Poster Presentation

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Local dynamics of proteins and DNA evaluated from crystallographic B-factors

B. Schneider[1], J. Gelly[2], A. de Brevern[2], J. Černý[1]

[1]Institute of Biotechnology AS CR, Prague, Czech Republic, [2]University Paris Diderot, Sorbonne Paris Cité, UMR_S 1134, Paris, France

Temperature displacement factors also known as B-factors provide information about local dynamics of atoms. Because dynamic behavior of biomolecules is as important as their static molecular structures we decided to analyze B-factors in almost a thousand non-redundant crystal structures of protein-DNA complexes from a well-curated dataset described in Schneider et al. Nucleic Acids Research, 42 (2014). Biopolymer residues, amino acids and nucleotides, were classified according to their molecular neighborhood as solvent-accessible, solvent-inaccessible (buried, i. e. forming the protein core), or lying at protein-protein or protein-DNA interfaces. In addition, water molecules were labeled as solely bound to the biopolymer surface as the first hydration shell or as water bridges binding protein and DNA molecules. Distributions of scaled B-factors for these types of residues confirmed several expected features of protein and DNA dynamics but they also revealed some surprising facts. Solvent-accessible amino acids have B-factors larger than residues at both biomolecular interfaces and amino acids forming protein core are restricted in their movement the most. A really unique feature of the buried amino acids is that their side chains are restricted in their movements more than the main chains. Protein interior is therefore packed significantly better than protein-protein or protein-DNA interfaces. Low values of B-factors of the waters bridging protein and DNA molecules contrast with extremely high values of DNA phosphates. Characteristic features distinguishing different types of residues quickly vanish in structures with lower resolution and some of the observed trends are a likely consequence of improper refinement protocols that may need rectifying. Acknowledgments. This study was supported by BIOCEV CZ.1.05/1.1.00/02.0109 from the ERDF and by grant P305/12/1801 from the Czech Science Foundation.

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