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Ramachandran plot on the web†

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ABSTRACT

Summary: A graphics package has been developed to display the main chain torsion angles phi, psi (ϕ, Ψ); (Ramachandran angles) in a protein of known structure. In addition, the package calculates the Ramachandran angles at the central residue in the stretch of three amino acids having specified the flanking residue types. The package displays the Ramachandran angles along with a detailed analysis output. This software is incorporated with all the protein structures available in the Protein Databank.

Availability: This package is available over the world wide web at http://144.16.71.146/rp/ or http://dicsoft1.physics.iisc.ernet.in/rp.

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Ramachandran plot (RP) is the display of the (ϕ, Ψ) angle pairs of the polypeptide chain in a given protein structure in an easily comprehensible way (Ramachandran *et al.*, 1963). Over the years, structural crystallographers and the protein modellers use the Ramachandran plot during every stage of model building to see whether the main chain torsion angles (ϕ, Ψ) are stereochemically feasible. Using the principles of the Ramachandran plot, the conformational preferences of glycyl residues in the globular proteins have been studied extensively (Ramakrishnan *et al.*, 1987). Wu and Kabat (1971, 1973) have paid considerable attention in order to elucidate the influence of the neighbouring amino acid residues ($n - 1$) and ($n + 1$) on the conformation of the middle residue n.

There are stand-alone packages to calculate the Ramachandran angles (for example PROCHECK; Laskowski *et al.*, 2001). In addition, programs like PDBSUM (Laskowski, 2001), and WEBMOL (Walther, 1997) can be used to produce Ramachandran plots over the world wide web for the protein structures available in the Protein Databank (PDB) (Berman *et al.*, 2000). To the best of our knowledge, there is no Internet-based web package to study some of the following options:

(a) Ramachandran plot for any particular residue or all the residues present in a particular chain (in the case of multimeric chain proteins) or fragment of the chain;

(b) Ramachandran plot for the central residue in a stretch of three residues with an option for the users to specify the flanking residue types;

(c) the occurrence of different amino acid residues at various regions of the plot;

(d) to display the multiple conformation angles adopted by an amino acid residue.

The graphics package, Ramachandran plot, has been developed to address these issues in detail.

This software is fully incorporated with all the protein structures (solved using both X-ray crystallography and NMR spectroscopy) available in the PDB. The package is written using Java (Servlets and Applets). The program is easy to use and runs on windows 95/98/2000, windows NT server, Linux and silicon graphics (SGI) platforms through NETSCAPE browser. The software runs on our Bioinformatics server (a 1.7 GHz Pentium IV processor, 1 GB of Random Access Memory, running in Redhat Linux 7.2). The front-end input data part of this package is written in HTML and JavaScript and allows user-friendly web forms.

There are two kinds of input streams available in the proposed software. For the structures available in the PDB, the user needs to enter the four character PDB-id code. The software takes the atomic coordinates from the locally available PDB-FTP anonymous server for the user inputted PDB-id code. For the second input stream 'Upload PDB file', the user needs to upload the three-dimensional atomic coordinates of the protein molecule (PDB format) of interest from the client machine through the browser. For the above two options, the package has three functions, namely, display the Ramachandran angles for (a) all the residues, (b) a particular residue and (c) $(n - 1) - n - (n + 1)$. The option 'particular residue' shows the Ramachandran plot for a particular amino acid residue type of interest, available in various parts of the protein molecule. The notable feature of this package is that it allows the user to calculate the conformation angle

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† This work is dedicated to Late Professor G. N. Ramachandran.

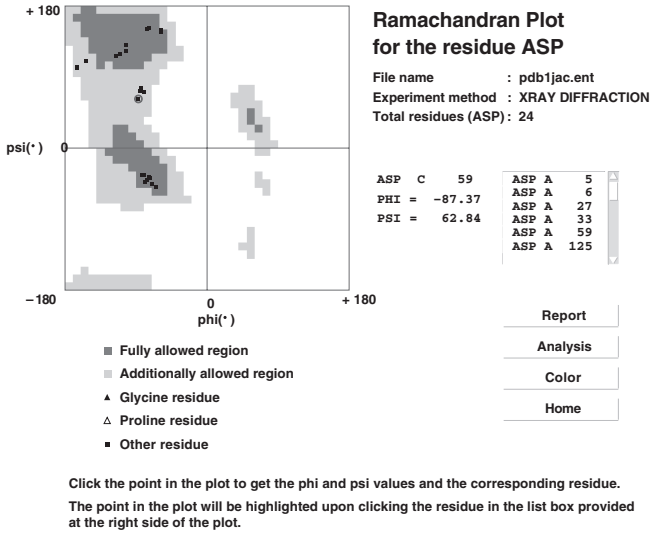

Fig. 1. A sample output showing the (ϕ, Ψ)—plot for the residue Aspartate in the protein structure, Jacalin (PDB—id code 1JAC—Sankaranarayanan *et al.*, 1996), a lectin from the seeds of the jackfruit. The highlighted (encircled) point in the plot corresponds to the residue Asp C 59.

of a residue, which is preceded and succeeded by any residues. The program calculates and displays the multiple conformations adopted by a single amino acid residue whose structure is solved and refined at atomic resolution. Once the plot is available on the client machine, the users can get the values (ϕ, Ψ) of a particular amino-acid by clicking the residue in the list box provided at the right side of the output screen and the corresponding point in the Ramachandran plot is highlighted. In addition, the user gets the complete information of the amino acid residue and its (ϕ, Ψ) value by clicking a point marked in the Ramachandran plot (Figure 1). Also, for NMR structures, an option has been provided to choose the model number for which the plot is desired. The analysis button shows a detailed output of the type and the number of residues present in various major secondary structural regions of the plot.

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