

SIGNATURE CONTACT COORDINATION PATTERNS FOR SECONDARY STRUCTURE ELEMENTS IN PROTEIN STRUCTURES

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The contact patterns within and around the secondary structure elements (SSE) might shade some light into the process of protein folding and nucleation. We present here analysis of pre-calculated values for the cross-links, previously stored in the STING_RDB. The Cross Links are defined as contacts (any type from possible 5 classes: Hydrophobic, Hydrogen Bonding, Aromatic Stacking, Salt bridging and Cystein-bridging) established among residues that are far apart in the protein primary sequence, but are close in its 3D fold. The order of cross link is identified as a number of such cross-links established among independent stretches of sequence (the size of which was fixed to 30 Amino Acids). The higher the order, the more important that residue must be for the protein folding/stability. Our procedure for this work was to first separate the proteins from the PDB according to their classes: all alpha or all beta. Special attention in analysis of collected data was given to the order of cross links along the secondary structure elements. We found a clear and opposing tendency for the value of cross links for alpha helices and beta strands, showing less and more, respectively, cross links in comparison to the other parts of proteins. Consequences of this finding are discussed in terms of structure prediction.