

P009 β -sheet capping: signals that initiate and terminate β -sheet formation

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In the present work, we address the question that whether different amino acids have different β -sheet initiating and terminating characteristics. Using a large scale analysis of parallel and antiparallel β -sheets in a non-redundant dataset of proteins, we observed that most of the amino acids show significant under- or over-representation in at least one of the positions at the two ends of β -sheets, which are denoted as N-cap and C-cap. In addition, based on statistical data and structural comparison, we found that certain amino acids, especially Asp, Asn, Gly and Pro have strong tendencies to block β -sheet continuation. Hence, we can consider these residues as β -sheet terminators. It was also proposed that the dipole moments in parallel β -sheets, whose direction is from C-terminal (partially negative) to N-terminal (partially positive), are much stronger than what previously has been suggested. In fact, enhancement of dipole moments in parallel β -sheets is a result of positioning of positively charged residues at N-cap and negatively charged residues at C-cap. This enhancement in dipole moment magnitude leads to strengthen dipolar interactions between parallel β -sheets dipoles and other partners especially β -helices dipoles. The results provide explanation for antiparallel alignment of parallel β -sheets with α -helices.