Unveiling the ω/ψ Correlation in High Resolution Protein Structures

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The planarity of the peptide group is one of the fundamental features of protein structures. Several investigations on peptide bond distortions have been reported [1]. Here we present a statistical survey of peptide plane deviations analyzed as a function of the local conformation of the backbone. By surveying a dataset of 163 non-homologous protein chains, determined at atomic resolution, we have identified the stereochemical conditions that favor significant deformations of peptide bond planarity. In particular, the values of the ω dihedral angle are found to be strictly correlated to the values of the adjacent ψ angle [2]. This trend is also observed in highly strained states such as those occurring in vicinal disulfide bridges. The dependence of the ω angle on the ψ angle is similar to that already observed for a different type of deviation from peptide planarity: the pyramidalization at the carbonyl carbon atom [3].

These findings provide direct evidence for the mutual influence of the geometrical parameters that describe protein structures.

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