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The fine structure of proteins: detection and implications

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Pictures of protein three-dimensional structures heavily decorate every biochemistry textbook. These representations highlight the complexity and the structural versatility of these fundamental biological players. As the remarkable molecular complexity of proteins is generally coupled with a fine structural regulation, a full understating of their functionality is a challenging task. Indeed, fundamental protein activities often rely on extremely subtle structural details that may fall in the low (or even sub) picometer scale. Investigations carried out over the last two decades by us and other groups have demonstrated that protein structures are endowed with important subtle features that have been somehow overlooked. Indeed, statistical surveys of protein structure ensembles and quantum chemistry calculations have unraveled the variability of some geometrical parameters of the protein backbone (bond lengths, bond angles and peptide bond planarity). These studies have highlighted clear and precise correlations between these parameters and the local conformation expressed in terms of (φ,ψ) values of the Ramachandran Space.

In our ongoing research activities, we are exploiting this conceptual framework to address basic questions related to protein structure. By analyzing the entire structural content of the Protein Data Bank we have shown that the analysis of protein fine structure represents a valuable tool for rapid structure quality assessment. A user friendly web server that performs these analyses is under development (QuiProQua – QUIck PROtein structure QUAlity assessment http://study.ibb.cnr.it/quiproqua/index.php). Moreover, we have also demonstrated that this fine structure plays a major role in dictating the secondary structure preferences of aminoacyl residues in proteins. Finally, we are evaluating the ability of force fields commonly used in molecular modeling and dynamics to reproduce these subtle, but important, structural features.