MD simulations of DNA recognition by the repressor AmtR

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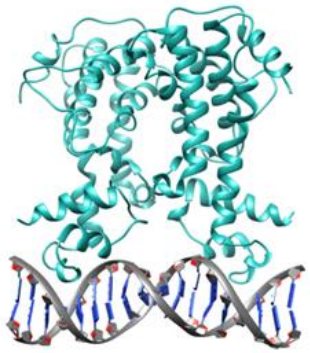
The protein AmtR occurs in the gram positive *Corynebacterium glutamicum* in which it is a master regulator and represses genes of the nitrogen metabolism and the signal transduction pathway. Each subunit of the dimeric AmtR recognizes a conserved four base motif ("CTAT"). A comparison between the known binding sites and those genomic sites that are not regulated by AmtR reveal significant differences for those bases that are adjacent to the CTAT recognition motif. Therefore, we investigated whether these adjacent bases also play a role for AmtR binding specificity.



Molecular simulations (MD) of free DNA and AmtR-DNA-complexes were used to study the dynamics of these two systems and the interactions between DNA and AmtR. There are several specific contacts to the flanking bases formed during the MD simulation. Besides direct base recognition also unspecific contacts to the phosphate backbone of the DNA were detected. These contacts correlate with a local deviation from the ideal B-DNA geometry which is not observed in the simulation of free DNA. This suggests that the specific DNA recognition by AmtR relies on a larger binding motif than previously known.