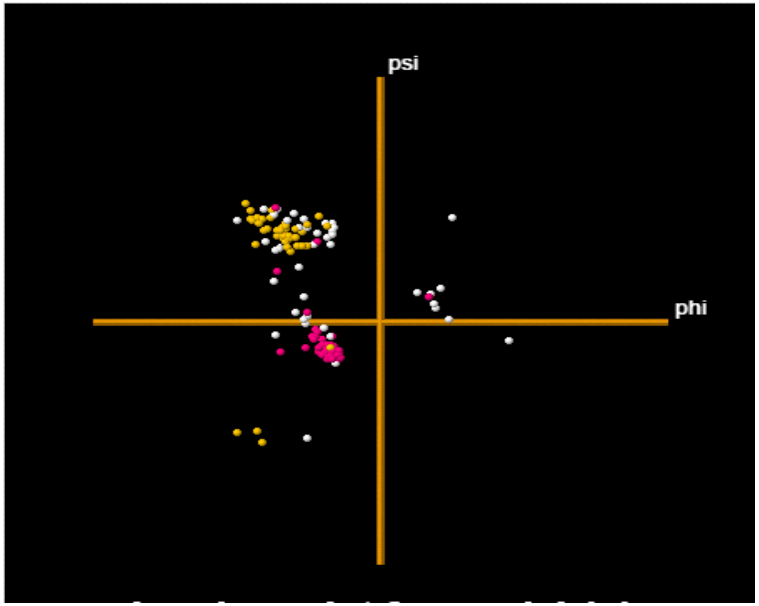
TAMIL NADU AGRICULTURAL UNIVERSITY

RAMACHANDRAN PLOT



Submitted by

Nishanth S

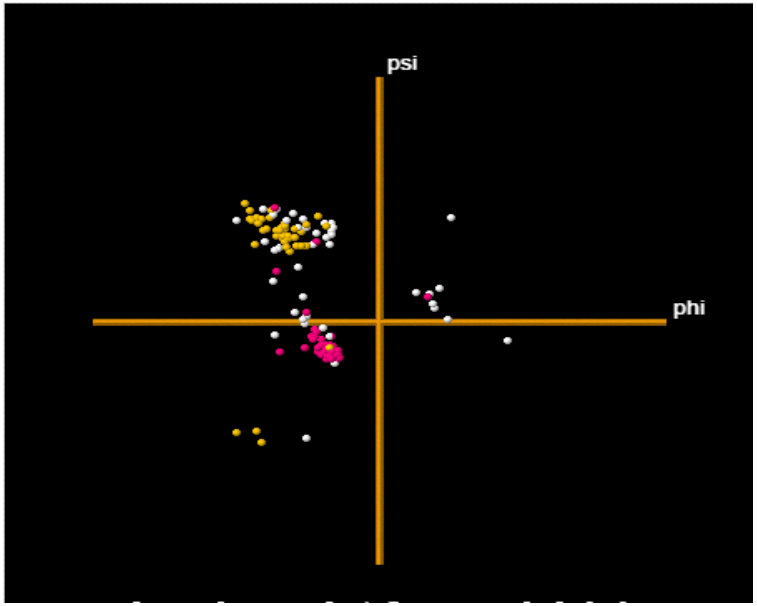
Introduction

- **Ramachandran plot** – to visualize the backbone of aminoacid residues (1963 - Collagen)

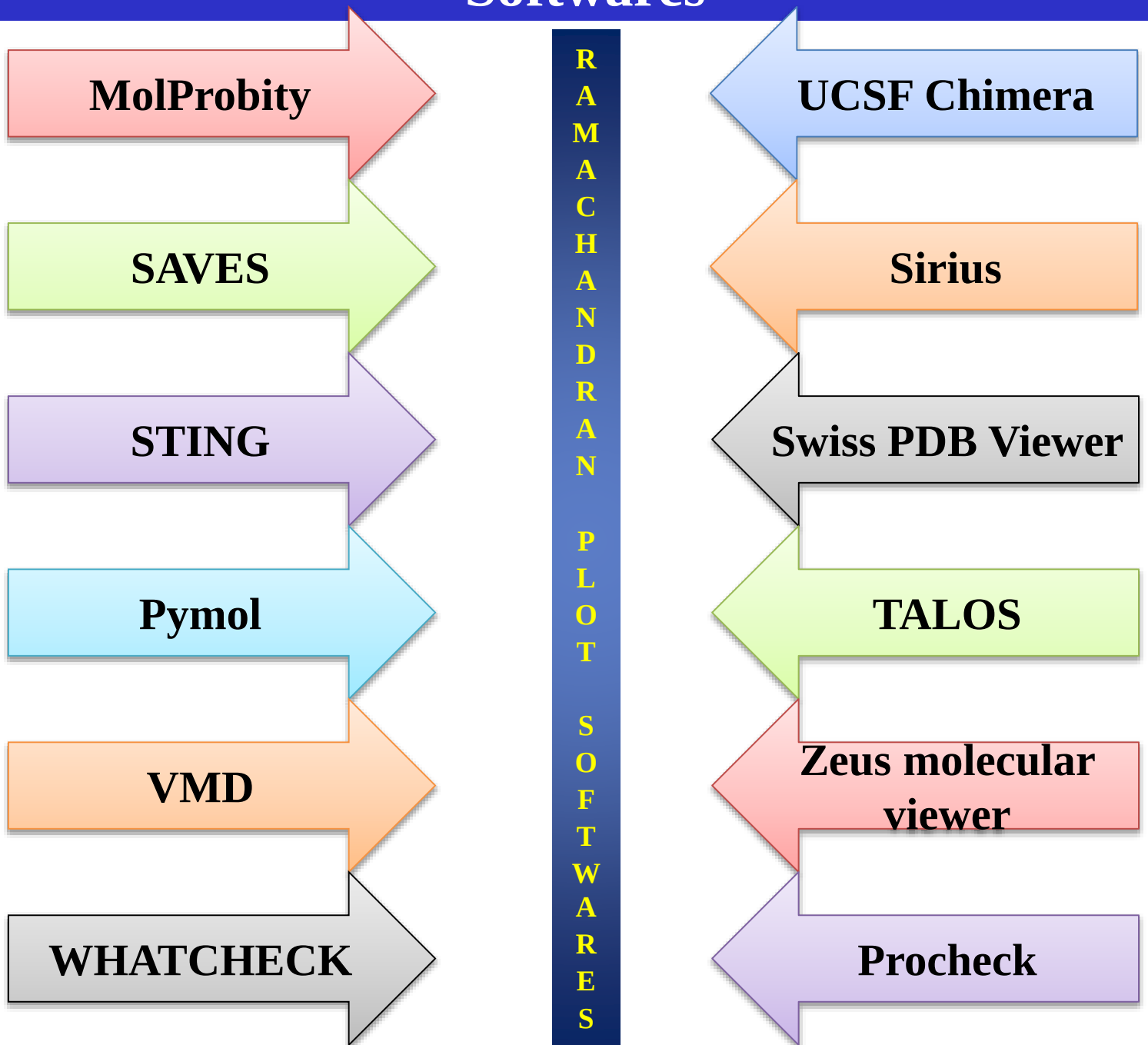
- Used for **structural validation** and to calculate the possible **phi and psi angles** that accounts for the aminoacid residues.

- Done by several software namely **WHATIF** RAMACHANDRAN PLOT

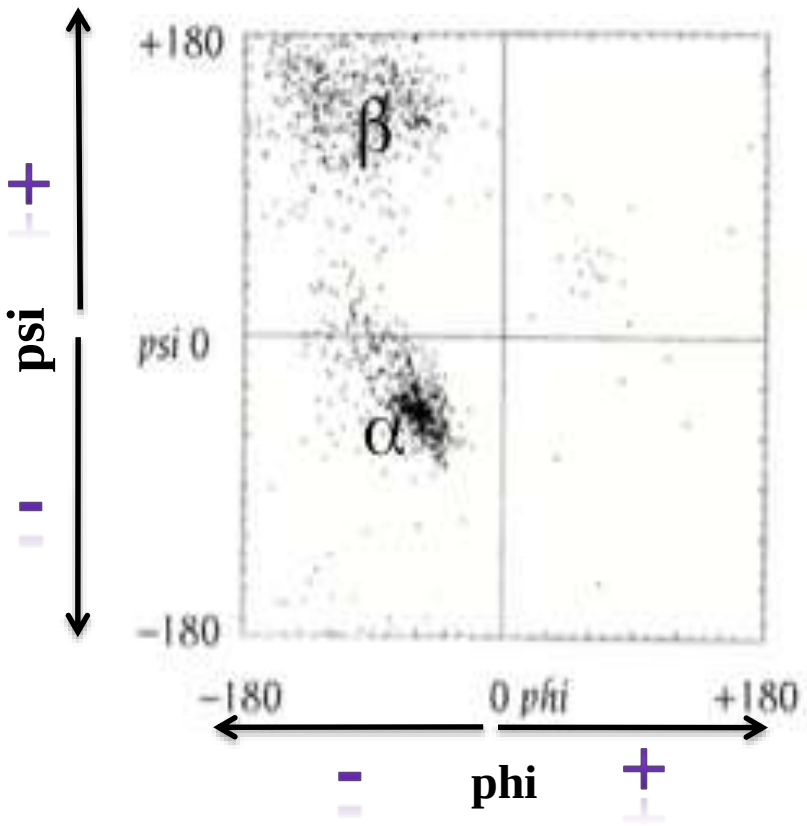
Ramachandran G N
Ramakrishnan C
Sasisekharan V



Softwares


MolProbity
SAVES
STING
Pymol
VMD
WHATCHECK
RAMACHANDRAN PLOT SOFTWARES
UCSF Chimera
Sirius
Swiss PDB Viewer
TALOS
Zeus molecular viewer
Procheck

Ramachandran plot



Horizontal axis - φ values

Vertical axis - ψ values

Dot on the plot - angles for an AA

Counting: -180 → +180

(vertical and horizontal axes)

Allowed / Low-energy region:

The regions on the plot with the highest density of dots

Steric clash: Additional interactions → to stabilize such structures.

(They may have ***functional significance*** and may be ***conserved within a protein family***)

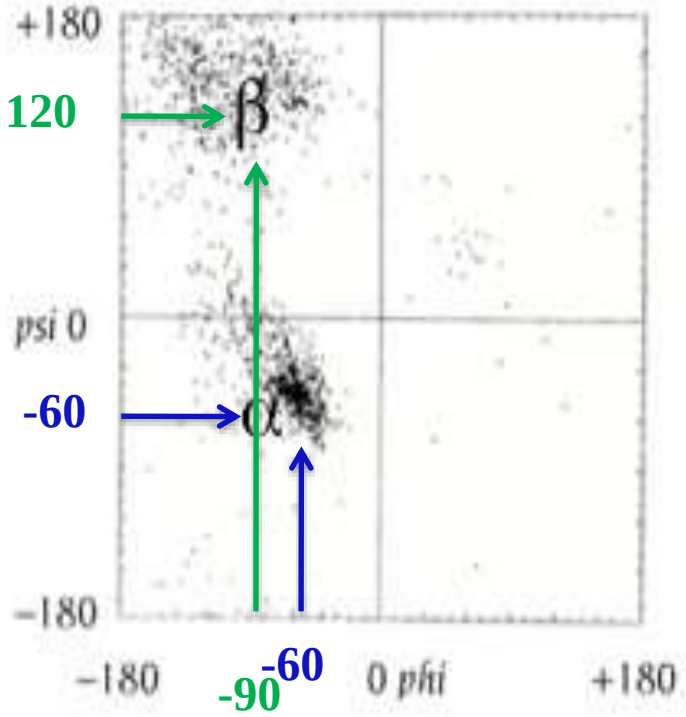
Pal and Chakrabarti (2002)

Distribution over the map

The distribution of phi and psi angles for a total of **9,156 AA residues** from **4,413 protein chains** – ***crystallographic data***.

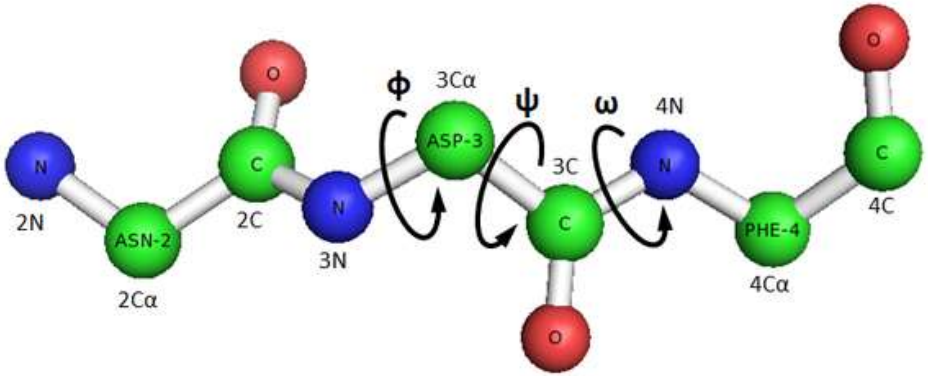
Two areas where the density of points are high:

1. Around **phi= -60** and **psi= -60** → alpha helix
2. Around **phi= -90** and **psi= 120** → beta structure

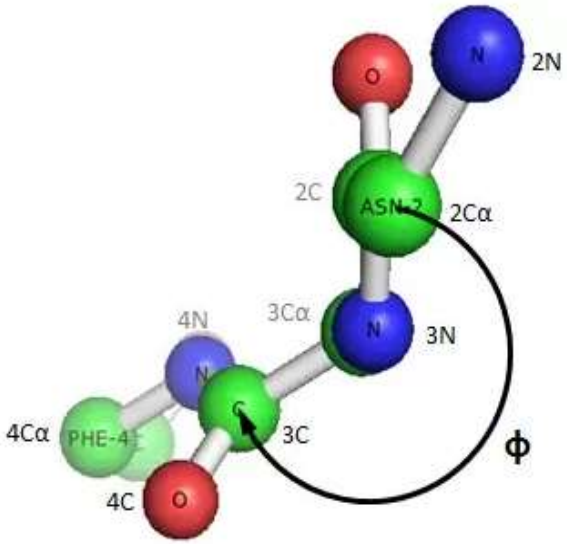


How to calculate phi and psi angles?

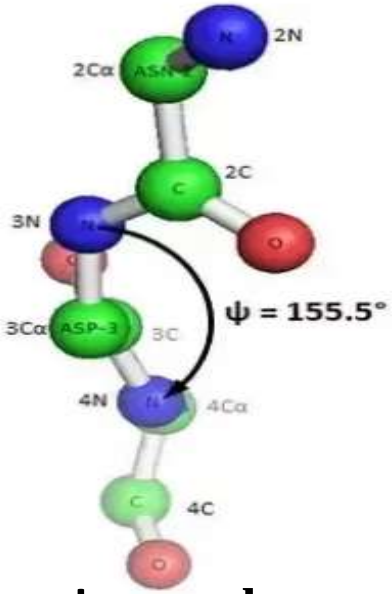
A simple tripeptide



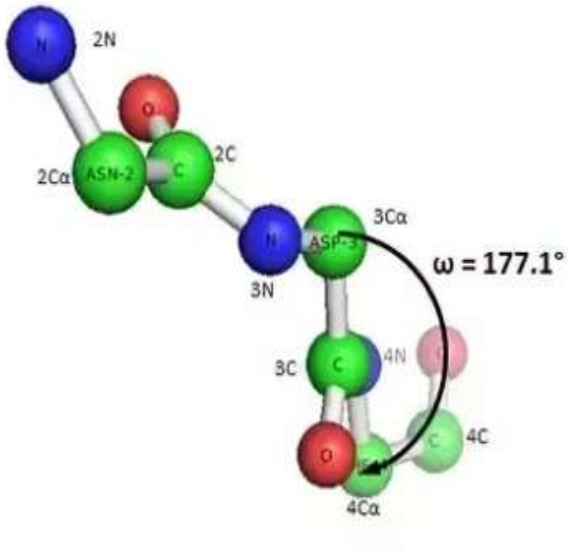
Proteins have **three types** of backbone dihedral angles



Φ - angle

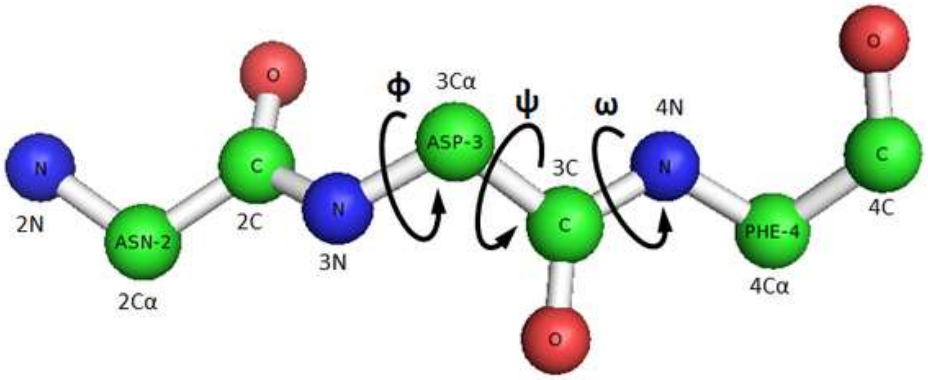


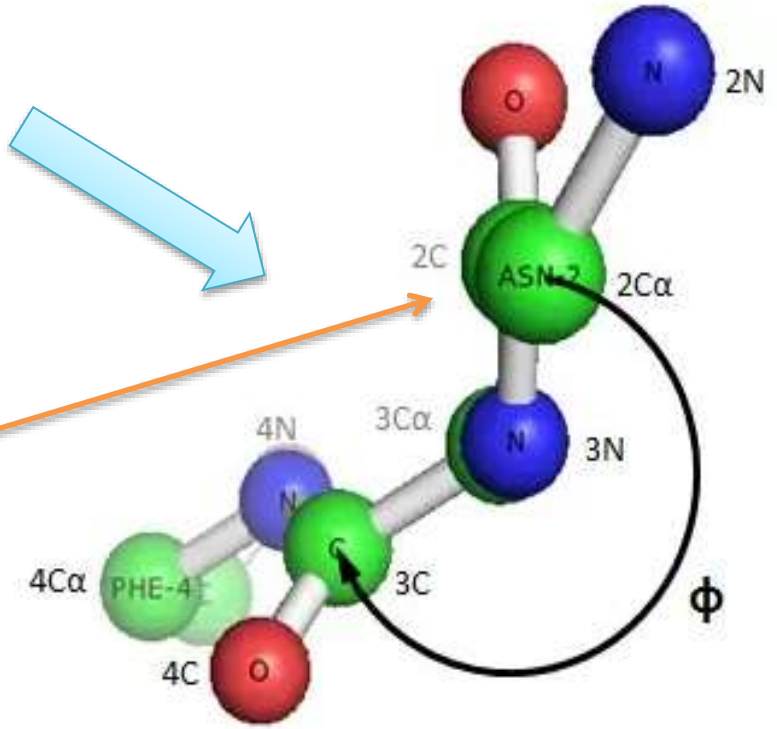
ψ - angle



ω - angle

Calculate Φ - angle



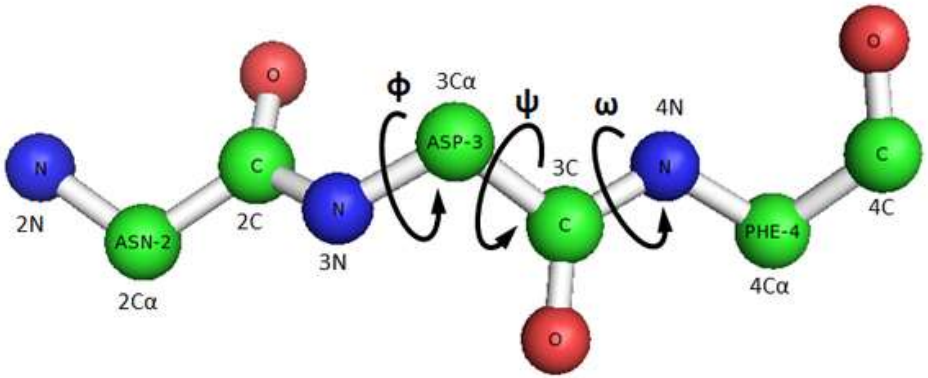


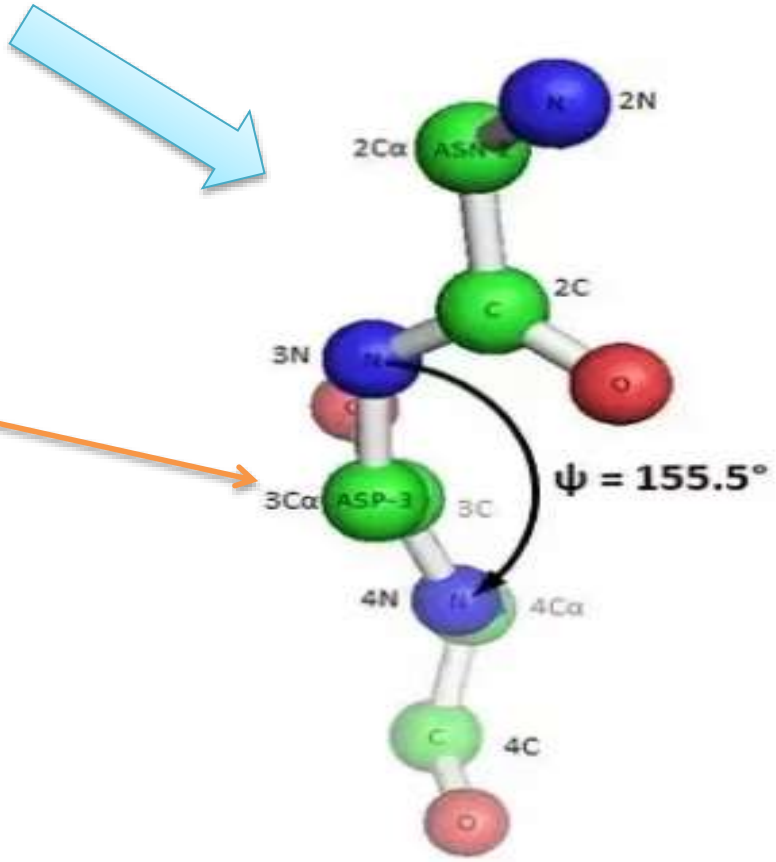
3N overlaps the 3Cα

φ - angle made between the **2C-3N bond** and the **3Cα-3C bond**.

The value of φ is 238.6° or -121.4°

Calculate ψ - angle



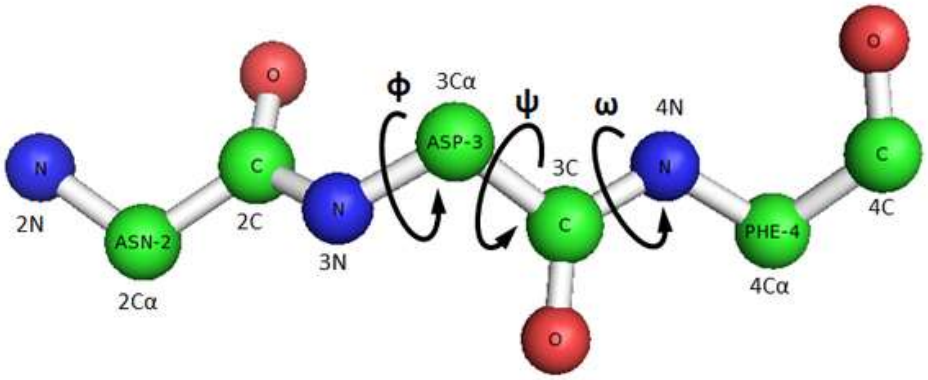


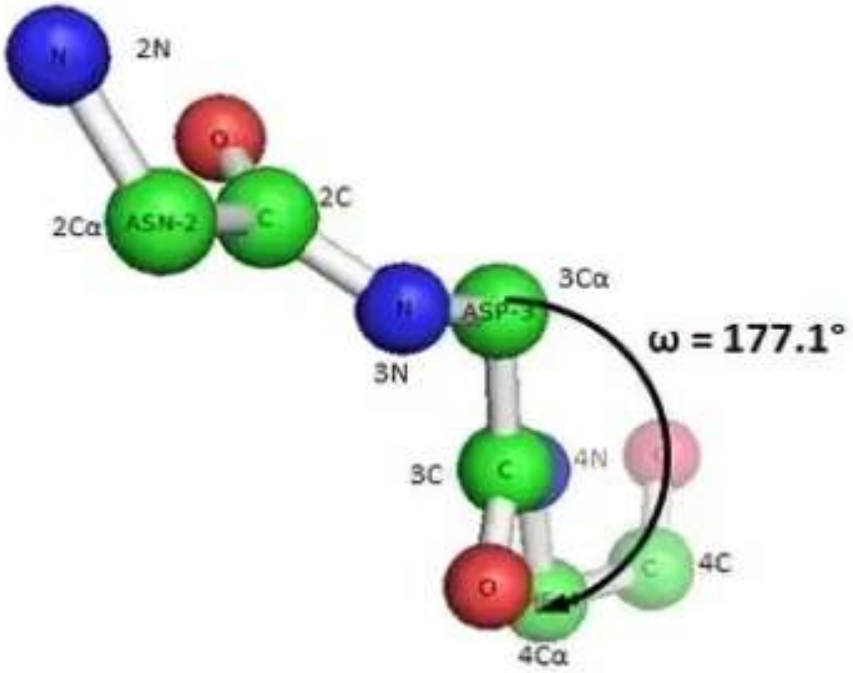
3Cα overlaps the 3C

ψ - angle made between the **3N-3Cα bond** and the **3C-4N bond**.

The value of ψ is 155.5 °

Calculate ω - angle

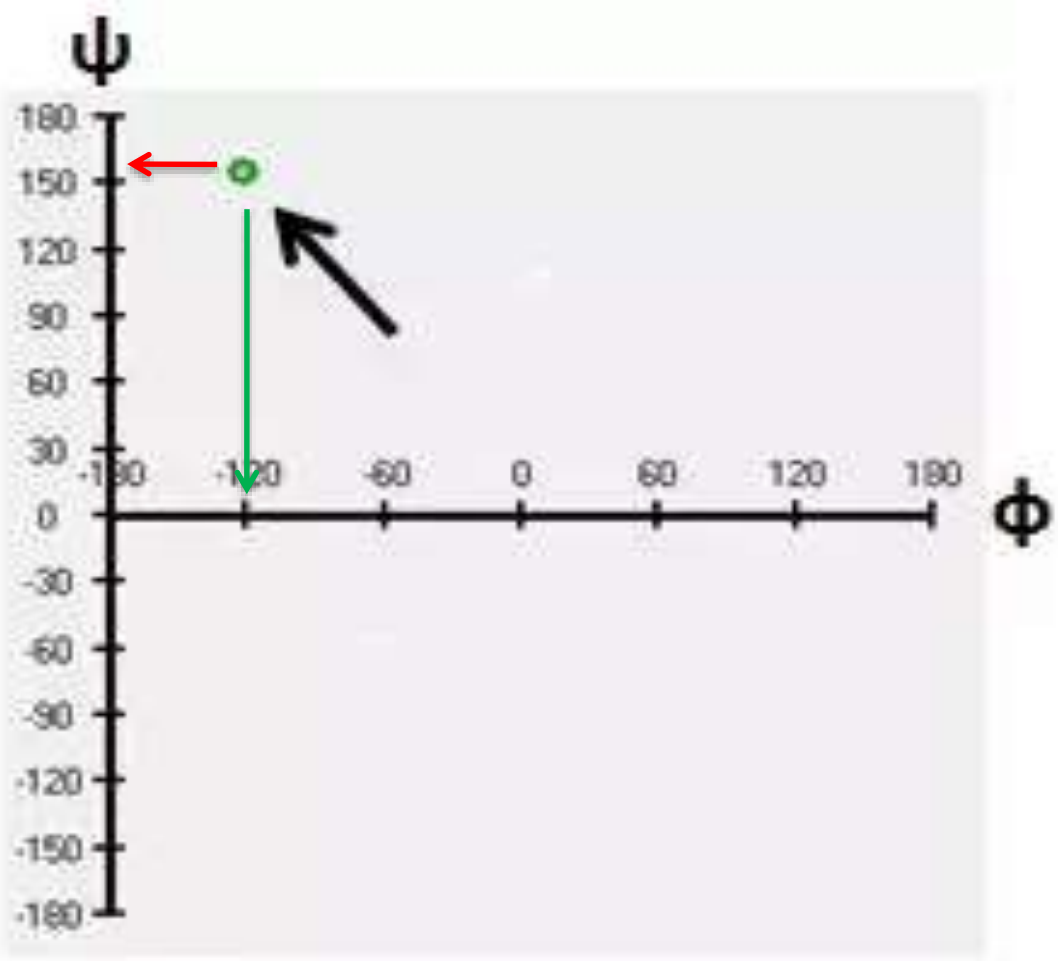




ω - represents the peptide bond

Its value is usually **close to 180° (*trans*) or 0° (*cis*)**

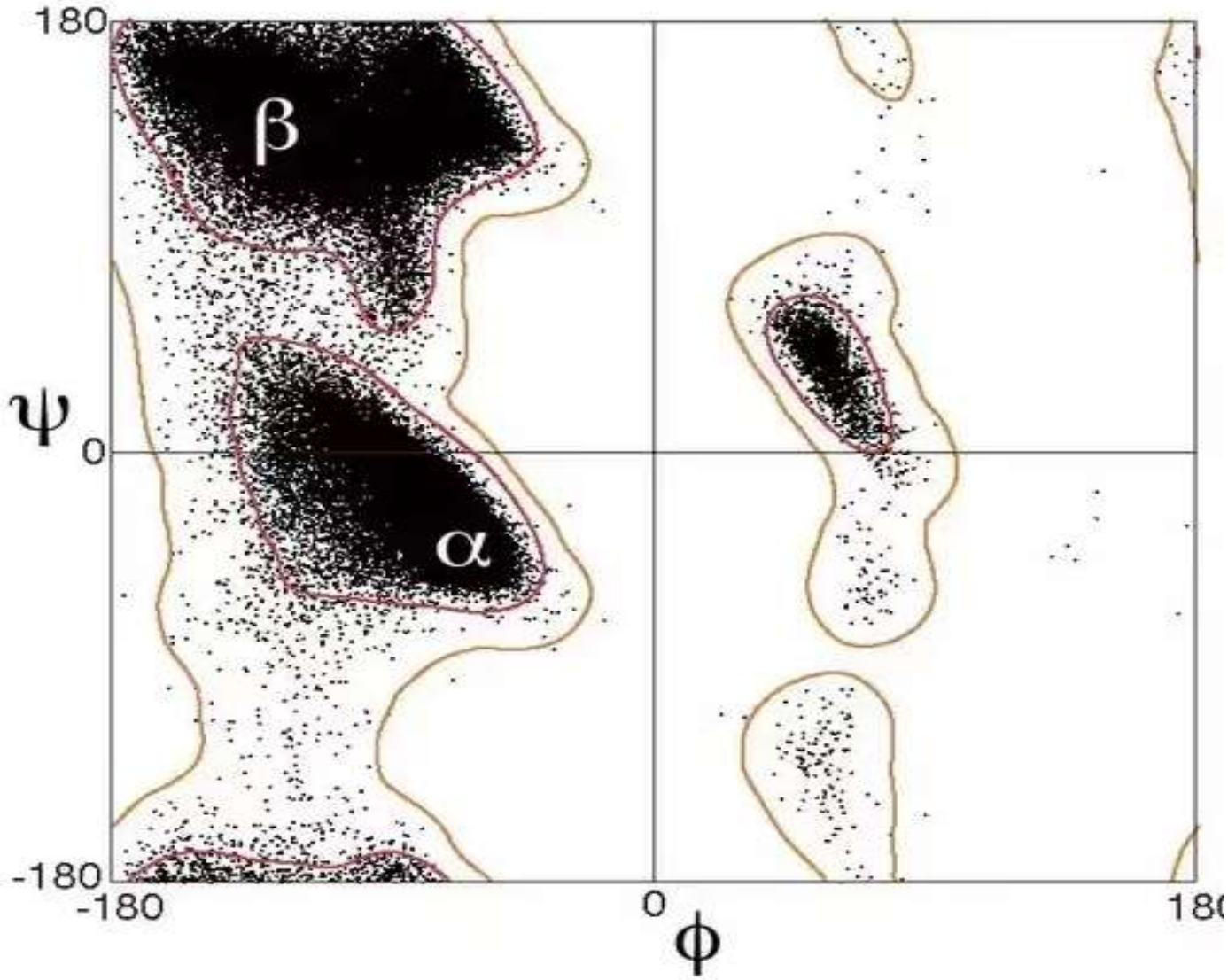
After plotting the angle (Single peptide)



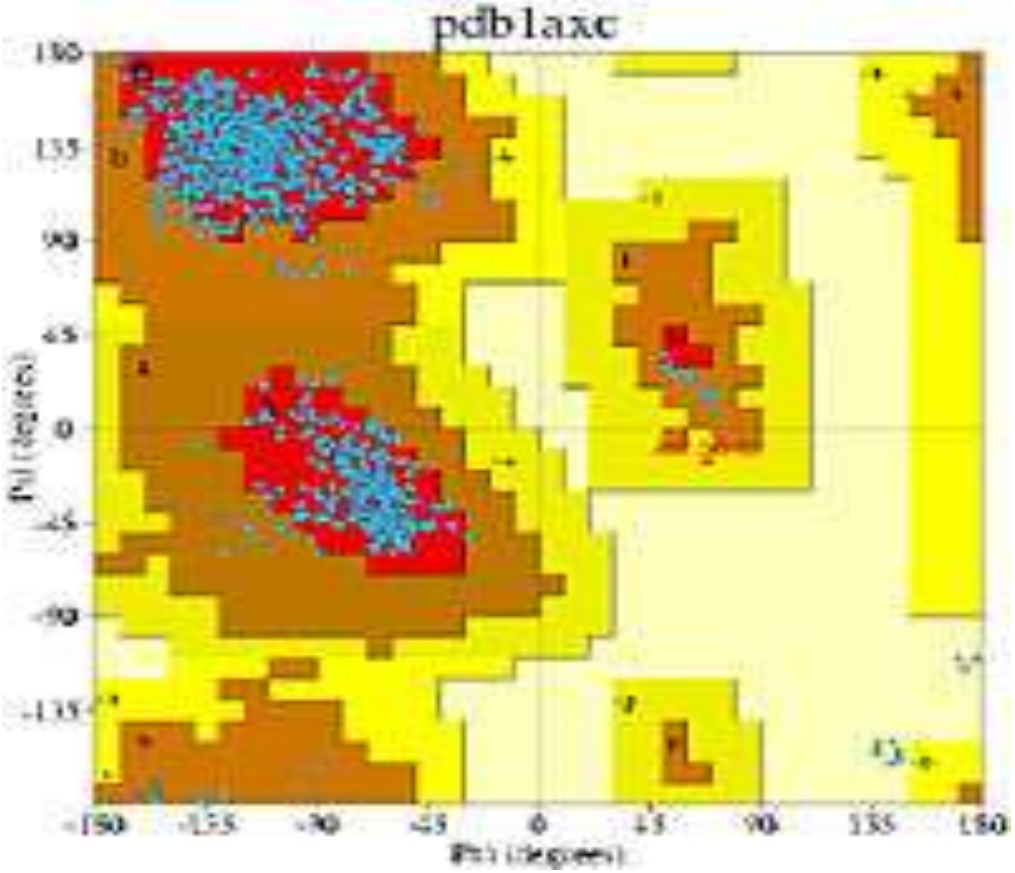
φ = 238.6° or -121.4°

ψ = 155.5 °

After plotting all the peptides



Regions of the plot



Red → favored region

Brown → allowed region

Yellow → generously allowed region

(defined by ProCheck)

Applications of Ramachandran plot

Validation of protein structures

✓Highly anomalous **φ and ψ values**
✓Assumed that a **mistake** might have occurred in the **determination of the position of atoms**.

Improvement of structure determination methods by NMR spectroscopy

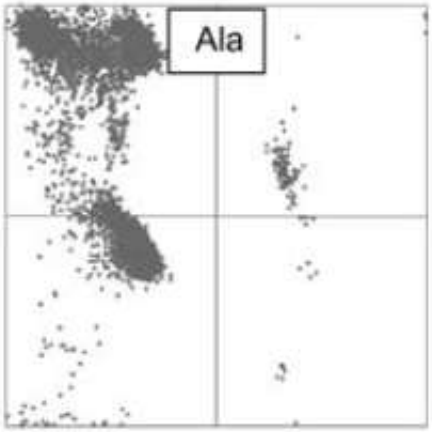
✓**φ and ψ restraints** - tools for protein solution structure prediction
✓**Importance:** Different amino acids exhibit different constraints due to

1. Variable flexibility
2. Steric effects from their side-chains.

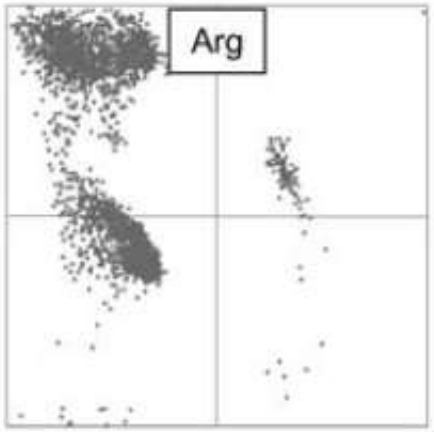
Assessing side-chains effects on the protein backbone

✓Certain **amino acids** prefer to *form a particular kind of secondary structure* over others
✓The effect of single residue substitutions on the backbone conformation, and protein function

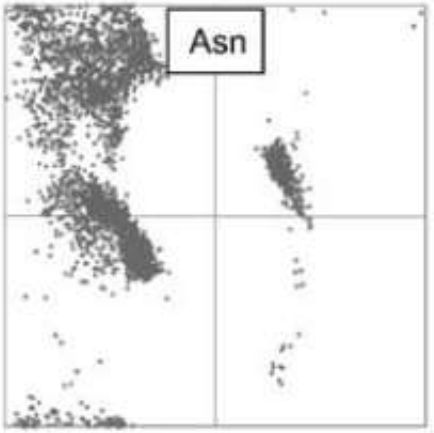
Individual residue distribution



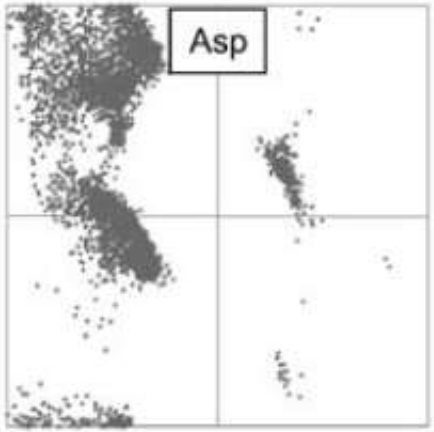
Ala 6781 residues



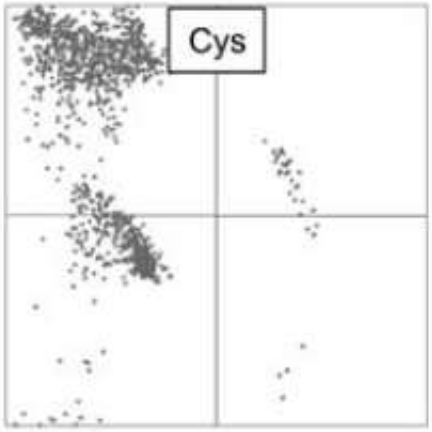
Arg 3208 residues



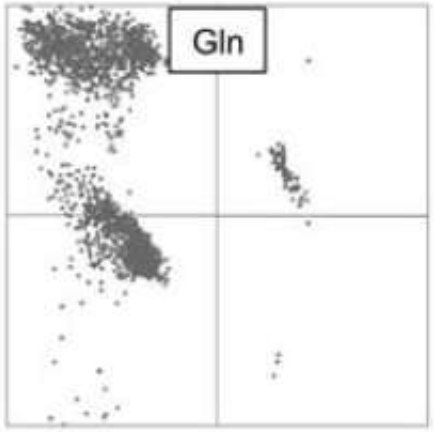
Asn 3267 residues



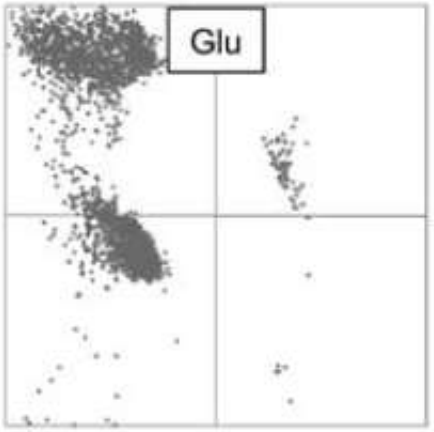
Asp 4300 residues



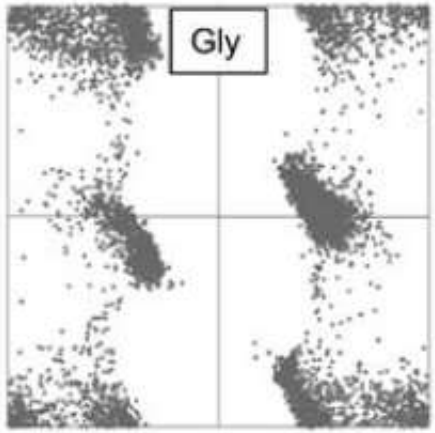
Cys 1167 residues



Gln 2540 residues



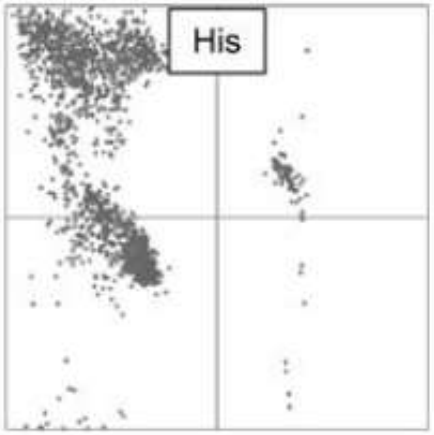
Glu 3819 residues



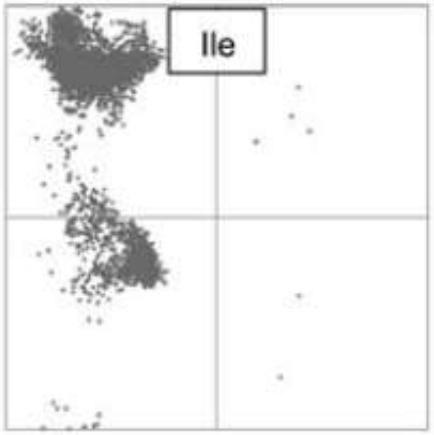
Gly 6046 residues

Hollingsworth *et al.*, (2010)

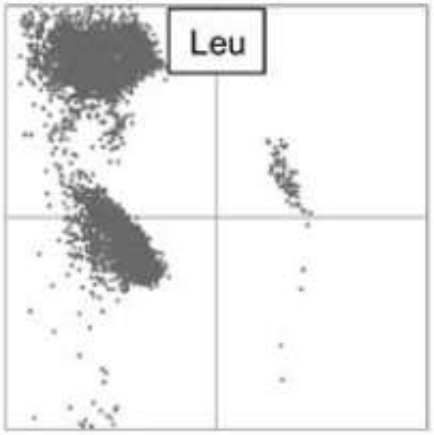
Cont.,



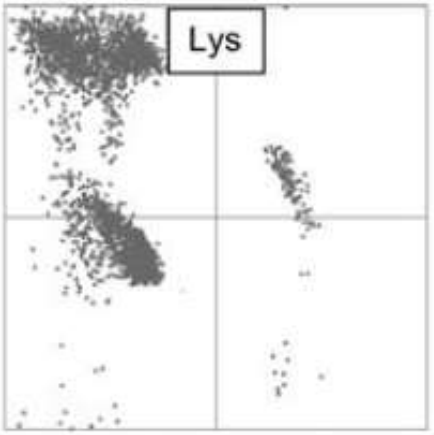
His 1748 residues



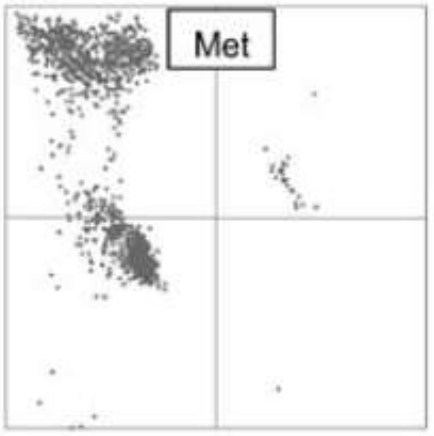
Ile 4128 residues



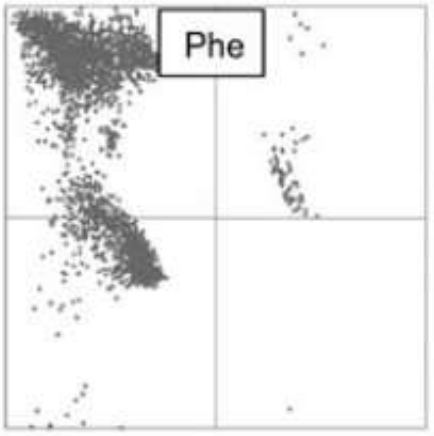
Lue 6334 residues



Lys 3287 residues

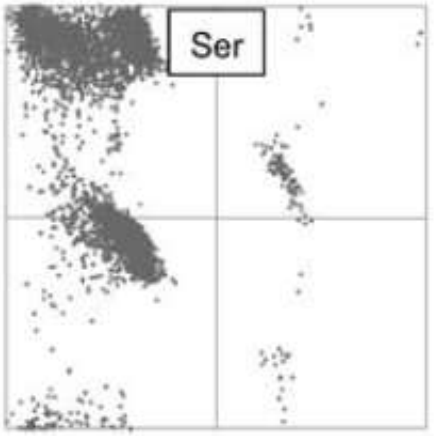


Met 1342 residues



Phe 2904 residues

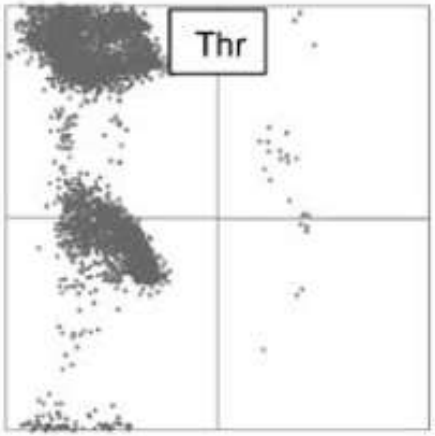
Pro 3185 residues



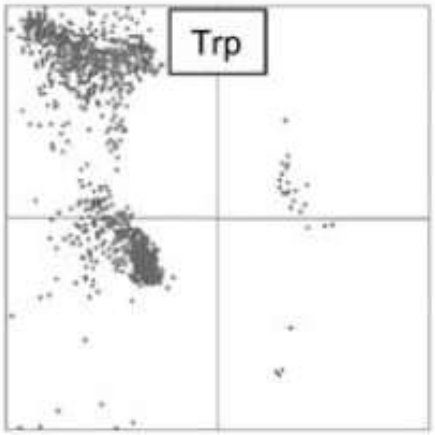
Ser 4340 residues

Hollingsworth *et al.*, (2010)

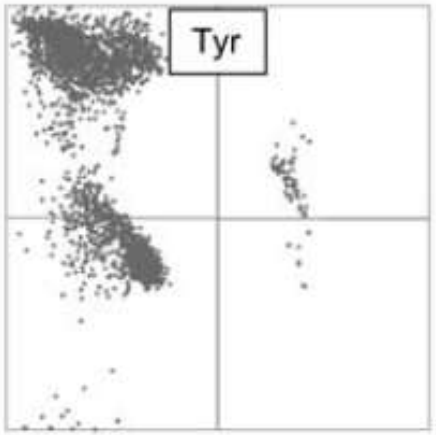
Cont.,



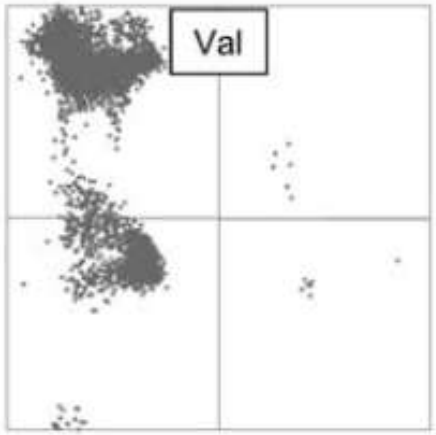
Thr 4545 residues



Trp 1197 residues

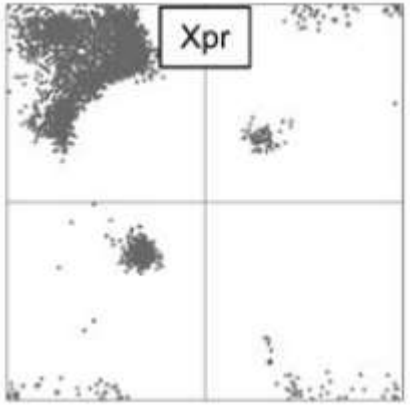


Tyr 2764 residues



Val 5474 residues

A

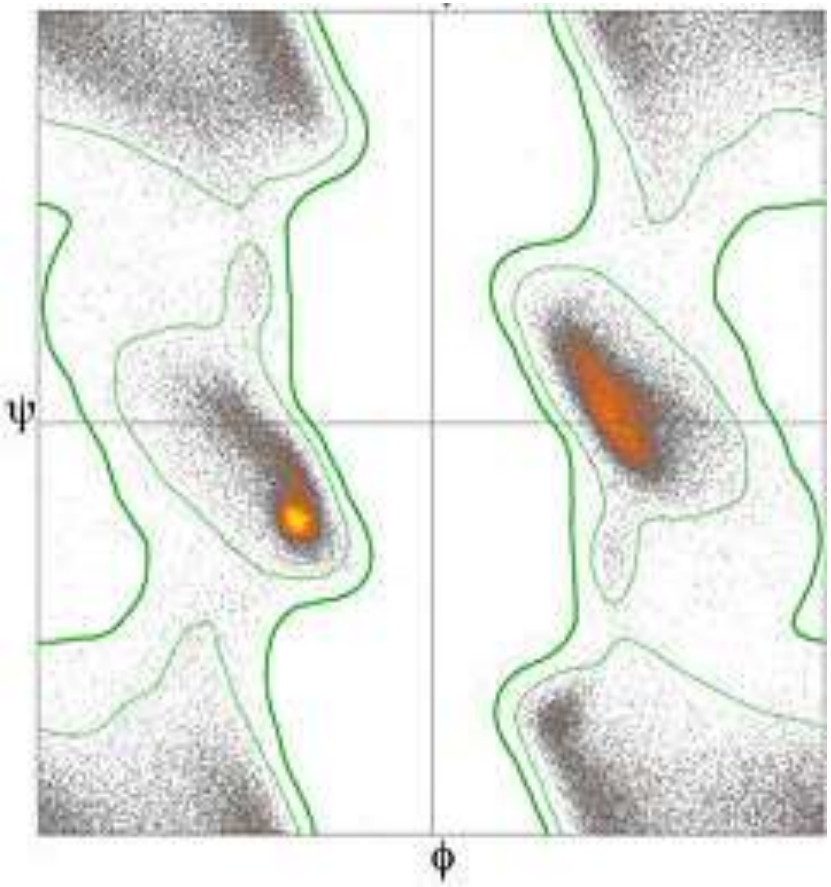


Xpr 3185 residues

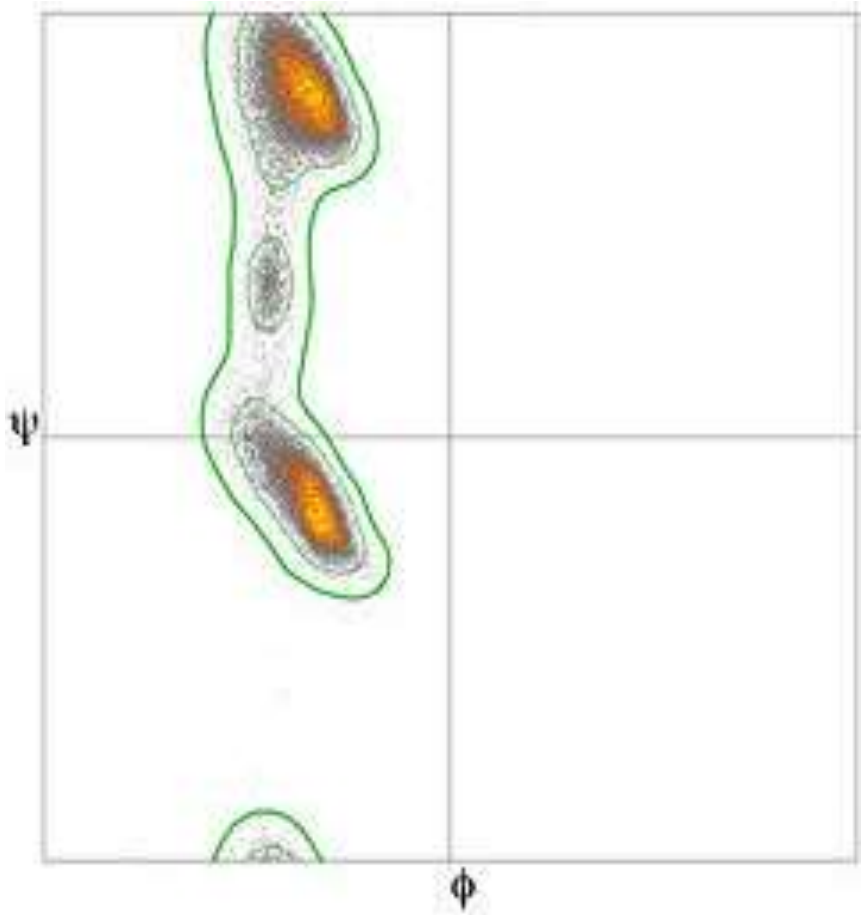
Hollingsworth *et al.*, (2010)

Exceptional Amino acids

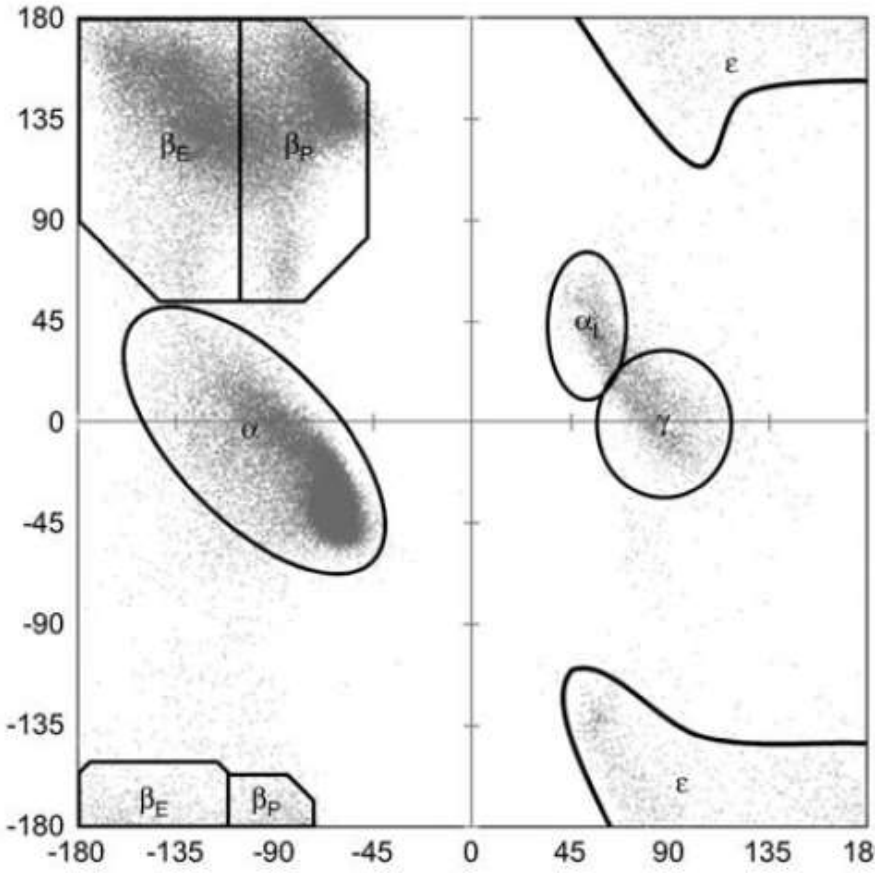
Glycine



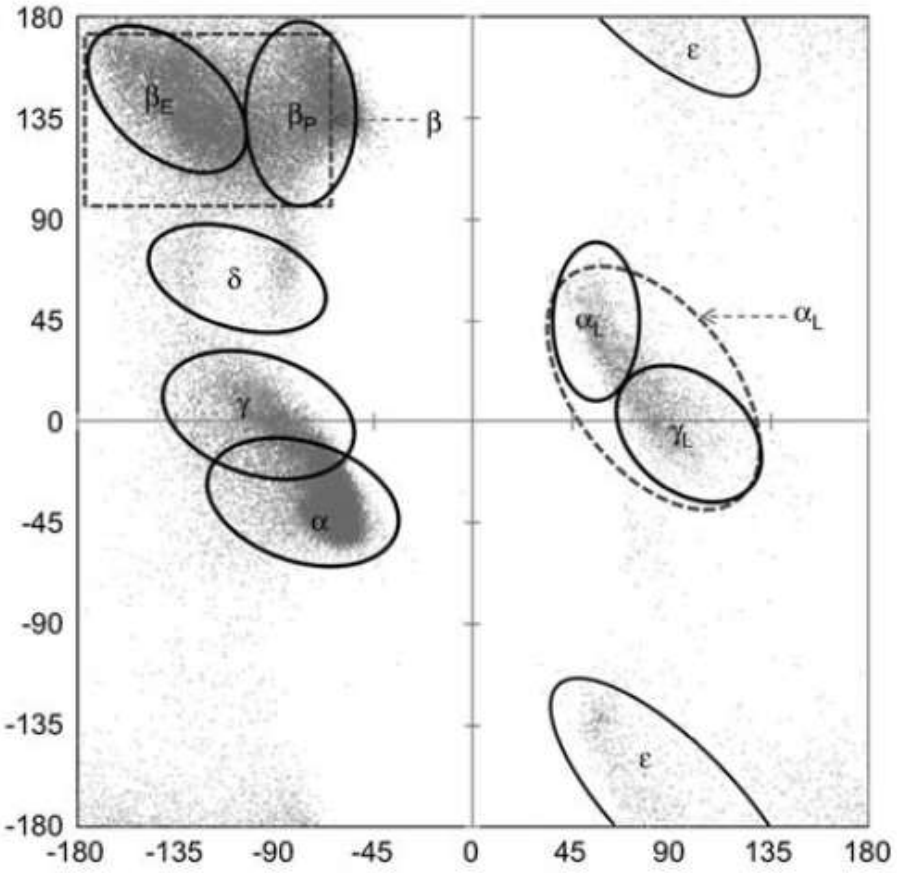
Proline



Nomenclature

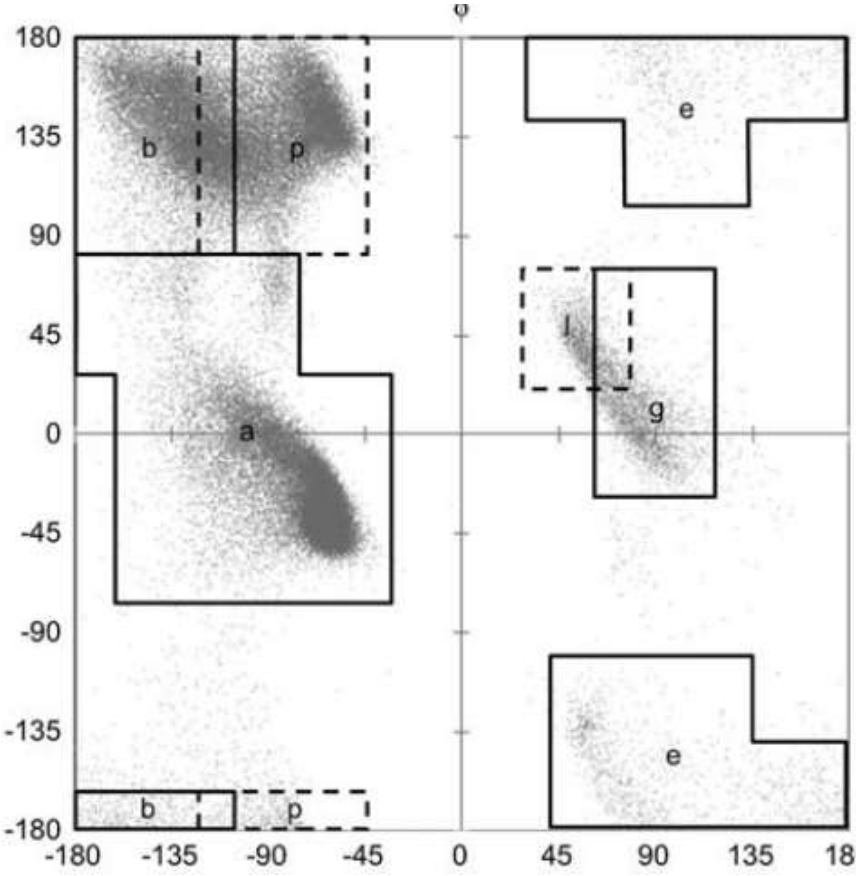


Wilmot and Thornton (1990)

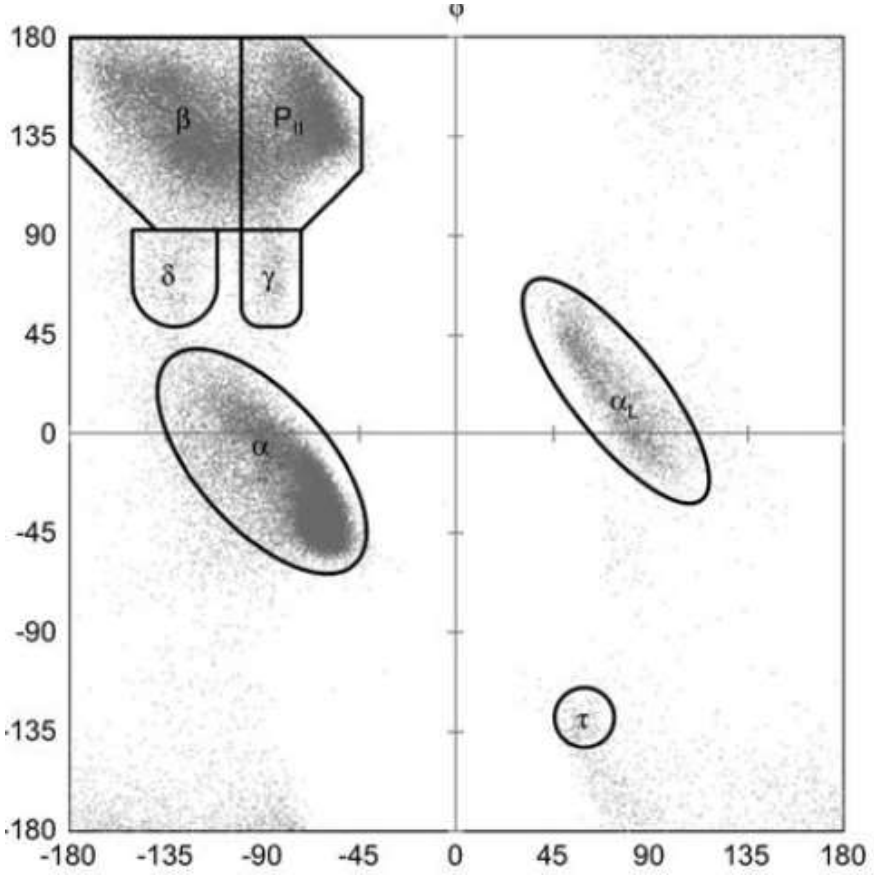


Efimov (1993)

Nomenclature

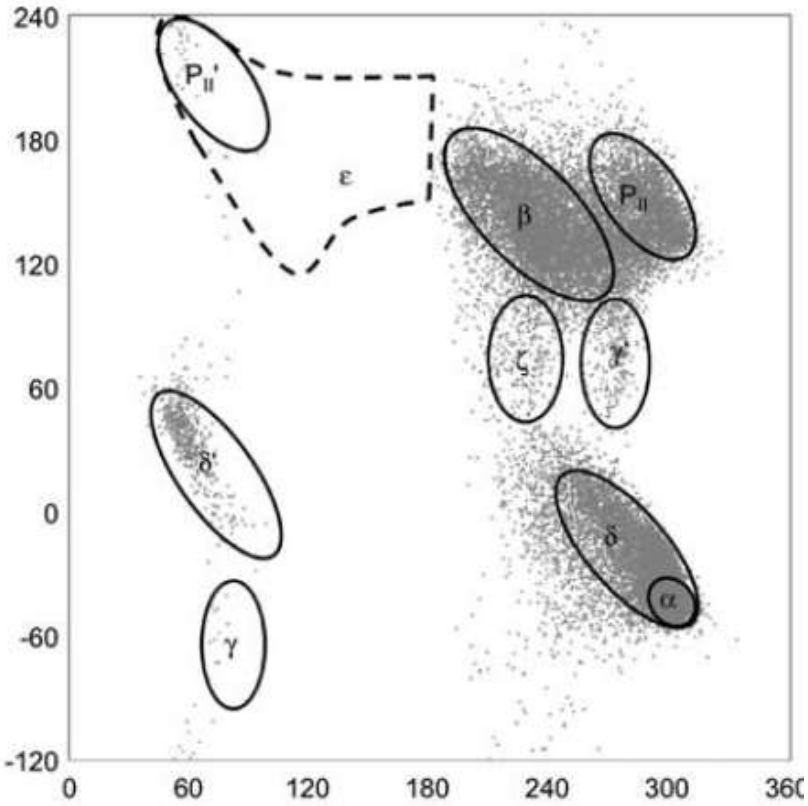


Oliva *et al.*, (1997)

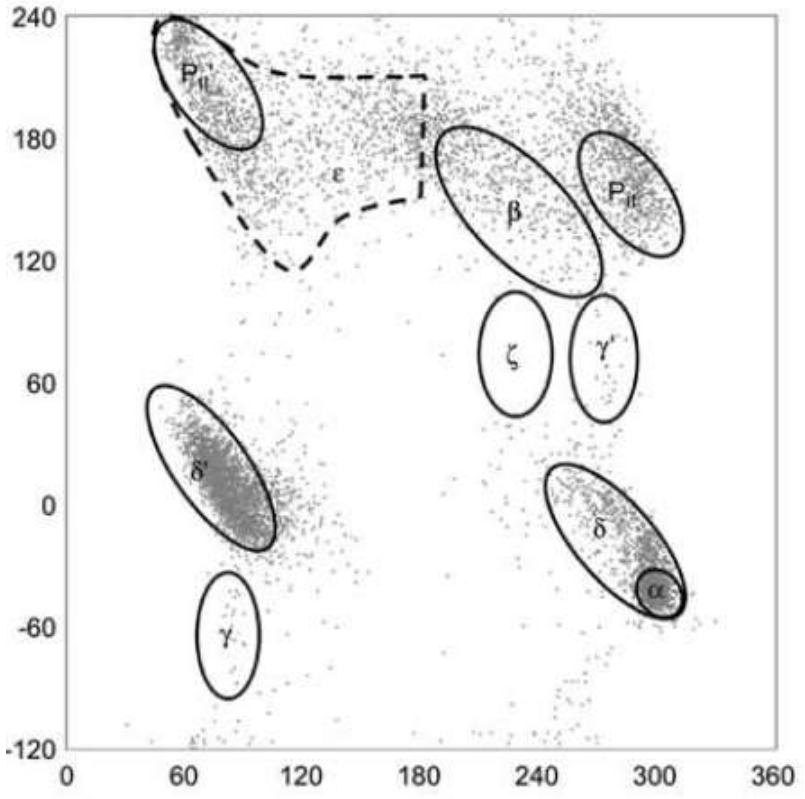


Perskie *et al.*, (2008)

Wrapped Ramachandran plot

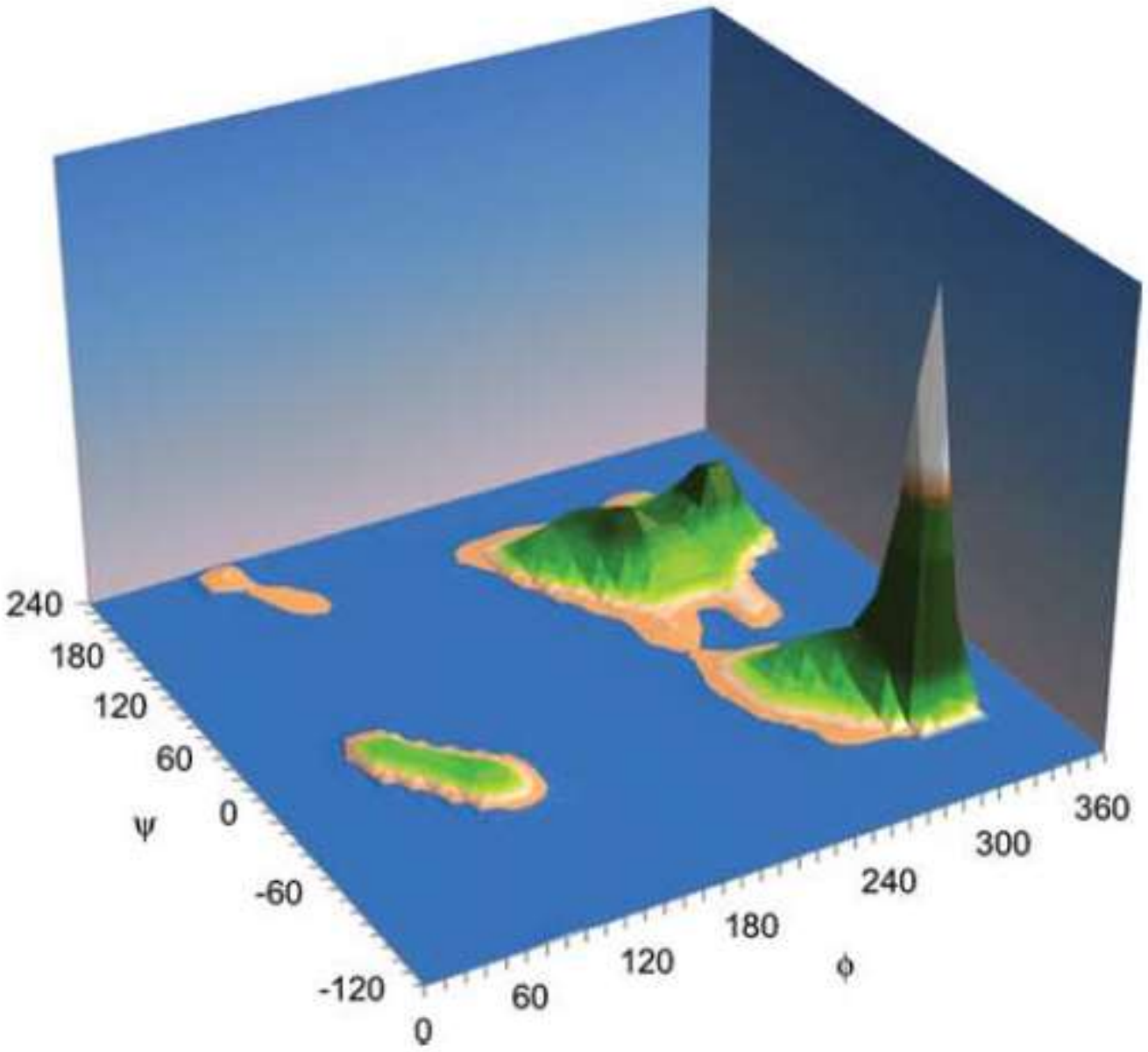


63,149 Ala-like residues (non-Gly, non-Pro)



6046 Gly residues

3D view of Ramachandran plot



References

Articles and review papers:

1. Efimov A V (1993). Standard structures in proteins. Prog Biophysics Molecular Biology **60:** 201–39.

2. Hollingsworth *et al.*, (2010). A fresh look at the Ramachandran plot and the occurrence of standard structures in proteins. Biological Molecular Concepts, **1:** 271–283.

3. Oliva *et al.*, (1997). An automated classification of the structure of protein loops. Journal of Molecular Biology **266:** 814–30.

4. Perskie LL, Street TO, Rose GD (2008). Structures, basins, and energies: a deconstruction of the Protein Coil Library. Protein Science **17:** 1151–61.

5. Wilmot C M, Thornton J M (1990). Beta-turns and their distortions: a proposed new nomenclature. Protein Eng **3:** 479–93.

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Websites:

6. http://www.proteinstructures.com/Structure/Structure/Ramachandran-plot.html

7. http://skuld.bmsc.washington.edu/~merritt/bc530/local_copies/Ramachandran_article.pdf

8. http://www.greeley.org/~hod/papers/Unsorted/Ramachandran.doc.pdf

THANK YOU