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The analysis of protein fine structure is a valuable tool for quality assessment

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Proteins combine molecular complexity and fine structural regulation. Although protein crystallography provided an enormous contribution to the development of structural biology, crystallographic data are generally not sufficient for effective protein structure refinements. In this framework, the assessment of the validity/quality of three-dimensional models represents a fundamental step in the structure determination process. Although impressive advances have been done [1], there are several unmet needs in this field. We and others have shown that backbone geometry and planarity of individual protein residues strongly depend on their local (φ,ψ) values [2-10]. By analysing the whole structural content of the Protein Data Bank (PDB), we here show that the variability of backbone geometry and planarity can be individually detected in the vast majority of protein structures including those refined at low/moderate resolution (Fig. 1). Our data demonstrate that the detection and the analysis of these fine structural elements are strongly correlated with the overall accuracy of individual structures. These findings clearly indicate that the evaluation of these subtle parameters represents an innovative and valuable tool for structure quality assessment. A web server for the automatic evaluation of the local and global quality of protein structures is under development (QuiProQua – QUIck PROtein structure QUAlity assessment).

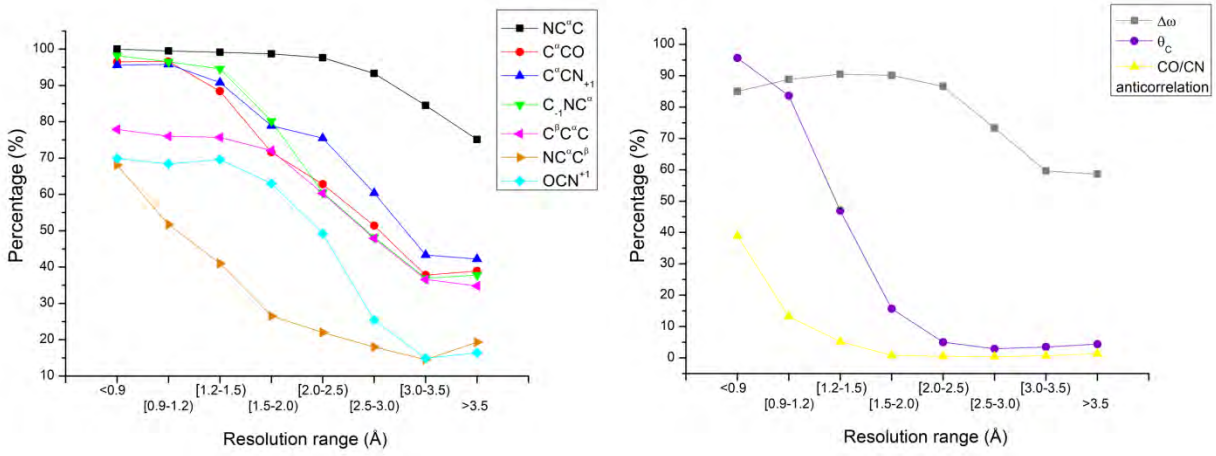

Figure 1. Percentage of PDB structures that show the geometry-conformation interplay for that parameter.

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