basis of the interactions observed in the enzyme-inhibitor complex, implicate the side chain of Leu-272 in active expulsion of uracil from DNA by penetrating the DNA helix from the major groove, with the uracil "flipping out" via the DNA minor groove. Recent results corroborate this hypothesis and suggest a mechanism for UDG recognition of promutagenic GU mismatch base pairs within the context of double-stranded DNA.

PS04.05.23 DNA POLYMERASE II FROM *ESCHERICHIA COLI*. C.R.A. Muchmore, M.M. Blair, L. Shuvalova, M.F. Goodman, W.F. Anderson, Northwestern University Medical School, Department of Molecular Pharmacology and Biological Chemistry, Chicago, Illinois and University of Southern California, Department of Molecular Biology, Los Angeles, California.

Polymerase II from *E. coli* is a member of the group B (α-like) DNA polymerases as indicated by conserved sequence motifs. It contains both polymerase and 3'->5' exonuclease activity on a single polypeptide chain of 781 amino acid residues and is induced by DNA damage. The βγ accessory protein complex of the polymerase III holoenzyme increases polymerase II processivity, raising questions about the nature of this interaction. Information about structure and function derived from the atomic structure of *E. coli* polymerase II may be applicable to other homologous group B polymerases like mammalian cellular DNA polymerase α, eucaryotic viral polymerases and bacteriophage T4 polymerase.

Polymerase II crystallizes by sitting drop vapor diffusion with PEG 400 and citrate as precipitating agents at pH 5.8. Three heavy atom derivatives were produced under these conditions. Recently, the crystals have been successfully transferred to solutions of lower ionic strength and higher pH thus improving conditions for derivatizing crystals with heavy atom compounds.

X-ray diffraction data have been collected from the wild type polymerase II crystals at room temperature and at 103K from flash-frozen crystals. The crystals are of space group $P2_12_12$ with one monomer per asymmetric unit. Initial phases for the wild type data were obtained by MIR methods. Phases were improved and extended to higher resolution by model building, phase combination and density modification techniques.

This work is supported by NIH GM48569, ES05355 and GM15075

PS04.05.24 REFINEMENT STRATEGIES FOR PROTEIN-NUCLEIC ACID COMPLEXES. G. N. Parkinson, B. Schneider, J. Vojtechovsky, R. H. Ebright, and H. M. Berman, Department of Chemistry, Rutgers University, Piscataway, New Jersey 08855.

Protein-DNA complex crystals offer an obvious path towards visualizing modes of recognition, stabilization, interaction, and conformation of nucleic acids and proteins. We are studying a series of such crystalline complexes containing Catabolite Activating Protein (CAP) and DNA with particular emphasis on understanding the detailed interactions between the amino acid side chains and the nucleic acid bases. To do this, it is necessary to exercise special care with the refinement process.

In order to achieve improved results, we created a nucleic acid parameter file (Parkinson, et al., Acta Cryst. D52, 57 1996) for use with X-PLOR that incorporated newly determined standard values for the bond distances, bond angles, and dihedral angles. More recently we have expanded the parameter file to include dihedrals for three DNA conformational classes.

The strategies for refinement of these complexes that allow for the correct balance between the macromolecular components will be discussed.

Supported by grants from NIH (GM 21589) and NSF (BIR 9305135).

PS04.05.25 THE BATTLE FOR IRON - CRYSTALLOGRAPHIC STUDIES OF THE IRON DEPENDENT REPRESSOR PROTEINS FROM *C. DIPHTHERIA* AND *M. TUBERCULOSIS*. Ehmke Pohl[a], Xiayang Qiu[a], Randall K. Holmes[c] & Wim G.J. Hol [a,b]. [a]Biomolecular Structure Center and [b]Howard Hughes Medical Institute, University of Washington, Box 357742, Seattle, WA 98195, USA; [c]Department of Microbiology, University of Colorado, Health Sciences Center, Denver, CO 80262, USA.

Iron is an essential nutrient for most virulent bacteria, however the availability of free iron in the mammalian hosts is extremely limited. A number of pathogens utilize the low-iron environment as a signal for the expression of virulence factor and proteins involved in obtaining iron from the host organism.

In *Corynebacterium diphtheria* the Diphtheria Toxin Repressor (DtxR) is activated at about 2 mM Fe^{2+}. The active dimeric protein binds specifically the *tox* and *irp* operators which encode the tox gene and the irp genes. The crystal structure of DtxR has recently been solved at 2.8 Å resolution [1]. High resolution data of DtxR in complex with different divalent metals have been collected at low temperature using conventional X-ray sources and synchrotron radiation. The metal binding sites have been unraveled in greater detail than previously reported.

A functionally homologous repressor from *Mycobacterium tuberculosis* has been cloned, expressed in *E. coli* and purified. This iron dependent repressor (IdeR) shares 60% sequence identity with DtxR [2]. Crystallization and preliminary analysis by X-ray crystallography will be presented.

[1] X. Qiu, C.L.M.J. Verlinde, Z. Zhang, M.P. Schmitt, R.K. Holmes & W.G.J. Hol (1995) *Structure* **3** 87-100.

[2] M.P. Schmitt, M. Predich, L. Doukhan, I. Smith & R.K. Holmes (1995) *Infect. Immun.* **63** 4284-4289.

PS04.05.26 STUDIES TOWARDS THE X-RAY CRYSTAL STRUCTURE OF HELICASES. Christopher Putnam and John Tainer, The Scripps Research Institute, Molecular Biology, MB4, La Jolla, California 92037

DNA helicases are an important, structurally uncharacterized class of biological molecular motors that use the energy of nucleotide triphosphate hydrolysis to the unwinding of nucleic acid double helicies. The function of helicases in general are critical in the synthesis, maintence and repair of the genome of all organisms. The RuvB DNA helicase from Escherichia coli has been chosen as a starting point for investigation of this class of enzymes. RuvB is a relatively small DNA helicase that forms homohexamers around DNA. In vivo, the ATPase activity of RuvB is responsible for migration of Holliday junctions during genetic recombination. Preliminary diffraction data will be presented.