Poster Presentation

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The Protein Geometry Database: exploring protein conformational features

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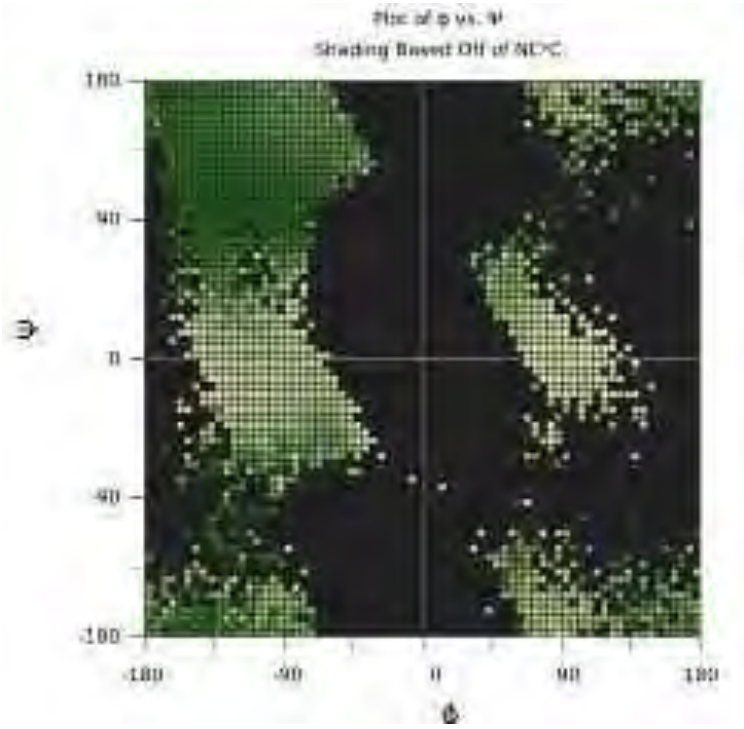
Have you ever seen a feature in your structure and asked, "I wonder how novel this is?" For instance a residue with a certain phi/psi angle, or an Asp residue followed by three further residues that make a tight turn centered on the side chain, or a peptide unit deviating 25˚ from planarity? If so, the Protein Geometry Database (PGD) is something you'll want to know about. The PGD web service (pgd.science.oregonstate.edu, Berkholz 2009a) manages access to a database containing the geometric details of 1.9 million amino acids. Working with the PGD involves two easy steps - using a search form to find a set of peptides matching your interests, and analyzing the geometric details of the set. The search form allows you to find examples of peptide fragments that have any specified combination of backbone conformations and sequence. Filtering can also be performed based on side chain conformations, or bond angles. You can also specify the quality of models included in the search. Once a set of peptides has been identified, their geometric properties can be analyzed on the web site. You can look at the averages and standard deviations for any bond length, bond angle, or conformational angle, or you can explore relationships between properties by displaying highly customizable plots. An option to export the search results allows you to perform any further analyses you might devise. We will show how the PGD has been used to develop a Conformation Dependent Library of main chain bond angle targets for crystallographic refinement (Berkholz 2009b), as well as to advance our understanding of peptide non-planarity, and of conformational preferences for pairs of residues and of cis-peptides. We will also describe how simple searches for outliers in bond lengths and angles are a powerful validation tool that can both uncovering errors in PDB models and can lead to the discovery of very interesting and real deviations from what is normally considered ideal geometry.

[1] *Berkholz, D.S., Krenesky, P.B., Davidson, J.R., et al., P.A. (2009a) Nucleic Acids Research, 38, D320-D325.,* ***[2]*** *Berkholz, D.S., Shapovalov, R.L. Jr, & Karplus, et al., P.A. (2009b) Structure, 17, 1316-1325.*



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