A conformational study of enkephalin

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The conformations of peptides can be described (Ramachandran, Ramakrishnan & Sasisekharan, 1963) by means of the torsion angles ϕ and ψ about the N—C and C—C bonds in the peptide chain, the torsion angle of the peptide bond being constrained by the planarity of the peptide group. In Figure 1 are shown ϕ, ψ-maps for glycine and alanine. The maps for other amino acids resemble that for alanine, though some amino acids are conformationally more restricted.

The maps can be used to test the configurational specificities of various conformations. For example, the type II β-bend (Venkatachalam, 1968) contains two residues and the conformations for each of these are shown in Figure 1. Each residue is plotted according to it being glycine, an L-amino acid or a D-amino acid. A D-residue is plotted on the map for an L-residue by inverting the ϕ and ψ angles before plotting. It is seen that a D-residue at position 1 and an L-residue at position 2 are disallowed.

Several possible conformations for the pentapeptide leucine-enkephalin have been examined and the configurational specificities predicted for each conformation using ϕ, ψ-maps have been compared with those observed from activity and receptor-binding measurements on leucine enkephalin and analogues containing D-amino acids. Thereby the extent to which the biological data may be explained in terms of the peptide conformation at the receptor has been examined.

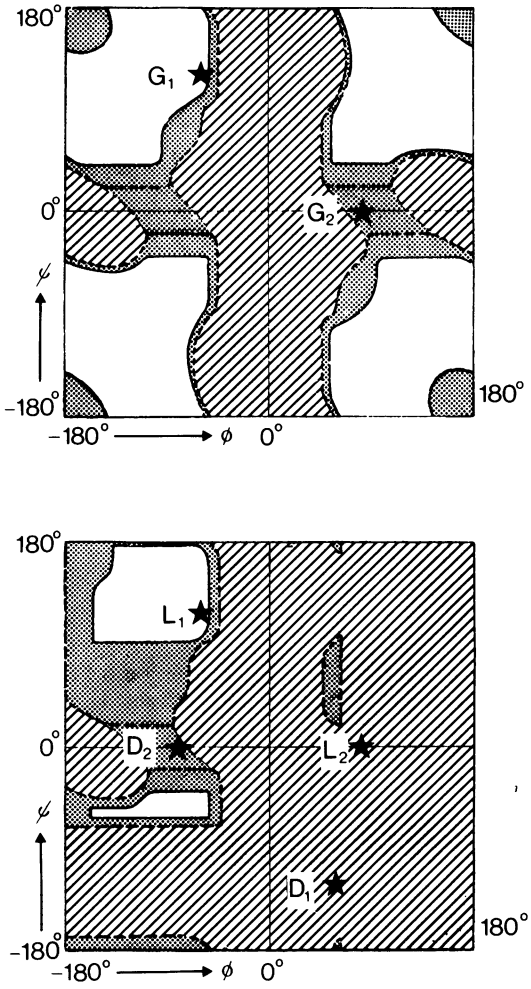

Figure 1 Conformational maps for glycine (top) and L-alanine. Disallowed combinations of ϕ and ψ are hatched. For these, atoms would be too close. Allowed areas are clear. Shaded areas (allowed) correspond to marginally close approaches (e.g. hydrogen bonds). The two residues (1,2) in a type II β-bend conformation are shown, each plotted as glycine (G), an L-amino acid (L) or a D-amino acid (D).

References

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VENKATACHALAM, C.M. (1968). Stereochemical criteria for polypeptides and proteins. V. Conformation of a system of three linked peptide units. *Biopolymers*, **6**, 1425–1436.