This week I worked mainly in analyzing some previous structures and learning some programming. Some of the structures are in the next pages; however, this is not a complete analyzes of the DNA in the complexes. Some examples are the CtsR, DnaA, SlyA and CSL. For this week (and probably next week as well), I plan on searching for newer structures on the pdb that contain features that I want, such as A-tracts, unwinding of the double helix, arginines inserted into the minor groove, applying some scripts in order to do so.
**CtsR/McsB**

**CtsR**
repressor binds to the promoter region of heat-shock genes with high affinity and inhibits transcription under normal conditions;

**McsB**: protein arginine kinase that phosphorylates residues in the DBD of CtsR, and inhibits the heat-shock regulator CtsR

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*Fuhrmann, … Clausen, Science 2009*
In the same paper by Fuhrmann et al., they observed that CtsR that was phosphorylated could not bind to DNA. Sites of phosphorylation were identified as arginines 28, 49 and 62. Interestingly, Arg62 is invading the minor groove, and when R62 → E62, mutant can no longer bind to DNA. New class of protein kinases acting on Arg residues?
Binding of DnaA to oriC regions result loading of DnaB and consequent DNA replication; In E coli, oriC contains several DnaA binding sites (some sites higher, others weaker affinity);

DnaA – conserved in bacteria.
In E. coli, DnaA-box is TTATNCACA, while in M. tuberculosis has larger number of box sequences. Across different mycobacteria, most conserved boxes are [T/C][T/C][G/A]TNCACA
Bending of DNA in the region is observed for E. coli and M tuberculosis

First 3 positions vary the most among M. tuberculosis and E. coli.

Lys436, if mutated, abolishes binding; in E coli it is substituted by an arg; Even though there is not a narrowing of minor groove of naked DNA on that region, the minor groove contact is important for this recognition.
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SlyA (3QF5)
3brg - consensus site

3iag - nonconsensus site