

BITS :: Call for Abstracts 2024 - Oral communication

<i>Type</i>	Oral communication
<i>Session</i>	Proteins
<i>Title</i>	Deciphering Beta Turn Diversity: Unveiling the Role of Carbonyl-Carbonyl Interactions
<i>All Authors</i>	D'Arminio N(1), Ruggiero V(1,2), Pierri G(1), Marabotti A(1), Tedesco C(1)
<i>Affiliation</i>	(1) Department of Chemistry and Biology "A. Zambelli", University of Salerno, Fisciano Italy (2) Present address: Department of Pharmacy, University of Salerno, Fisciano Italy

Motivation

A folded polypeptide chain adopts specific conformations characterized by backbone torsion angles ϕ and ψ , forming secondary structures like helices, strands, and turns. Beta turns, a prevalent non-repetitive secondary structure, involve four consecutive residues where the chain reverses direction, with the distance between α -carbon atoms of residues i and $i+3$ lower than 7 Å.

Venkatachalam (1968) identified three beta turn conformations (types I, II, III) defined by specific ϕ , ψ angles and intraturn hydrogen bonding. Lewis et al. (1973) expanded this definition, identifying additional turn types (IV-VII), with some lacking the intraturn hydrogen bond.

Richardson (1981) categorized beta turns, confirming type VI's cis-proline residue and further dividing it into VIa (mostly H-bonded) and VIb (mostly not H-bonded). Wilmot and Thornton (1988) added type VIII, then, Hutchinson and Thornton (1994) distinguished VIa1 and VIa2. The current classification (Hutchinson & Thornton, 1996) includes eight types plus a miscellaneous type, considering deviations from ideal ϕ , ψ values.

De Brevern (2016) identified four new types from the miscellaneous group. Shapovalov et al. (2019) proposed 11 more types, introducing a new nomenclature based on Ramachandran regions.

Newberry and Raines (2019) highlighted weak interactions' role in protein folding, such as C-H...O hydrogen bonding and $n \rightarrow \pi^*$ interactions. These interactions influence beta turn classification. Carbonyl-carbonyl interactions, including $n \rightarrow \pi^*$ and reciprocal carbonyl-carbonyl ones, are crucial in peptides, proteins, and polymers.

This work surveys carbonyl-carbonyl interactions in peptides and beta turns, suggesting a classification based on these interactions alongside backbone dihedral angles.

Methods

The examination of beta turns in protein structures relied on a meticulously curated dataset sourced through PISCES, comprising 1424 X-ray protein structures meeting stringent criteria for resolution, R-factor, and sequence identity, resulting in a finalized dataset named TotalSet, housing 28,828 beta turns.

From this TotalSet, a subset named CuredSet was created, isolating 9440 non-overlapping and non-adjacent beta turns from 1386 protein chains for subsequent analysis. Computational tasks were executed using R programming with the Bio3D package and in-house scripts.

Protein PDB files were segregated by chains as per PISCES selection criteria. Beta turns were identified using BetaTurnTool18, a Python2-based software relying on DSSP.

Each beta turn's carbonyl-carbonyl distances were calculated, including reciprocal distances, alongside the distance between the first and fourth residues' carbonyl oxygen and amino nitrogen atoms, respectively. Torsion angles and Bürgi-Dunitz angles within detected beta turns were measured using Bio3D.

Beta turns of similar types were grouped, and statistical analyses were conducted, encompassing carbon and oxygen distances' minimum, maximum, mean, median, mode, standard deviations, and percentages meeting certain distance criteria.

Results

Several interaction patterns emerged for each beta turn type, indicating distinct structural characteristics. For instance, type I and type I' beta turns exhibited direct carbonyl-carbonyl interactions between the first two residues and hydrogen bonding between the first and fourth residues. Our study uncovered a previously unrecognized type II beta turn, featuring direct carbonyl-carbonyl interactions between the second and third residue, and hydrogen bonding, distinguishing it from other types. An analysis of the amino acid distribution for this new type II beta turn revealed predominance of glycine residues on second position. Type VI beta turns were clustered into subgroups based on structural features. Specifically, the PcisD type involves carbonyl interactions between the first and second residue, both direct and reciprocal ones. The BcisP type exhibits bimodal values in both distances between the third and fourth residue, while the PcisP type displays bimodal values for both interactions between the first and second residues and between the third and the fourth one. Type VIII beta turns were categorized into AB1, AB2, AG, and AZ subgroups, each with unique structural motifs. For this type of turn, hydrogen bonding is absent, while interactions between carbonyl groups are present, emphasizing their role in stabilizing the structure. These findings expanded the classification of beta turns and provided insights into their structural diversity, shedding light on their significance in protein folding and stability. Finally, these new discoveries pave the way for the development of novel tools capable of more precisely identifying these important secondary structures. Such advancement is crucial in the fields of structural biology and drug design as it

allows for a more accurate understanding of protein structure and its interactions.

<i>Info</i>	
References	
D'Arminio N, Ruggiero V, Pierri G, Marabotti A, Tedesco C. Emerging role of carbonyl-carbonyl interactions in the classification of beta turns. Protein Sci. 2024 Feb;33(2):e4868. doi: 10.1002/pro.4868. PMID: 38100281; PMCID: PMC10806932.	
<i>filename</i>	-
<i>Figure</i>	
-	
<i>Availability</i>	-
Dissemination Material	
<i>Social</i>	
-	
<i>Summary</i>	
-	
Corresponding Author	
<i>Name, Surname</i>	Anna , Marabotti
<i>Email</i>	amarabotti@unisa.it
<i>Submitted on</i>	02.05.2024

Società Italiana di Bioinformatica

C.F. / P.IVA 97319460586

E-mail bits@bioinformatics.it

Sede legale Viale G. Mazzini, 114/B - 00195 Roma

Website bioinformatics.it

message generated by sciencedev.com for <https://bioinformatics.it> 14:33:18 02.05.2024
