

CHARACTERISTICS AND ROLE OF CONFORMATIONALLY PREDETERMINED SEGMENTS OF A POLYPEPTIDE CHAIN IN PROTEINS

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A beta-hairpin that includes a beta-bend can be viewed as an example of a composite local structure whose components play a different structural, energetic, and geometric role. In accordance with our concept, a fragment of an antiparallel beta-structure characterized by increased stability imposes a specific set of conformations on the linker. At the same time, the number of independent conformational variables decreases due to the formation of a pseudocycle of hydrogen bonds. As a result, the total number of conformations in this system does not exceed two for the main types of beta turns. Thus, the conformation of the beta-turn is determined by the context. It should be emphasized that beta-turn is in a certain conformation, regardless of the sequence, even if this conformation is sterically unprofitable (the so-called “forbidden” conformations). In this study, we studied the amino acid sequences and three-dimensional structures of beta turns of four types: I, I', II, and II'. Based on a representative dataset, we found that the sequence and structure together ensure the stability of the context part. In spite to predetermined character of the beta-bend some peculiarities in amino acid composition rather than in sequence take place. Contacts within beta-hairpin and its part as well as long-distance contacts were estimated by Voronoi-Delaunay tessellation. Degree of residues conservation in beta-structural part and in beta-bend separately was determined by the position-weight matrices. Possible biological implementations are discussed. This work was supported by the Russian Foundation for Basic Research (projects No. 17-04-02105 and 18-54-00037).

References

1. Torshin, I. Y., Batyanovskii, A. V., Uroshlev, L. A., Esipova, N. G., & Tumanyan, V. G. Noncanonical and Strongly Disallowed Conformations of the Backbone in Polypeptide Chains of Globular Proteins // *Biophysics* **63(2)**, 2018. Pp. 149-153.
2. Torshin, I. Y., Batyanovskii, A. V., Uroshlev, L. A., Esipova, N. G., & Tumanyan, V. G. The relationship between the sign of the polypeptide backbone angle omega and the type of the side chain radical of amino-acid residues // *Biophysics* **62(3)**, 2017. Pp. 342-347.
3. Torshin, I. Y., Uroshlev, L. A., Esipova, N. G., & Tumanyan, V. G. Descriptive statistics of disallowed regions and various protein secondary structures in the context of studying twisted beta-hairpins // *Biophysics* **61(1)**, 2016. Pp. 6-12.
4. Uroshlev, L. A., Torshin, I. Y., Batyanovskii, A. V., Esipova, N. G., & Tumanyan, V. G. Disallowed conformations of a polypeptide chain as exemplified by the beta-turn of the beta-hairpin in the alpha-spectrin SH3 domain // *Biophysics* **60(1)**, 2015. Pp. 1-9.