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Revisiting India's pride: The Ramachandran map - all over again *

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

It is now known for over 50 years that not all possible (ϕ, ψ) combinations are equally preferable for polypeptide backbone. The classic work by Ramachandran and co-workers in early 1960s, in which one of us (CR) participated, was performed at a time when no globular protein structure was available at the atomic level. However, the impactful ideas from this work are being used routinely in a number of practical applications in the present-day protein structural science especially in validating protein structures. As George Rose reckons, this is one of very few instances in biological sciences where a discrepancy between theory and experiment raises doubt about the experimental result!

Presently Ramachandran validation of protein structures is commonly performed effectively by developments such as MolProbity which corresponds to “experimental Ramachandran map”. We suggest tailoring such analyses by position-wise, geometry-specific steric-maps which show (ϕ, ψ) regions with steric-clash at every residue position. These Ramachandran maps are different from the classical Ramachandran steric-map since they are highly sensitive to bond-length and angle values which are used, in our steric-maps, as observed in the residue positions in super-high-resolution peptide and protein structures. The (ϕ, ψ) outliers observed in such structures seldom have steric-clash. Therefore, we propose that a (ϕ, ψ) outlier is acceptable if the (ϕ, ψ) point is located within the steric-clash free region of geometry-specific steric-map for a residue position. We also observe that same residue with very different (ϕ, ψ) values, in different structural forms of a protein, lie within steric-clash-free regions in the corresponding position-specific map. Hence, these steric-maps define position-specific accessible (ϕ, ψ) space. The PARAMA resource performs in-depth position-wise analysis of protein structures using bond geometry-specific steric-maps.

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