RAMACHANDRAN PLOT

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INTRODUCTION

- A Ramachandran plot (also known as a Ramachandran map or a Ramachandran diagram or a [φ,ψ] plot)
- Developed by Gopalasamudram Narayana Ramachandran and Viswanathan Sasisekharan is a way to visualize dihedral angles ψ against φ of amino acid residues in protein structure
- Used computer models of small polypeptides to systematically vary φ and ψ with the objective of finding stable conformations
- For each conformation, the structure was examined for close contacts between atoms
- Atoms were treated as hard spheres with dimensions corresponding to their van der Waals radii
- Therefore, φ and ψ angles which cause spheres to collide correspond to sterically disallowed conformations of the polypeptide backbone

BACKBONE TORSION ANGLES

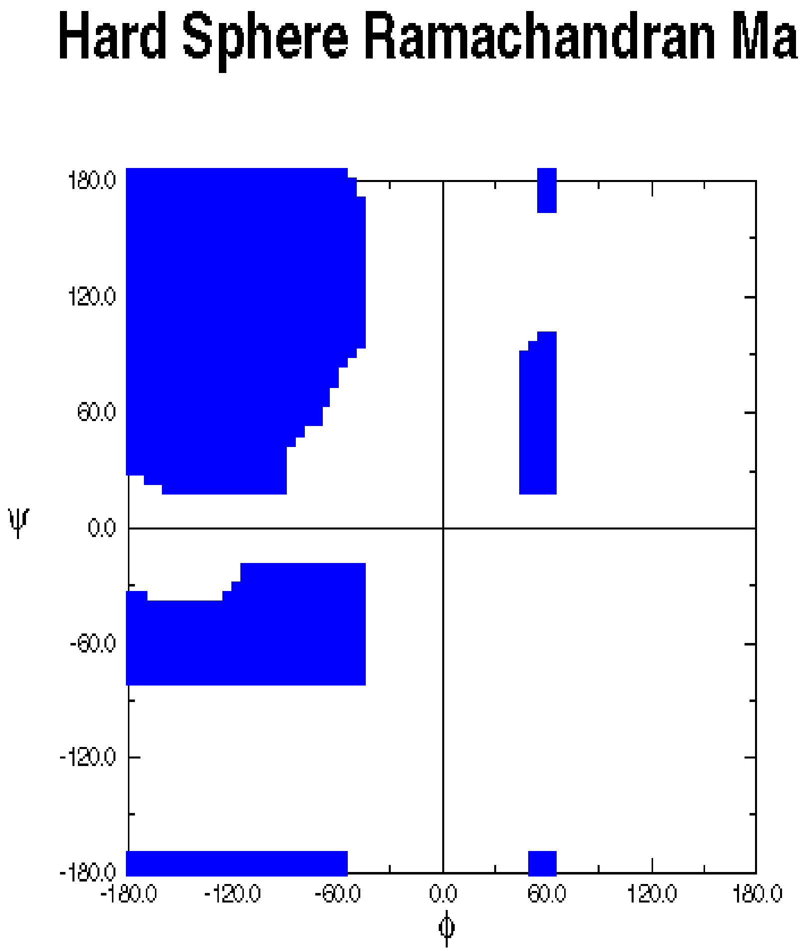
- ω angle tends to be planar (0º - cis, or 180 º - trans) due to delocalization of carbonyl pi electrons and nitrogen lone pair
- φ and ψ are flexible, therefore rotation occurs here
- However, φ and ψ of a given amino acid residue are limited due to steric hindrance
- Only 10% of the {φ, ψ} combinations are generally observed for proteins
- First noticed by G.N. Ramachandran

RAMACHANDRAN PLOT

- Plot of φ vs. ψ

- The computed angles which are sterically allowed fall on certain regions of plot

Computed Ramachandran Plot

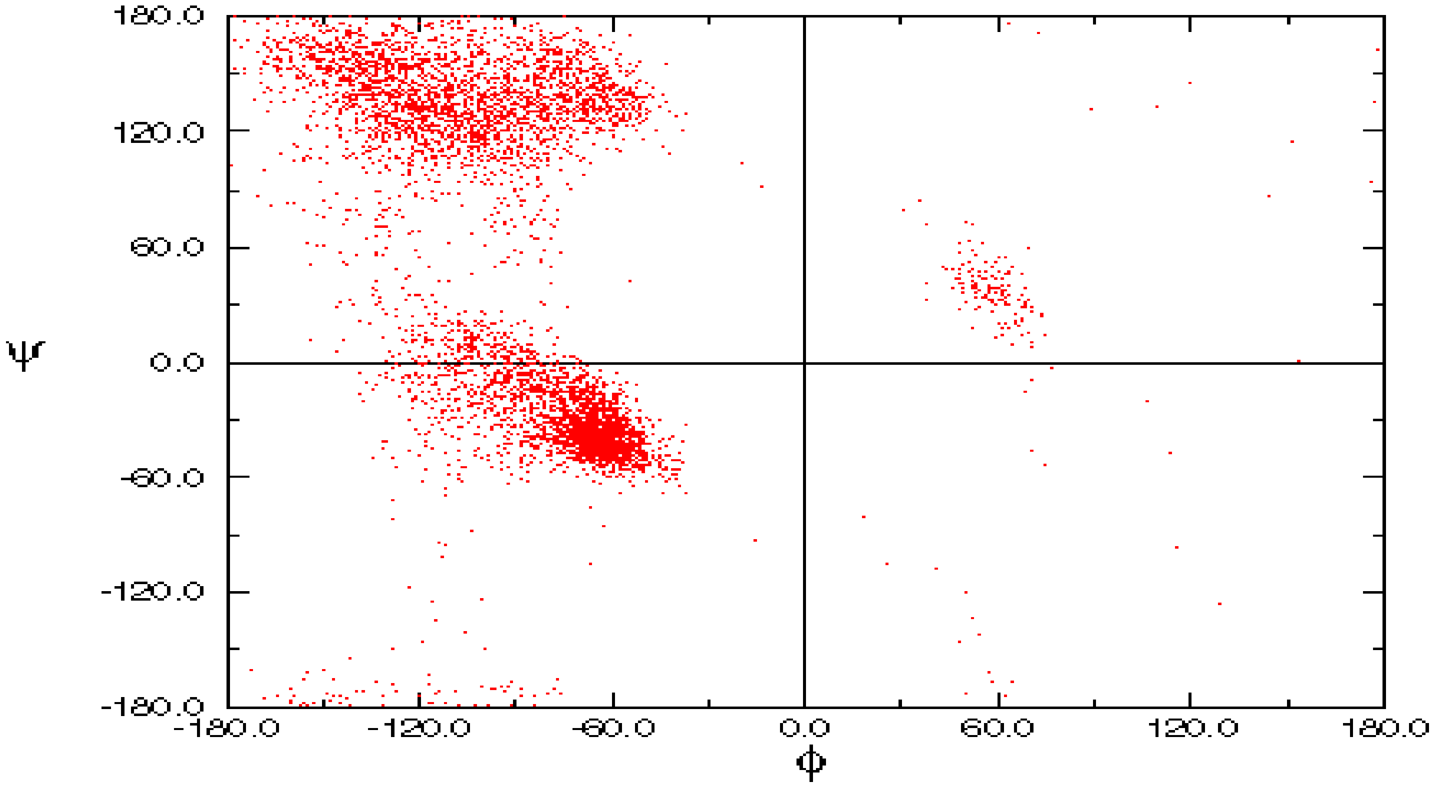


- White = sterically disallowed conformations (atoms come closer than sum of vander Waals radii)
- Blue = sterically allowed conformations

RAMACHANDRAN PLOT

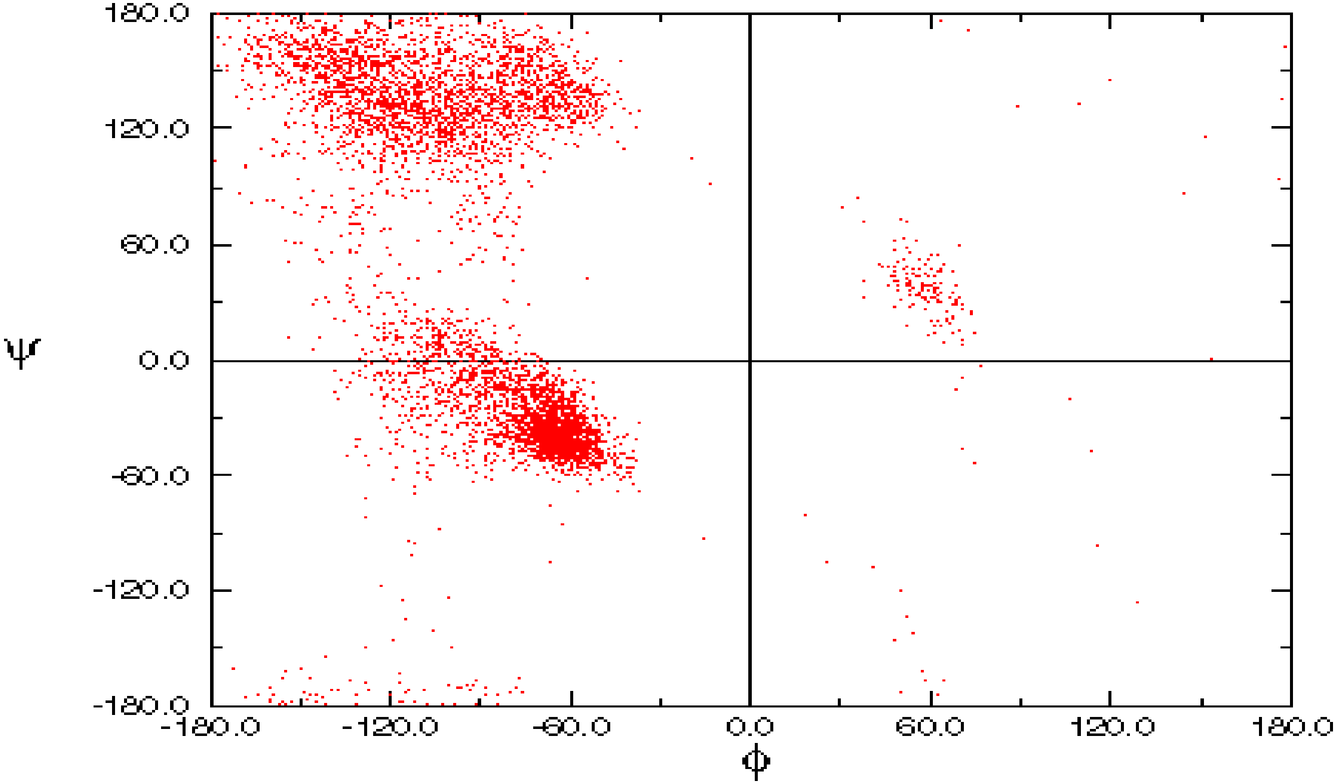
- Plot of φ vs. ψ
- Computed sterically allowed angles fall on certain regions of plot
- Experimentally determined angles fall on same regions

φ, ψ DISTRIBUTION IN 42 HIGH-RESOLUTION PROTEIN STRUCTURES (X-RAY CRYSTALLOGRAPHY)



EXPERIMENTAL RAMACHANDRAN PLOT

Φ, Ψ DISTRIBUTION IN 42 HIGH-RESOLUTION PROTEIN STRUCTURES (X-RAY CRYSTALLOGRAPHY)



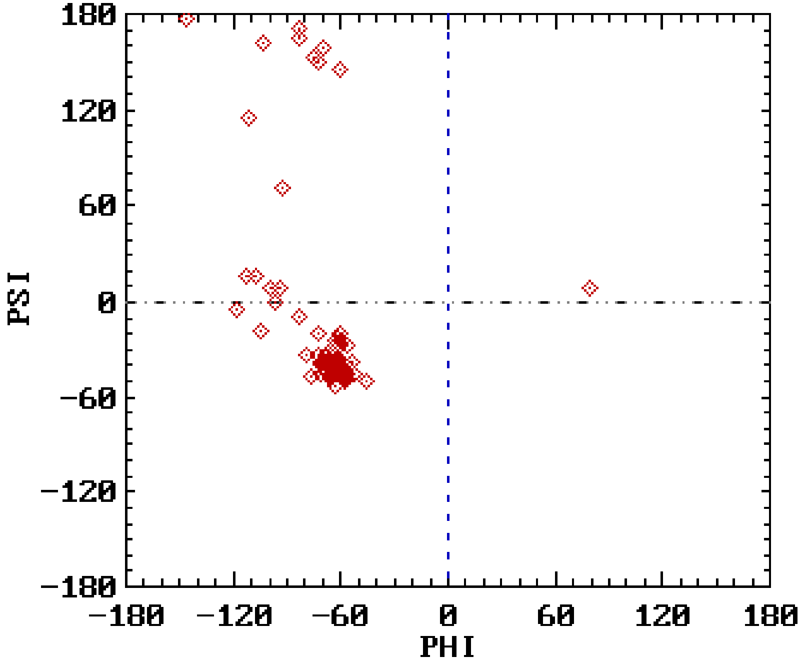
RAMACHANDRAN PLOT AND SECONDARY STRUCTURE

- Repeating values of φ and ψ along the chain result in regular structure

- For example, repeating values of φ ~ -57° and ψ ~ -47° give a right-handed helical fold (the alpha-helix)

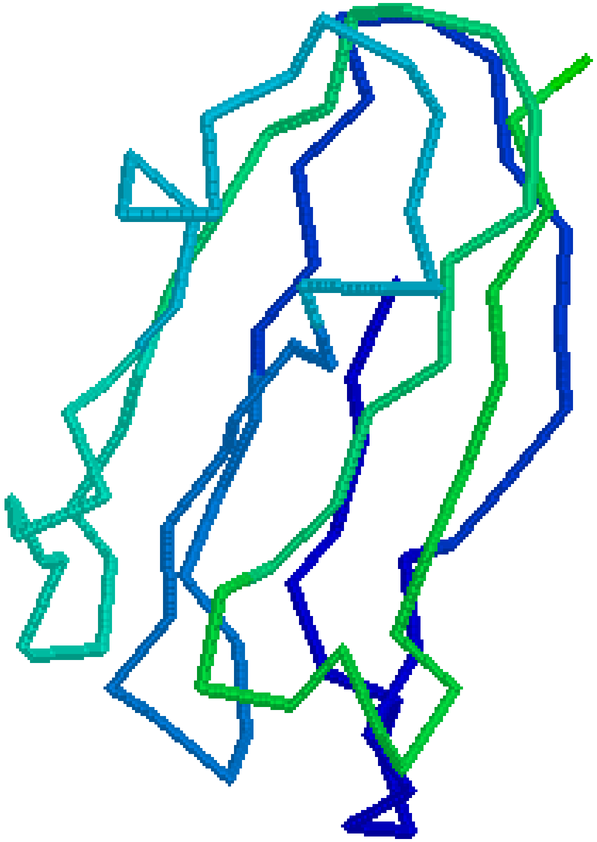
The structure of cytochrome C shows many segments of helix and the Ramachandran plot shows a tight grouping of φ, ψ angles near -50,-50

alpha-helix

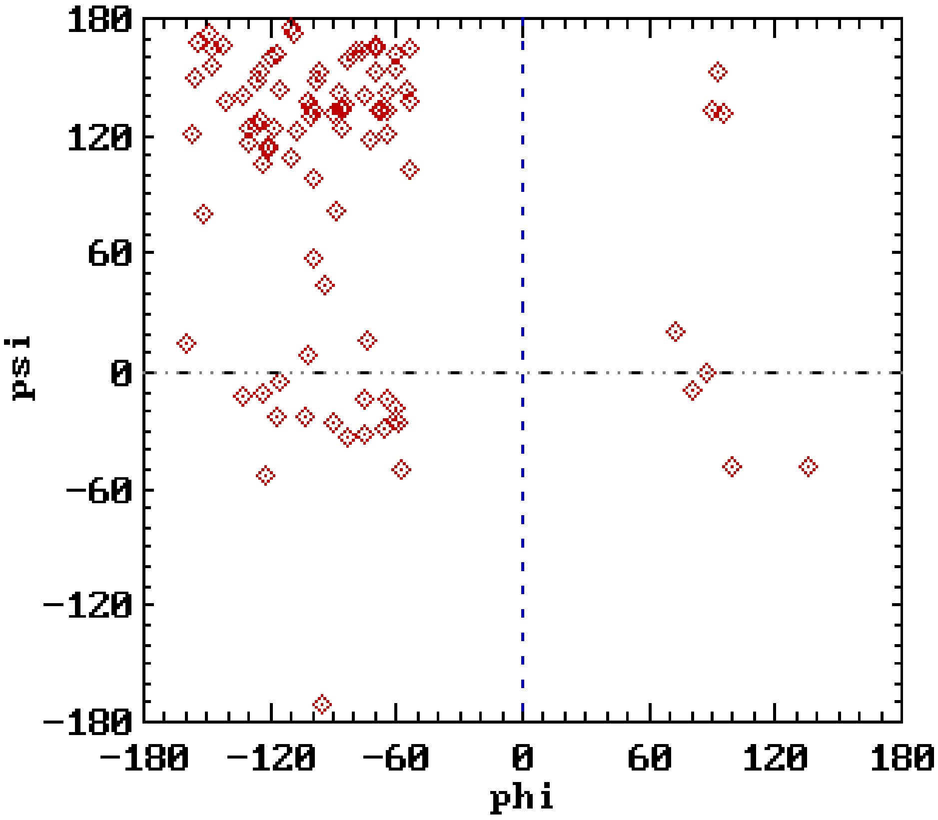


cytochrome C
Ramachandran plot

Similarly, repetitive values in the region of φ = -110 to –140 and ψ = +110 to +135 give beta sheets. The structure of plastocyanin is composed mostly of beta sheets; the Ramachandran plot shows values in the –110, +130 region:

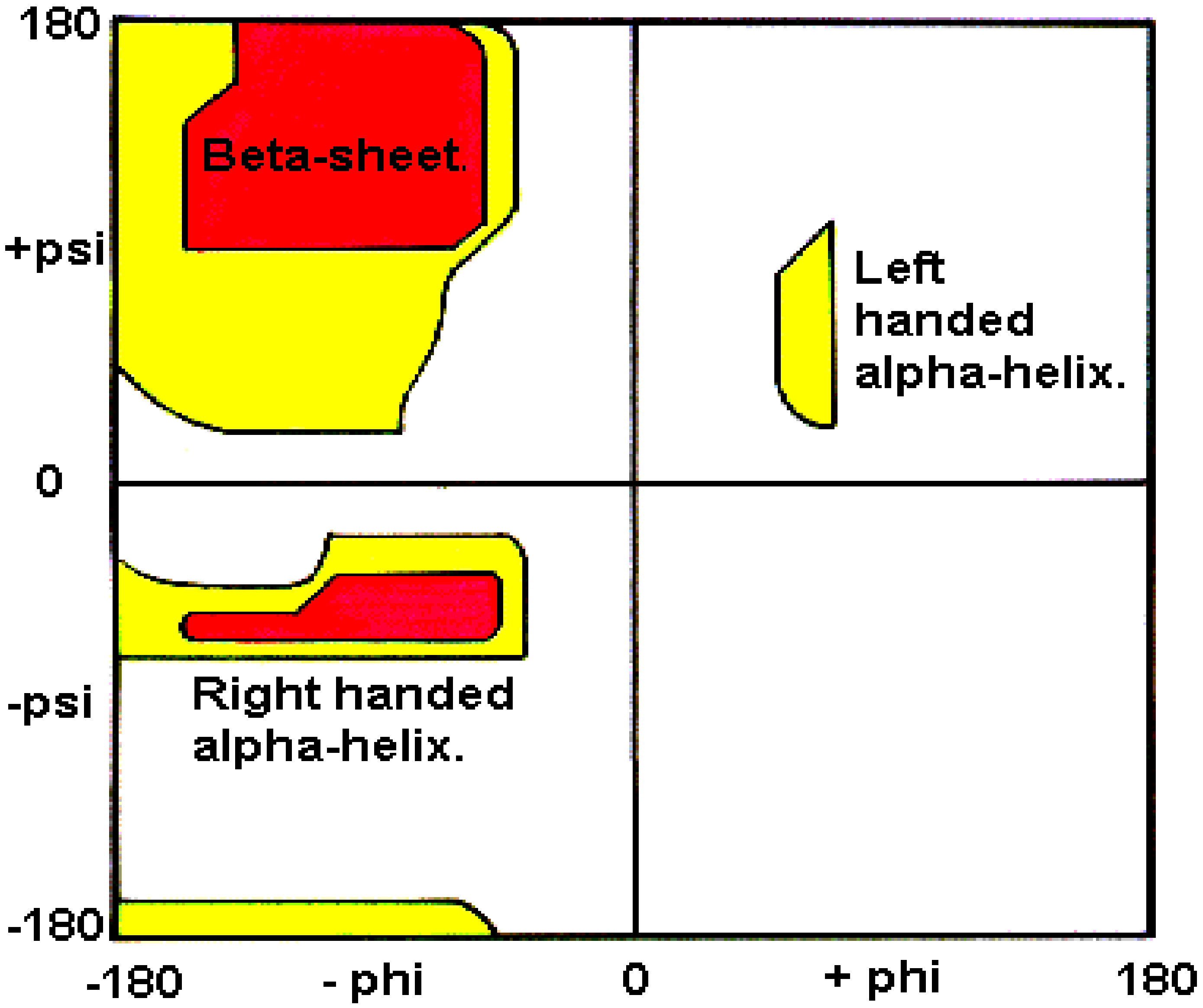


beta-sheet



plastocyanin
Ramachandran plot

The Ramachandran Plot.



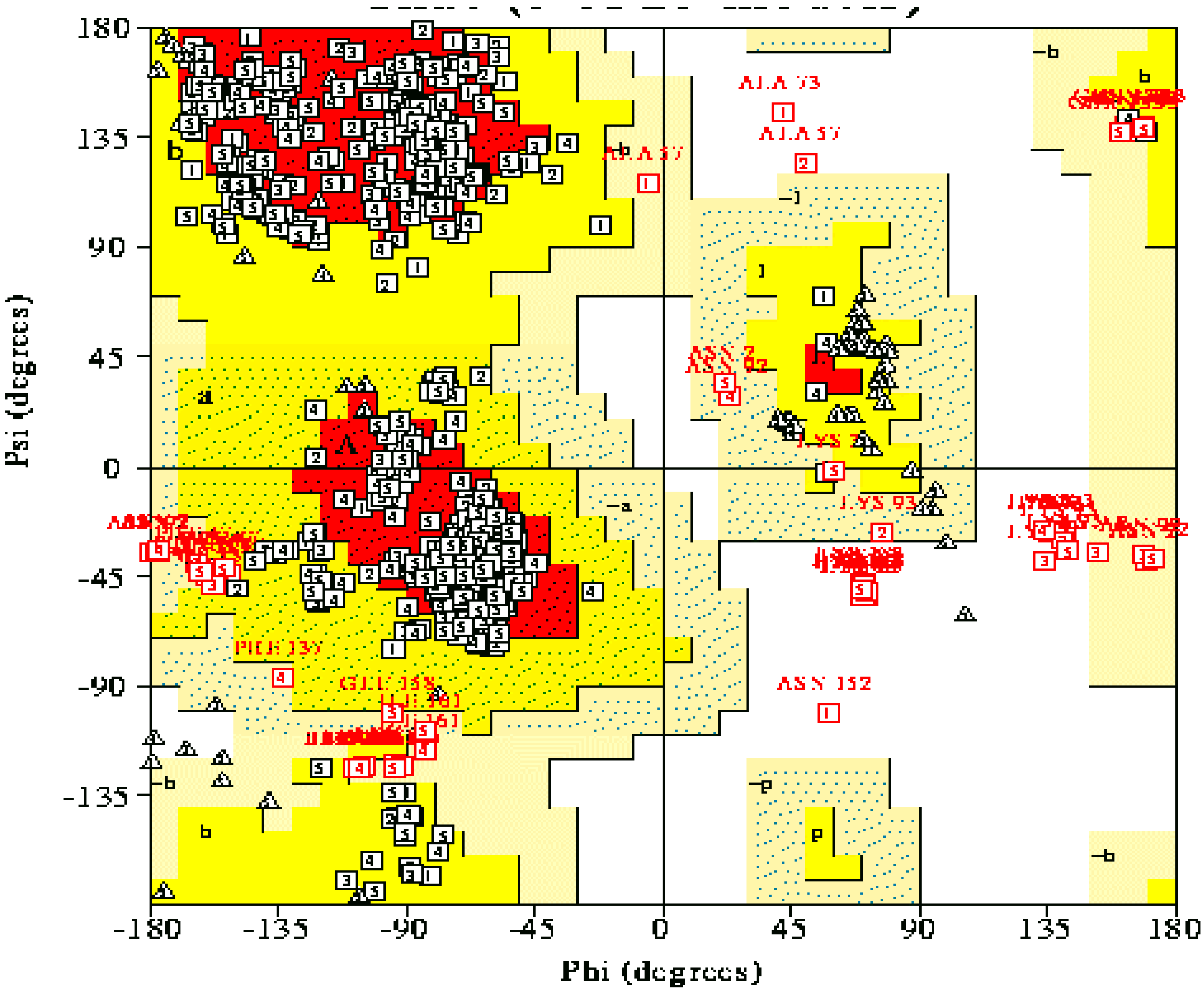
RAMACHANDRAN PLOT AND SECONDARY STRUCTURE

- White = sterically disallowed conformations

- Red = sterically allowed regions if strict (greater) radii are used (namely right-handed alpha helix and beta sheet)

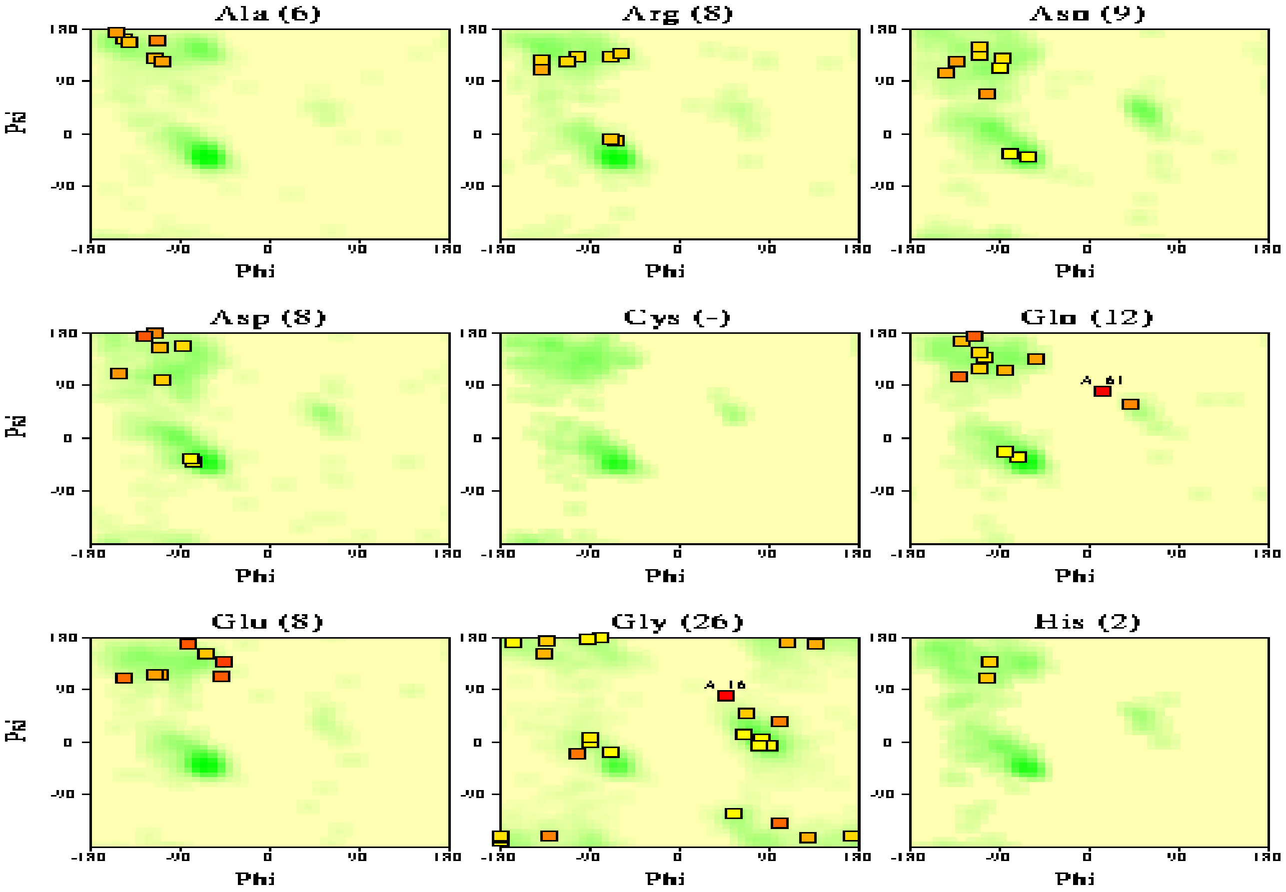
- Yellow = sterically allowed if shorter radii are used (i.e. atoms allowed closer together; brings out left-handed helix)

SAMPLE RAMACHANDRAN PLOT



Ramachandran plots for all residue types

1abc



Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0Å or better.