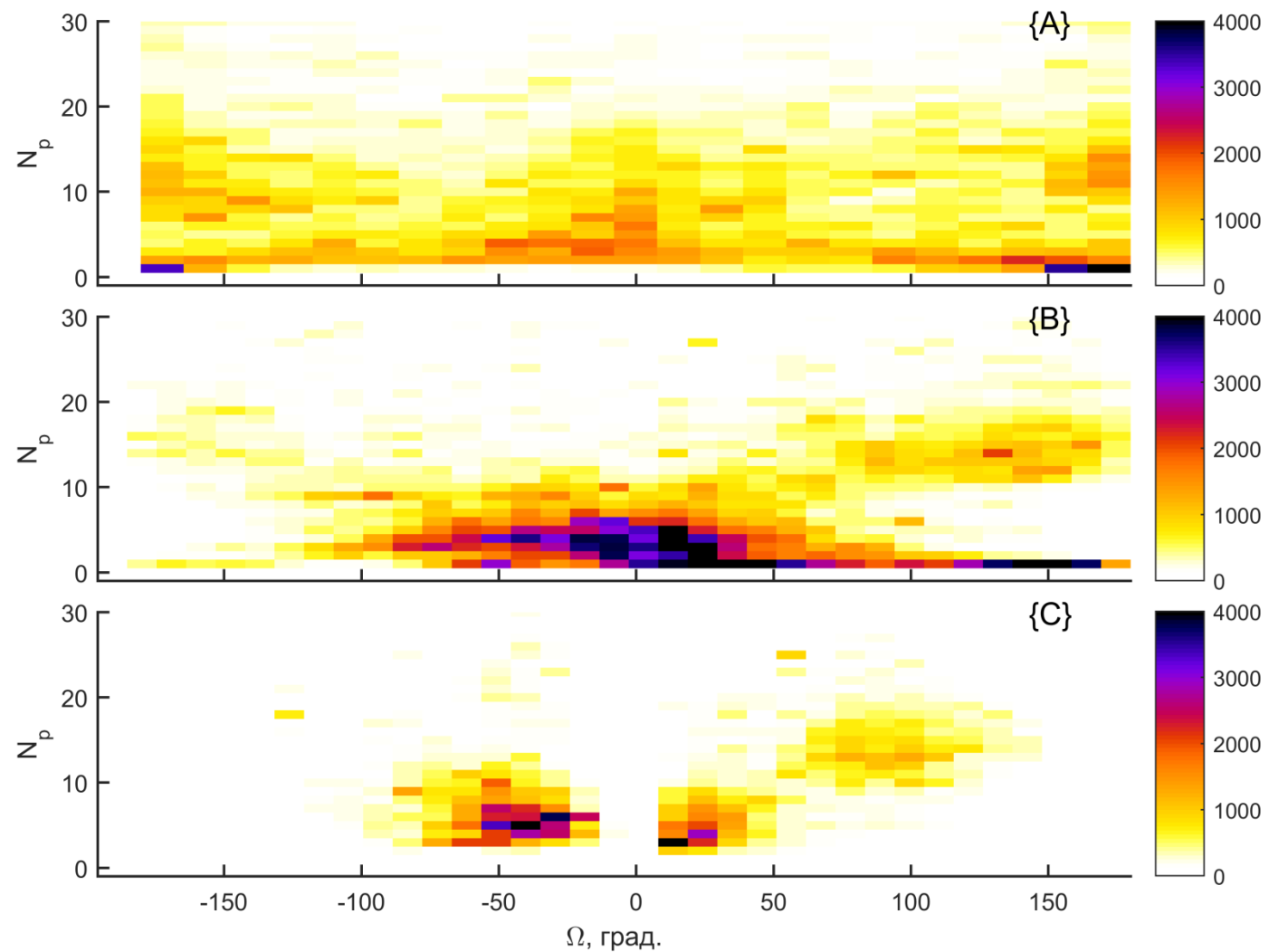
Distribution of different-type structures belonging to different subsets depending on the torsion angle Ω

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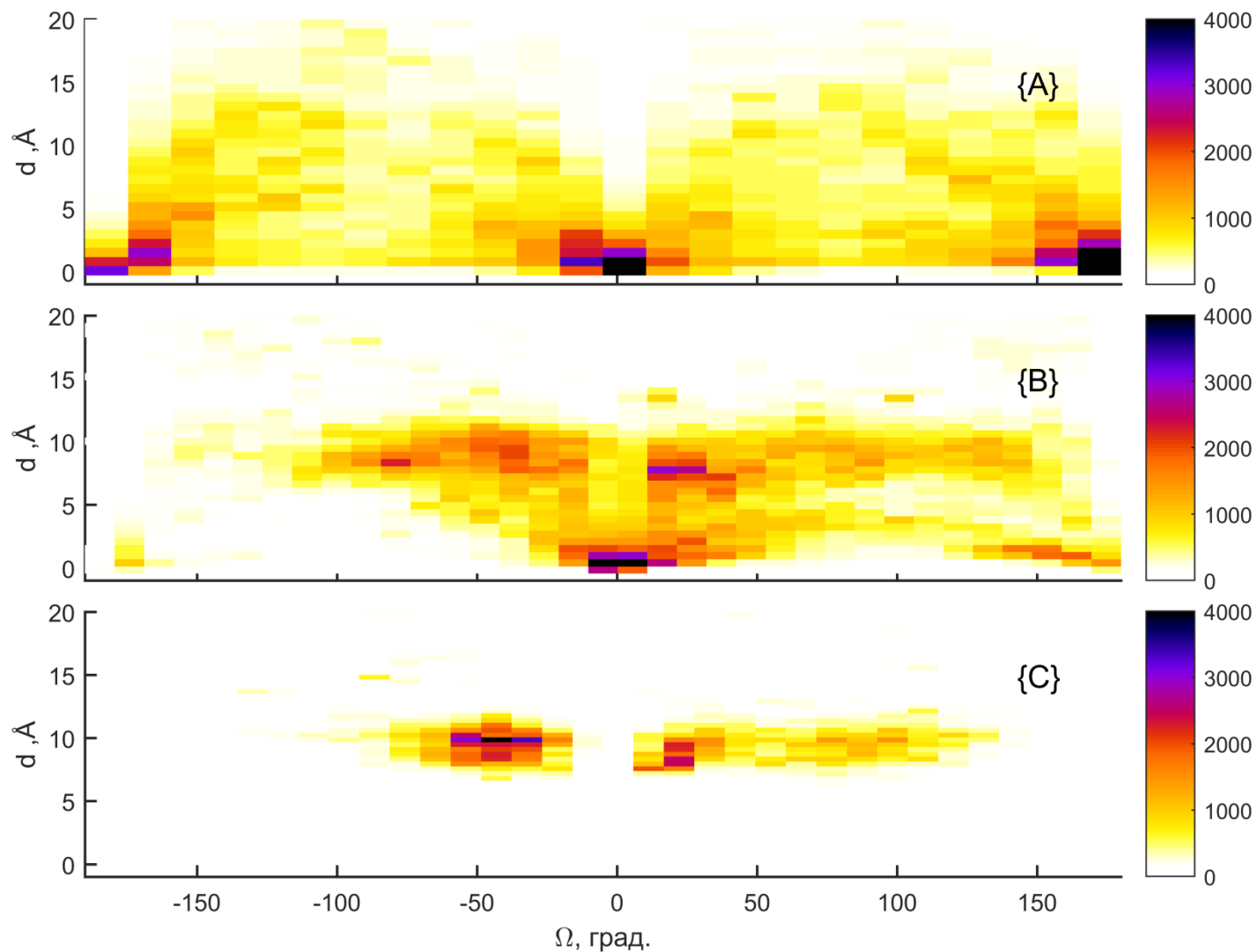
Distribution of helical pairs of HH type belonging to different subsets depending on the torsion angle Ω and the connection length N_p

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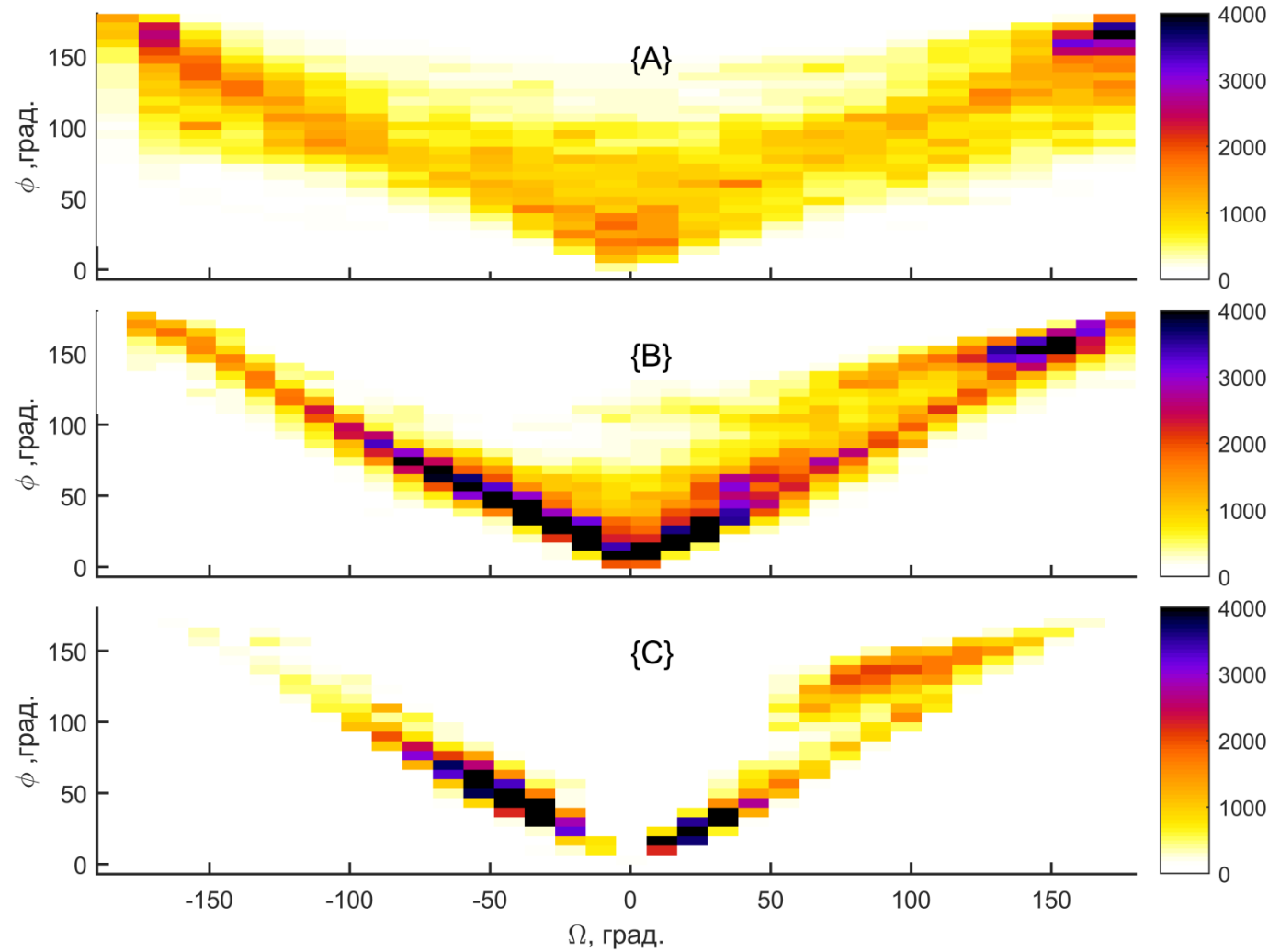


Distribution of helical pairs of HH type belonging to different subsets depending on the torsion angle Ω and the interplace distance d

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Distribution of helical pairs of HH type belonging to different subsets depending on the angle ϕ and the torsion angle Ω between the helical axes



In this study, an analysis of distribution of the torsion angles Ω between helical axes in pairs of connected helices found in known proteins has been performed. The database for helical pairs was compiled using the Protein Data Bank taking into account the definite rules suggested earlier. The database was analyzed in order to elaborate its classification and find out novel structural features in helix packing. The database was subdivided into three subsets according to criterion of crossing helix projections on the parallel planes passing through the axes of the helices. It was shown that helical pairs not having crossing projections are distributed along whole range of angles Ω , although there are two maxima at $\Omega = 0^\circ$ and $\Omega = 180^\circ$. It is shown that the distribution of all the helical pairs having the crossing helix projections has a maximum at $20^\circ < \Omega < 25^\circ$. The distribution of only α -helical pairs having crossing axes. projections has three maxima, at $-50^\circ < \Omega < -25^\circ$, $20^\circ < \Omega < 25^\circ$, and $70^\circ < \Omega < 110^\circ$.

Thank you for your attention!

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