Poster Presentation

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Hidden Hoogsteens in the Data

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Although extremely rare in the crystallographic database, Hoogsteen (HG) base pairs have been modeled, especially at duplex termini, protein-DNA interfaces, damaged DNA and DNA mismatches. Formation of HG base pairs in duplex DNA requires a 180 degree rotation along the glycosidic bond of the purine relative to the canonical Watson-Crick (WC) base-pair. In a recent survey of the PDB we identified 75 HS base pairs in 2,910 x-ray derived models. Recent evidence suggests that the prevalence of HG base pairs in nature to be greater than previously thought. Due to electron density density ambiguity at mid to low resolution, it is possible for bases to be modeled incorrectly. We have developed a high-throughput method which examines the difference density around DNA to identify mis-modeled bases. Here we show where bases were incorrectly modeled and our subsequent fixes which show pairs modeled as WC that really are HG, vice versa, and evidence of WC-HG alternates. This research shows that base pairing conformations in DNA are more heterogeneous than previously thought.

Keywords: Hoogsteen base pairs, DNA, electron density