

DNA phosphate crowding correlates with protein cationic side chain density and helical curvature in protein/DNA crystal structures

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Proteins that undergo sequence-specific binding to DNA targets do so by processes that are categorized as either direct readout, when the protein makes direct contact with the DNA groove, or indirect readout, which involves recognition of DNA shape. A subset of 58 protein-DNA crystal structures was used to investigate the relationship between protein cationic residue density (Cpc) and DNA phosphate crowding (Cpp). These values were quantified for each structure, and the correlation between Cpc/Cpp was calculated. Structures with a strong correlation ($>\pm 0.25$) contained a DNA helical curvature, and the factor sign indicated the direction of helical curvature (concave or convex).