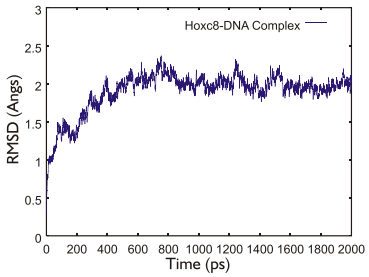
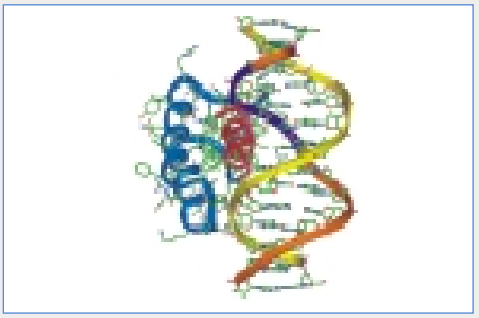
Homology modeling:

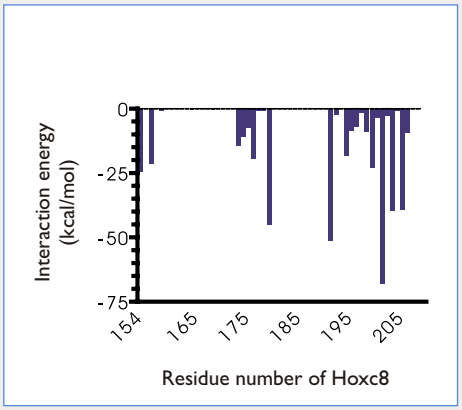
Homology modeling is a very effective method of generating the 3D structure of a protein for which experimental (X-rays crystallographic or NMR) structure is not available but the crystal structure of homologue is available. Then using that as the template the 3D structure of the protein of interest is generated by homology modeling based method. Here is an example where the homology-based model of a DNA-protein complex (DNA-HOXc8) is presented.

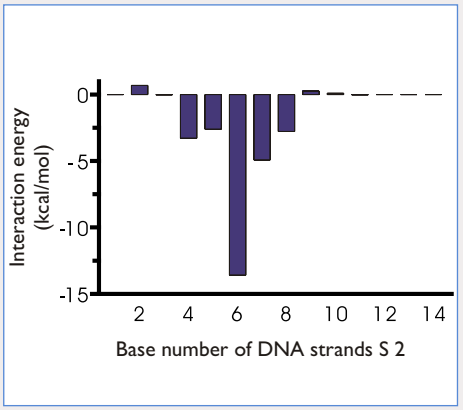


Time evolution of the RMSD of the Hoxc8-DNA complex over the 2.0ns trajectory obtained by MD simulation in explicit aqueous solvent.



Stereo view of the Hoxc8 - DNA complex obtained by Homology modeling





The top right hand figure represents the pattern of the interaction energies of the individual bases of the strand (S2) of the DNA that is mostly interacting with Hoxc8 in the model. This plot clearly indicates the relative importance of the different bases of S2 in the recognition process. The software CHARMM-27 did the computation of the energies.