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Low-Resolution Refinement of the DNA and Protein Complex Structures

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Macromolecular complexes of protein and DNA are often resolved in a low resolution structure (3.0 angstroms or lower). Because nucleic acids suffer radiation damage more than amino acids, the resulting temperature factors for DNA are generally higher than those for protein. Recognition of DNA-specific interactions with protein is a challenge at low resolution. The use of low-resolution refinement ([1]) or the reference high resolution model could improve DNA densities. A number of DNA/protein and nucleosome complexes (i.e. RAGE-DNA [2], CENP-C-NCP[3]) that we have recently refined demonstrated the validation of these methods.

[1] *Brunger AT, Adams PD, Fromme P, et al. "Improving the accuracy of macromolecular structure refinement at 7 angstroms resolution". Structure, 20:957-966, 2012,* ***[2]*** *Sirois C, Jin T, Miller AL, et al. "RAGE is a nucleic acid receptor that promotes inflammatory responses to DNA". Journal of Experimental Medicine, 210(11):2447-2463, 2013,* ***[3]*** *Kato H, Jiang J, Zhou BR, et al., Straight AF and Bai Y, "A conserved mechanism for centromeric nucleosome recognition by centromere protein CENP-C". Science, 340:1110-1113, 2013*

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