

Variation of conformational propensity of different amino acids within disallowed and allowed regions of the Ramachandran Plot

by

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Introduction

➤ The backbone conformation of amino acids in proteins is represented mainly by two torsion angles; ϕ and ψ . Ramachandran map is a way to visualize these torsion angles in protein structures.

➤ Here we analyze the nature and distribution of disallowed and allowed/disallowed Ramachandran conformations of amino acids observed in protein structures.

Material & Method

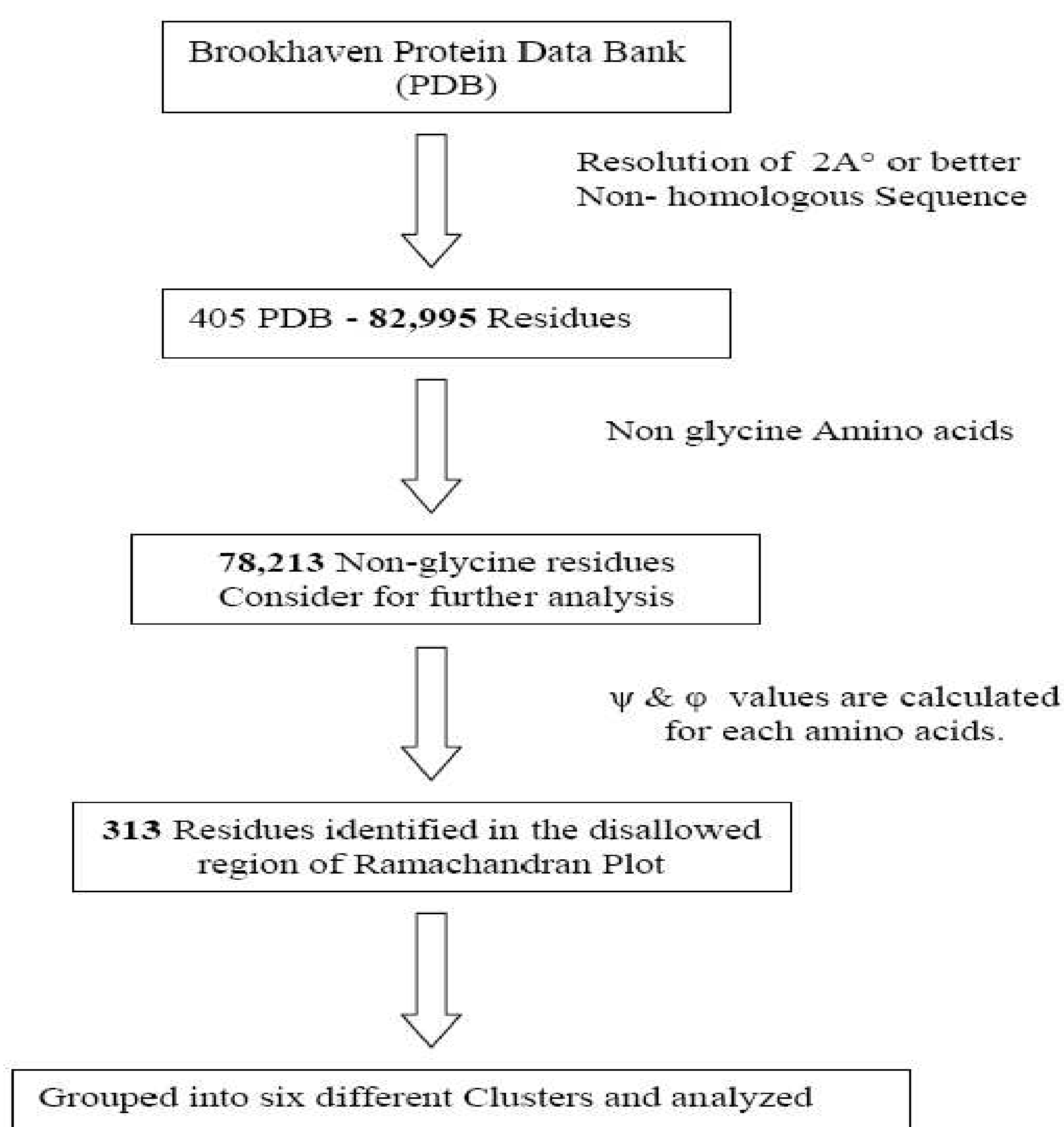


Fig -1: Flow chart depicting the scheme used in the selection of 313 disallowed residues from the Brookhaven Protein Data Bank

Analysis of Conformational Propensities in Disallowed & Allowed regions

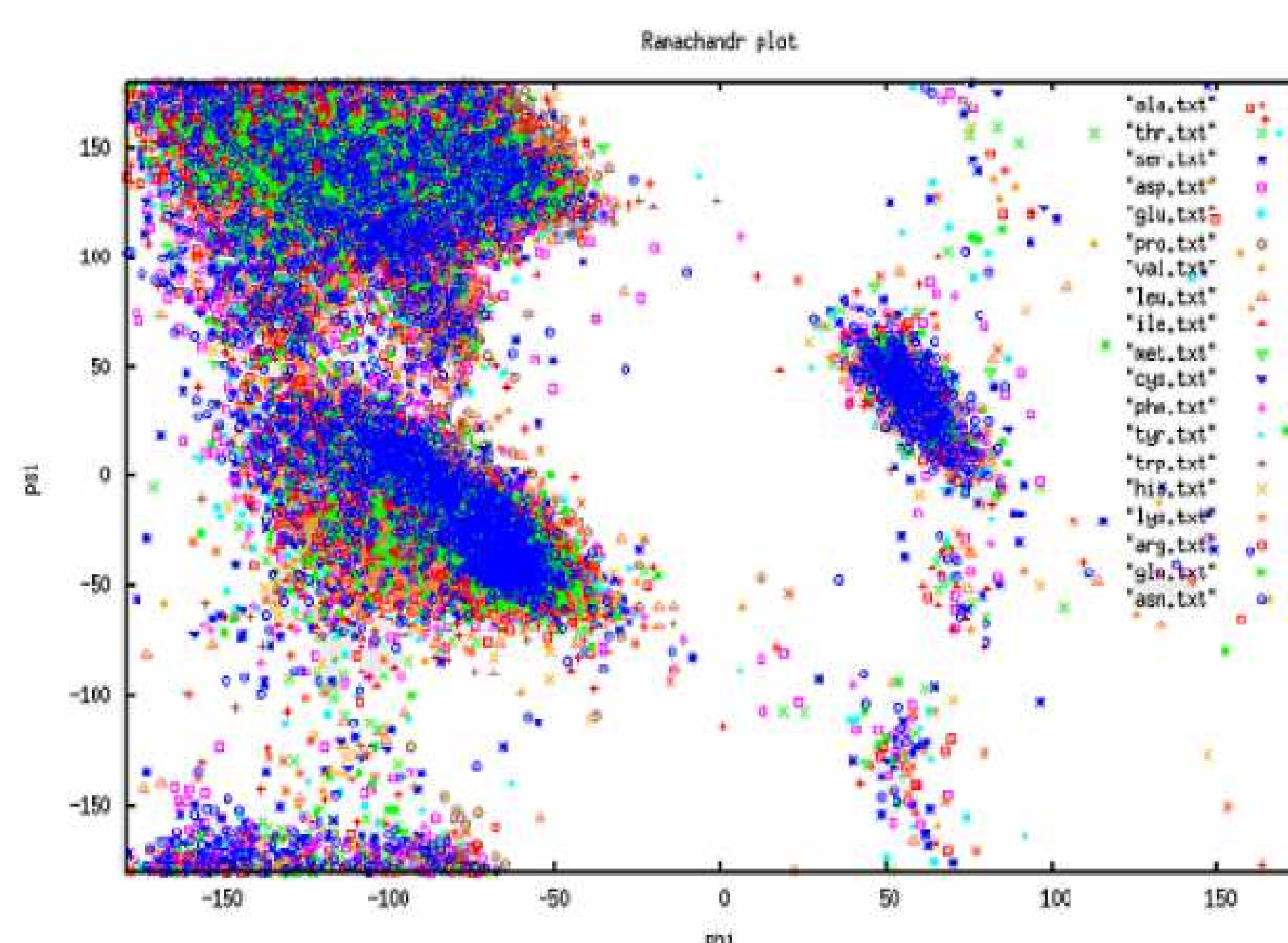


Fig-2: Conformational propensity of 78,213 non-Gly residues (Ramachandran Plot)

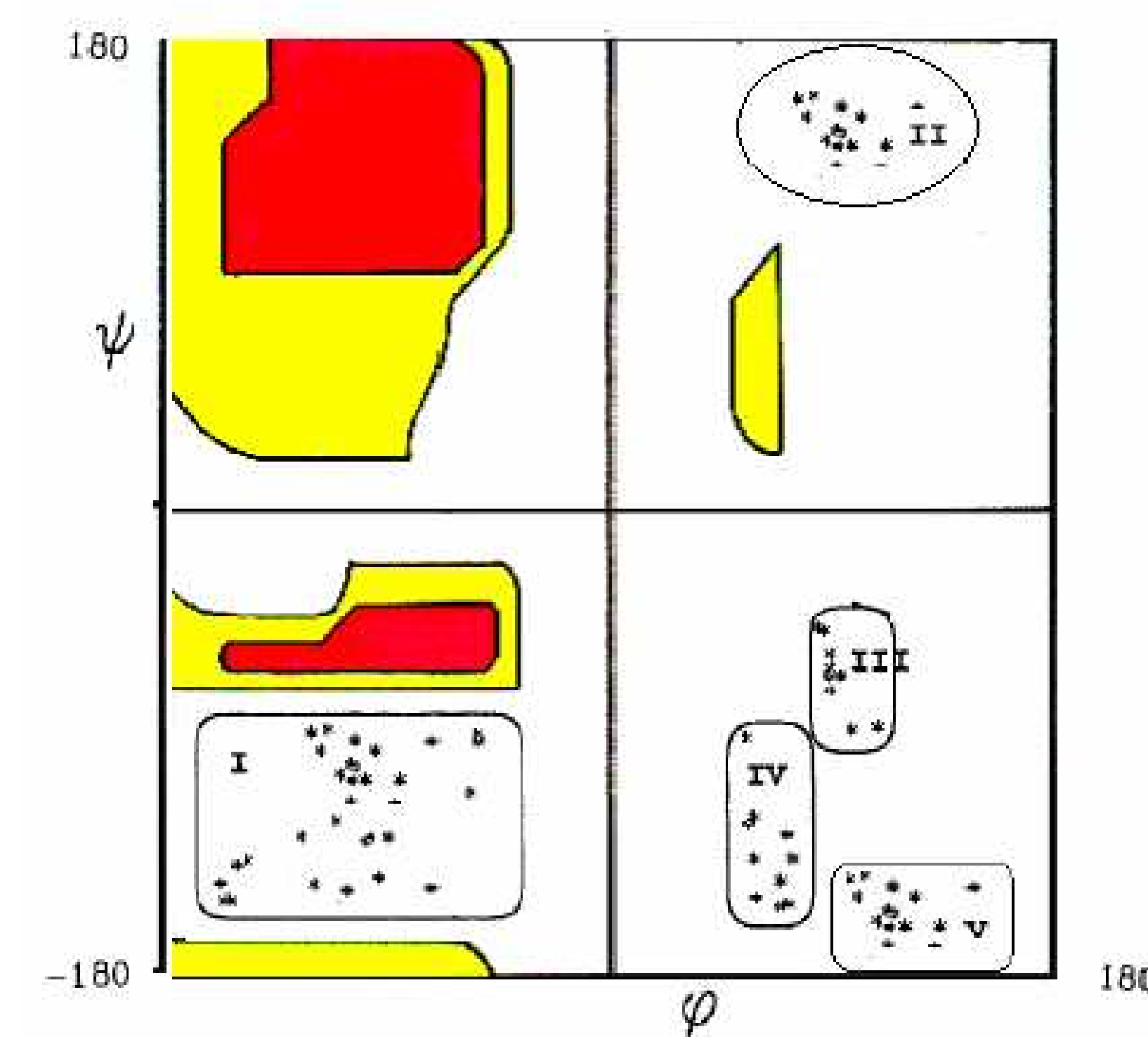


Fig-3: Showing Clustering in the disallowed region of Ramachandran Plot

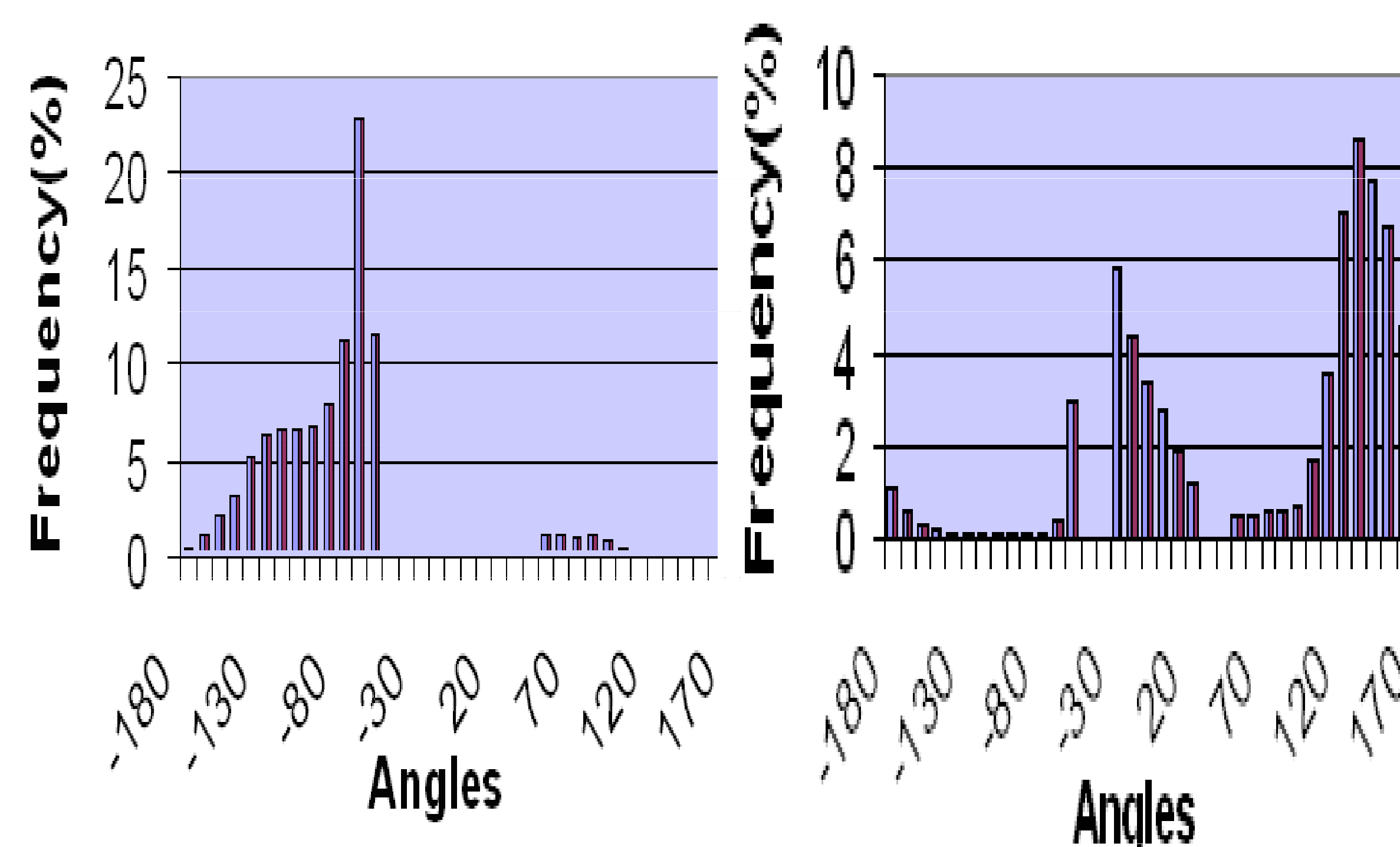


Fig -4: Distribution of ϕ & ψ angle in the allowed region

Analysis

Residue	C-I	C-II	C-III	C-IV	C-V	*C-VI	Frequency
ALA	8	2	3	1	3	9	26
THR	6	5	6	2	3	4	26
SER	10	8	3	1	14	4	40
ASP	8	4	7	4	13	5	41
ASN	10	4	4	0	9	12	39
PRO	1	0	0	0	0	1	3
LEU	8	0	2	0	2	3	15
ILE	0	0	6	0	0	2	8
MET	1	0	0	0	2	0	3
CYS	4	2	0	0	2	0	10
PHE	0	0	1	0	0	2	3
TYR	1	0	1	0	0	1	5
TRP	1	0	1	0	0	1	3
HIS	7	1	0	0	1	7	16
LYS	10	0	2	0	5	8	25
ARG	1	3	1	0	6	0	11
GLN	4	1	1	0	5	3	14
VAL	0	3	1	0	1	3	8
GLU	4	1	1	1	5	2	14
Total	84	34	40	9	71	75	313(Outliers)
Count							

*C-VI-Corresponds to the rest of the portion of Ramachandran plot

Table-1: Analysis of Disallowed Residues

Conclusion

- Very small fraction of residues (~0.4 %) lie in appreciably disallowed regions
- Small polar/charged residues Asn, Asp, Ser, Thr showed greater probability of adopting unusual backbone.
- The bulky charged residues Glu, Lys, Gln and Arg have a relatively low propensity for backbone distortions.
- Bulky hydrophobic residues, found predominantly in well packed interiors of proteins like Ile, Val and other aromatic amino acids like Phe, Trp and Tyr do not generally adopt disallowed conformation
- In the allowed region irrespective of the type of amino acid except Gly:

For ϕ : { -70,-60}
For ψ : {140:150}