



IIT Guwahati

Lecture 6

Course BT 631

Protein Structure function and Crystallography

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Ramachandran plot

Ramachandran Plot was given by Professor G.N. Ramachandran in 1969.
(published in Journal of Molecular Biology).



Ramachandran Plot defines Sterically allowed and disallowed Φ and Ψ angles calculated by vander Waals distances. **e.g. distances allowed for C---O is 2.8 \AA and C---C is 3.0 \AA .**

Similarly, CH_3 group has a radius of 1.7 \AA , so any other methyl group (alanine) coming below 3.5 \AA is sterically disallowed.

While all the allowed range of conformation is defined as contour area which include α -helix and β -Sheet.

Ramachandran plot

There are restrictions induced by side chain of amino acids which is meant for selective allowed value of Φ and Ψ angles.

The intra-molecular interactions cause some deviations in Φ and Ψ angles and make unfavorable conformation.

Glycine with H which is the smallest atom as side chain can adopt any Φ and Ψ angle.

Ramachandran plot

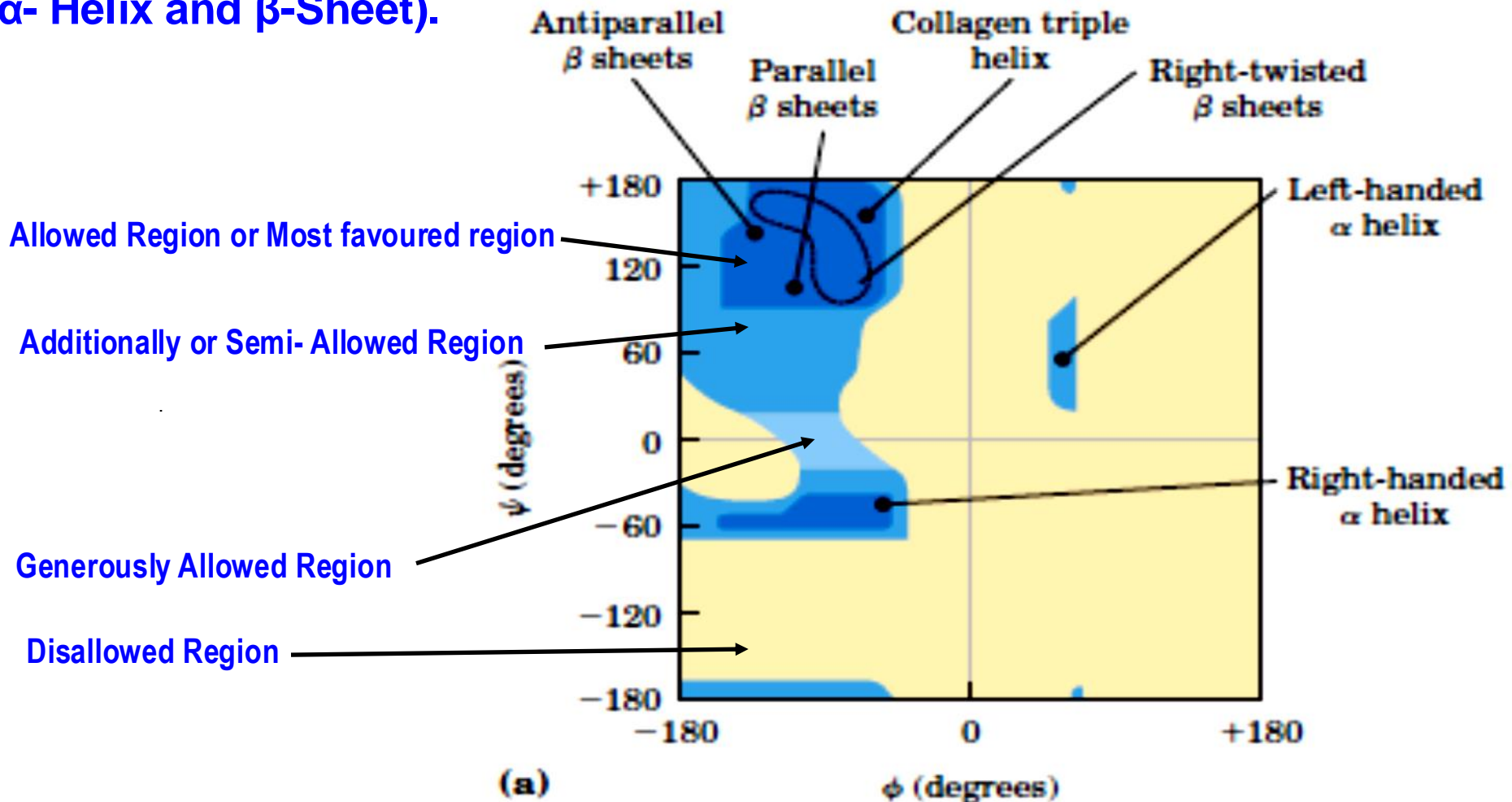
Ramachandran plot explains the **conformational angle of the amino acid residue** that appears in the primary structure.

The region with normal vander walls distances comes under the allowed region, while the outer limit of vander walls distances fall under semi-allowed region.

Ramachandran plot

Significance of Ramachandran Plot

Ramachandran plot is used to calculate the probability of a polypeptide to form secondary structure (α - Helix and β -Sheet).



Ramachandran plot

Softwares for validating protein structure

1. Procheck
2. Molprobit
3. Rampage

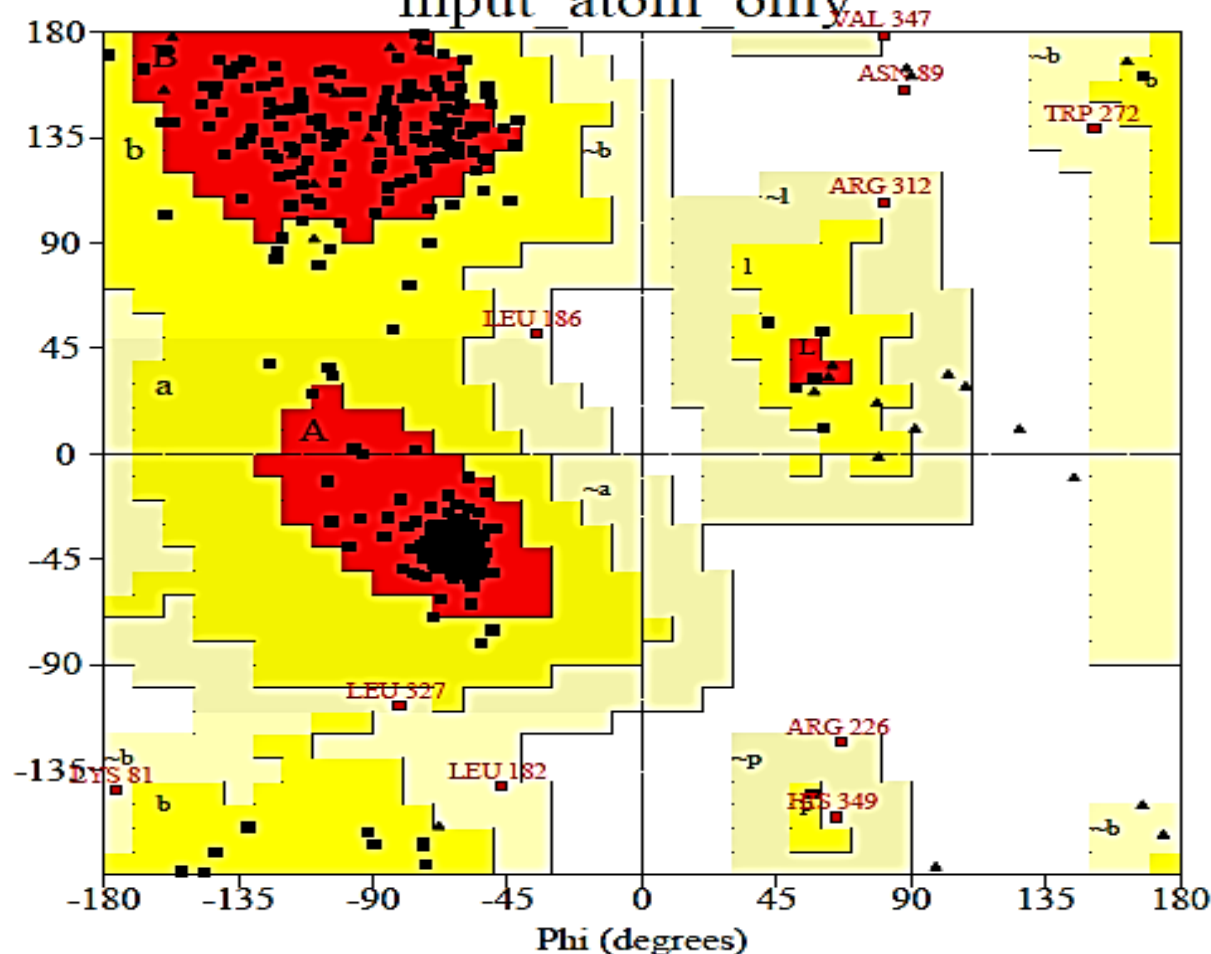
Ramachandran Plot

Xylanase (Family 10 Glycoside Hydrolase, GH10)

PROCHECK

Ramachandran Plot

input_atom_only



Plot statistics

Residues in most favoured regions [A,B,L]	Red	282	84.9%
Residues in additional allowed regions [a,b,l,p]	Yellow	40	12.0%
Residues in generously allowed regions [~a,~b,~l,~p]	Light Yellow	8	2.4%
Residues in disallowed regions	Blue	2	0.6%
<hr/>			
Number of non-glycine and non-proline residues		332	100.0%
Number of end-residues (excl. Gly and Pro)		2	
Number of glycine residues (shown as triangles)		32	
Number of proline residues		11	
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Total number of residues		377	

Note the Glycine residues as triangles in disallowed region