ELECTROSTATIC POTENTIAL AT THE ALPHA CARBON ATOMS ALONG THE ALPHA HELICES AND BETA STRANDS

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The process of protein folding might be investigated by analyzing the secondary structure elements (SSE). We present here analysis of pre-calculated values for the electrostatic potential at the alpha carbons, previously stored in the STING_RDB. We have constructed the new module added to the BlueStarSTING suite, named "Java Secondary Structure Dossier", where a user may visually and numerically observe and analyze per residue reported structure descriptors for the SSE: alpha helices and beta strands. Our procedure was to first separate the proteins from the PDB according to their classes: all alpha, all beta, alpha + beta and alpha/beta. All SSE were grouped and aligned with respect to their length. All aligned SSE, were then analyzed in terms of 47 sequence/structure descriptors (grouped in 32 major classes) such as: electrostatic potential, sequence conservation, hydrophobicity, accessibility, dihedral angles, internal contacts etc. Special attention in analysis of collected data was given to electrostatic potential at different atoms: alpha carbons (EPac), Last Heavy Atoms in the side chain, average value over all atoms of the residue and the EP at the protein surface of the residue which is accessible to solvent. We found a clear tendency for EPac for alpha helices and beta strands, both having negative values but showing distinct form. Consequences of this finding are discussed in terms of structure prediction.