Is there a connection between peptide bond geometry and aminoacid residue conformational preferences?

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Abstract

The definition of the structural basis of the conformational preferences of the genetically encoded aminoacid residues is crucial to decipher the physical code of protein folding and would have a huge impact on our understanding of protein structure and function. Indeed, although a large number of computational and experimental investigations have highlighted that the different protein residues show distinct conformational propensities, none of the current hypotheses is able to satisfactorily explain these preferences.

In the last decades, we and others have clearly demonstrated that several geometrical parameters of protein backbone (bond angles, peptide bond distortions from planarity, and pyramidalization of the carbonyl carbon atom) are heavily dependent on the local conformation (φ/ψ dihedral angles) [1-8]. Moreover, a correlation between bond distances such as CO and CN has been detected in ultrahigh resolution protein structures [9]. Concerning bond angles, most of these investigations have been focused on the $NC^{\alpha}C$ (τ) angle, shown to be significantly affected by both φ/ψ dihedral angles. In this framework, we here evaluated the impact of the local geometry on the residues conformational preferences by performing statistical analyses on a dataset of non-redundant protein chains selected from the Protein data Bank (PDB). Our data highlight a clear link between residue conformational preferences and local geometry.

References

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