Twisted ribbon structure stablized by C12 helical turns in γ/α peptide

Junaid ur Rahim,[a,b] Gazanfor ali,[d] Sudha Shankar,[a,b] Umesh Prasad Singh,[c] Rajkishor Rai*[a,b]

[a] Medicinal Chemistry Division, CSIR-Indian Institute of Integrative Medicine Jammu, India.
[b] Academy of Scientific and Innovative Research, New Delhi, India.
[c] CSIR-Indian Institute of Chemical Biology, Kolkata, India.
[d] National Institute of Technology Srinagar, India.
Email Id. iiim.junaid@gmail.com

Abstract: The β-bend ribbon, formed by the repetition of -turns, is a structural element in proteins. Such kind of structures has been examined in the peptaibols isolated from fungi.[1] Theoretical studies have suggested that successive -turns in proteins form the flat or twisted ribbon structures, depending on the type of -turns.[2] The ribbon structures have been generated by the repetition of Pro-Xxx and Xxx-Pro (Xxx=Aib, Ala, or D-Ala) sequences, in which Pro residue interrupts the conventional hydrogen bonding pattern in helices at alternate positions in β-peptide sequences.[3] Proline (Pro) residue plays an important role in the design of peptides due to presence of pyrrolidine ring restricting the ϕ value to ~ -60°± 20°.[4] Herein, we describe the solid state conformations of peptides, Boc-γ^4-L-Phe-L-Pro-NHMe (**P1**) and Boc-γ^4-L-Phe-L-Pro)$_2$-NHMe (**P2**) as determined by X-ray crystallography. Peptide **P1** adopts twelve membered (C_{12}) helical turn over γα segment, while **P2** folds into twisted ribbon structure involving two expanded C_{12} helical turns.In addition, CH...π and π-π interactions are observed between the same pair of symmetry related molecules. The helical γα turns observed may be extended to generate twisted ribbon structures involving C_{12} intramolecular hydrogen bonds.

Keywords: hybrid peptides; folded conformation; expanded turn; twisted ribbon; C_{12} conformation.

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