DNA ‘glass transition’ and the LL critical point of water

--- a simulation study

Previous work on DNA

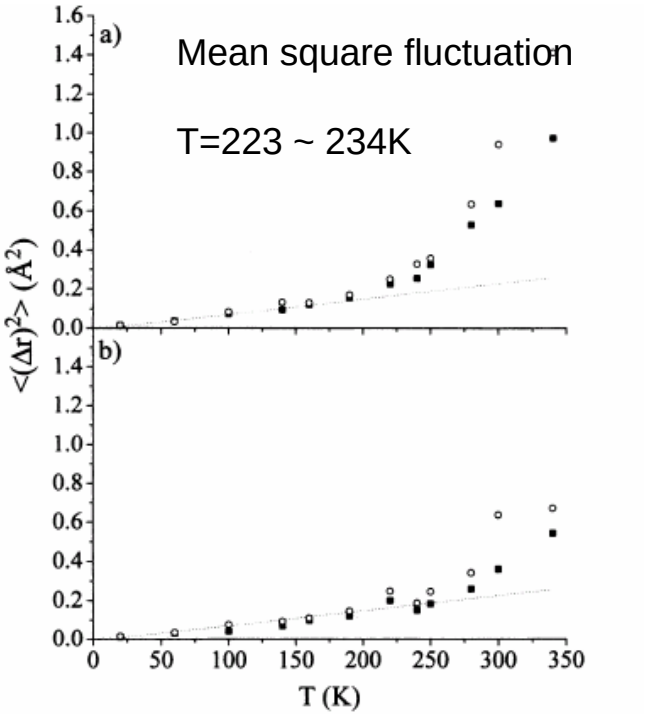
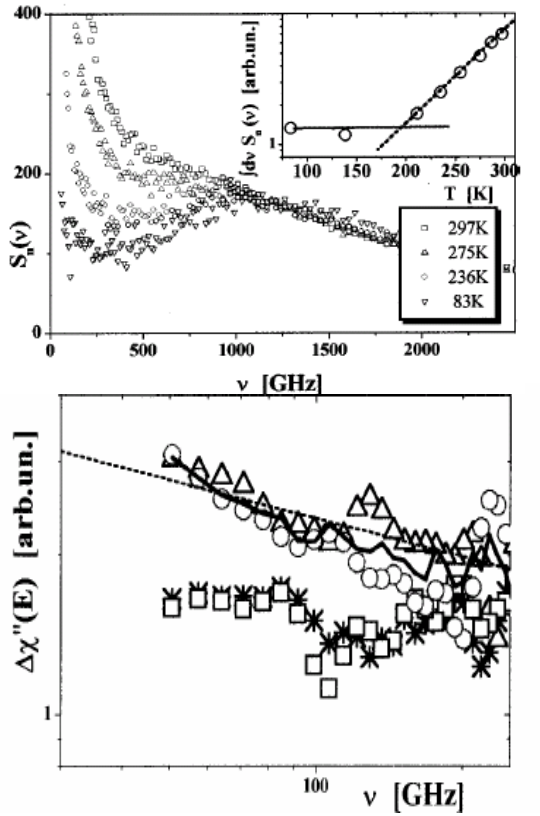


FIG. 2. Mean square atomic fluctuation averaged over the (*a*) phosphate groups (○) and sugar riboses (■) and over the (*b*) cytosine (○) and guanine (■) bases.

- **Glass transition in DNA from molecular dynamics simulations.**
  Norberg J, Nilsson L,
  Proc Natl Acad Sci U S A.
  1996 Sep 17;93(19)

[6 nucleotides: $(CGCGCG)_2$ duplex]
TIP3P



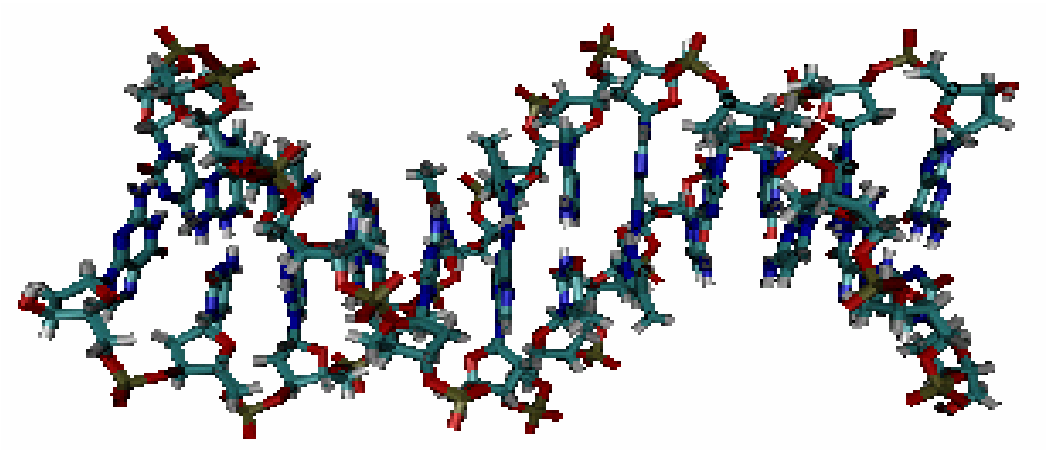
Inelastic neutron scattering spectra of DNA-fibers
A.P. Sokolov, H. Grimm,
A. Kisliuk and A.J. Dianoux
J CHem Phys
Volume 110, Issue 14, pp. 7053-7057 (1999)

Differences of the susceptibility spectra

Glass transition T=180-200K,
Dynamic crossover T=230K, (MCT ?)

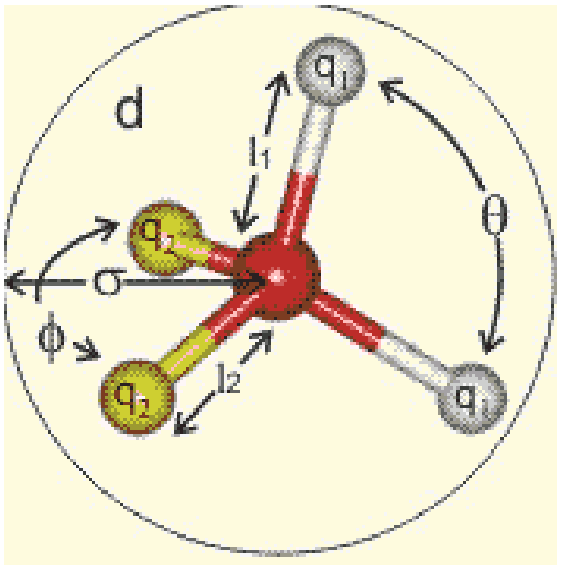
Our Model of DNA: Dickerson Dodecamer

- 12 nucleotides: CGCGAATTCGCG
- mass:7270.756 amu



Drew, H. R., Wing, R. M., Takano, T., Broka, C., Tanaka, S., Itakura, K. & Dickerson, R. E. (1981).
Structure of a B-DNA dodecamer: conformation and dynamics.
Proc. Natl. Acad. Sci. USA 78, 2179-2183.

Water: TIP5P



1488 water molecules,

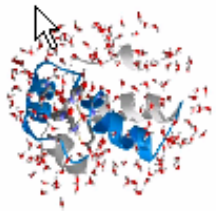
Hydration:1488*18/7270.756=368%

Model	Type	σ Å [6]	ε kJ mol^{-1} [6]	l_1 Å	l_2 Å	q_1 (e)	q_2 (e)	θ °	ϕ °
TIP5P [180]	d	3.12000	0.6694	0.9572	0.70	+0.2410	-0.2410	104.52	109.47

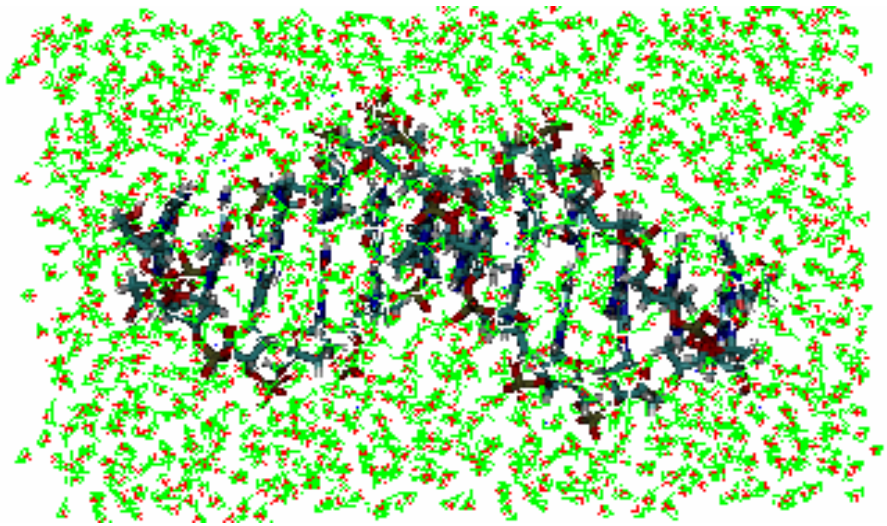
M. W. Mahoney and W. L. Jorgensen, A five-site model for liquid water and the reproduction of the density anomaly by rigid, nonpolarizable potential functions,
J. Chem. Phys. **112** (2000) 8910-8922.

Simulation:
AMBER force field ports for the GROMACS

AMBER homepage

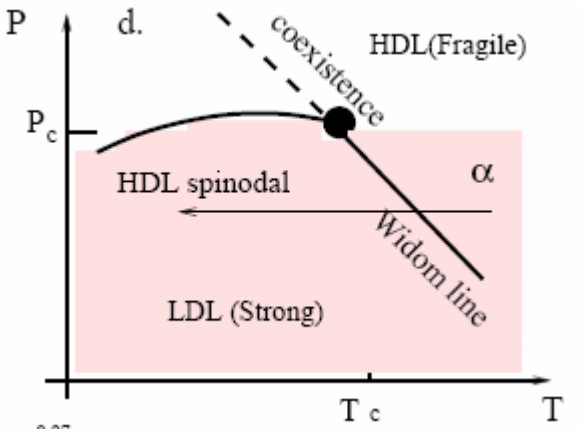


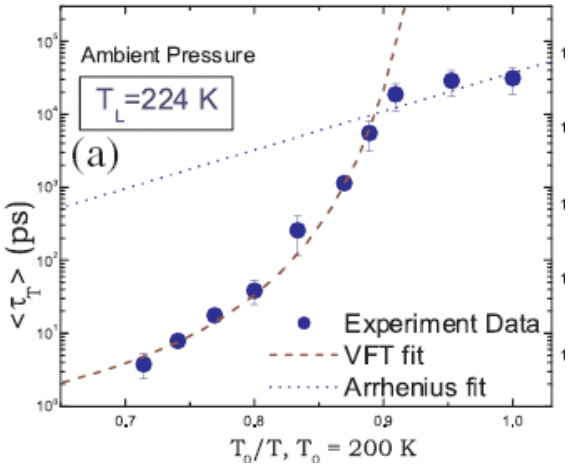
GROMACS homepage

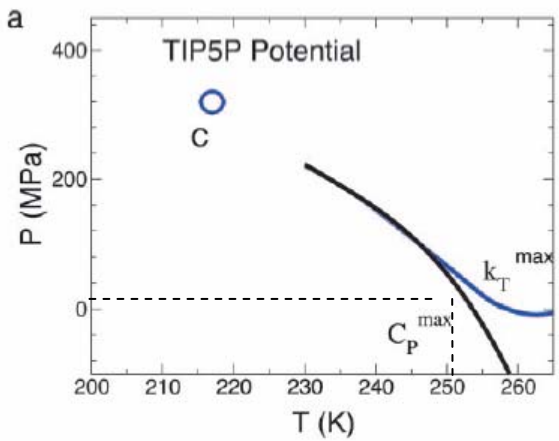


Details to see: http://folding.stanford.edu/ffamber/
http://www.gromacs.org/

LL critical point



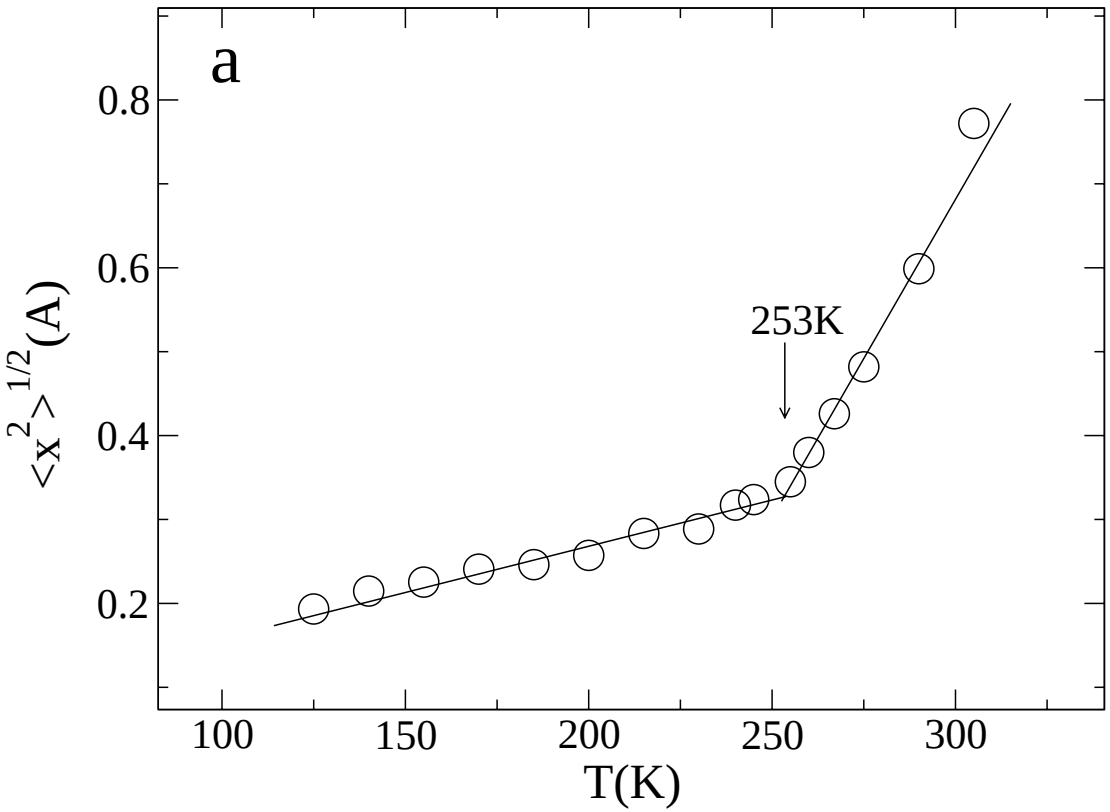




TIP5P, ambient pressure
T crossover=255K

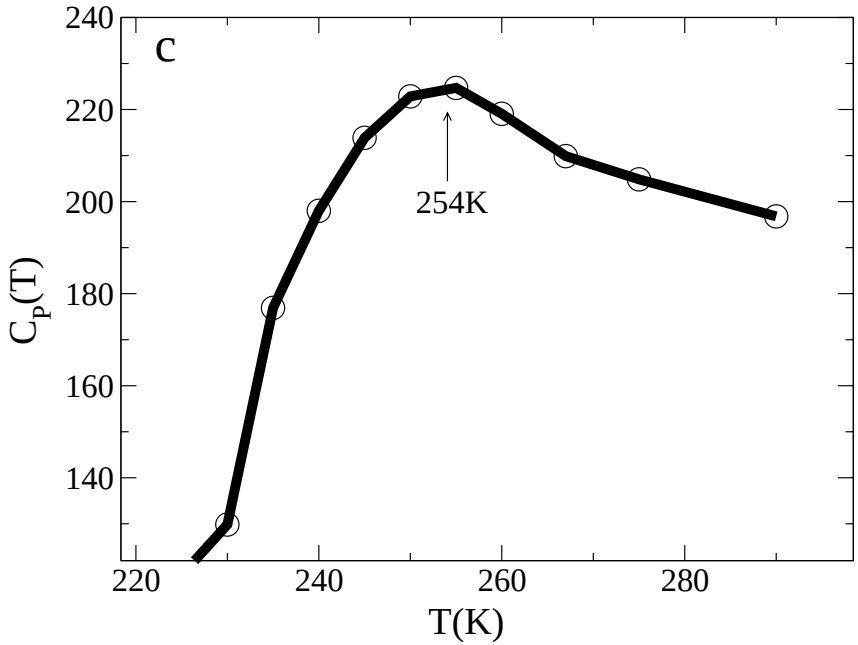
Li Liu, Sow-Hsin Chen, Antonio Faraone, Chun-Wan Yen,and Chung-Yuan Mou
Phys. Rev. Lett. **95**, 117802 (2005)
L. Xu, P. Kumar, S. V. Buldyrev, S.-H. Chen, P. H. Poole, F. Sciortino, and H. E. Stanley,
"Relation between the Widom Line and the Dynamic Crossover in Systems with a Liquid-Liquid Critical Point,"
Proc. Natl. Acad. Sci. 102, 16558-16562 (2005).
Pressure Dependence of Fragile-to-Strong Transition and a Possible Second Critical Point in Supercooled Confined Water

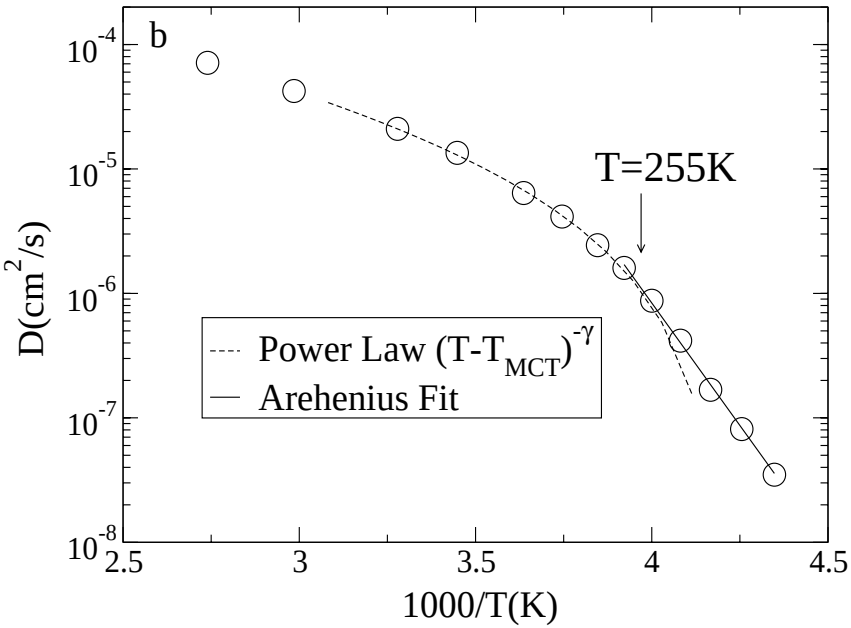
Results: root mean square fluctuation



root mean square fluctuation (RMSF, i.e. standard deviation) of atomic positions after first fitting to a reference frame

Results: thermodynamics and dynamics

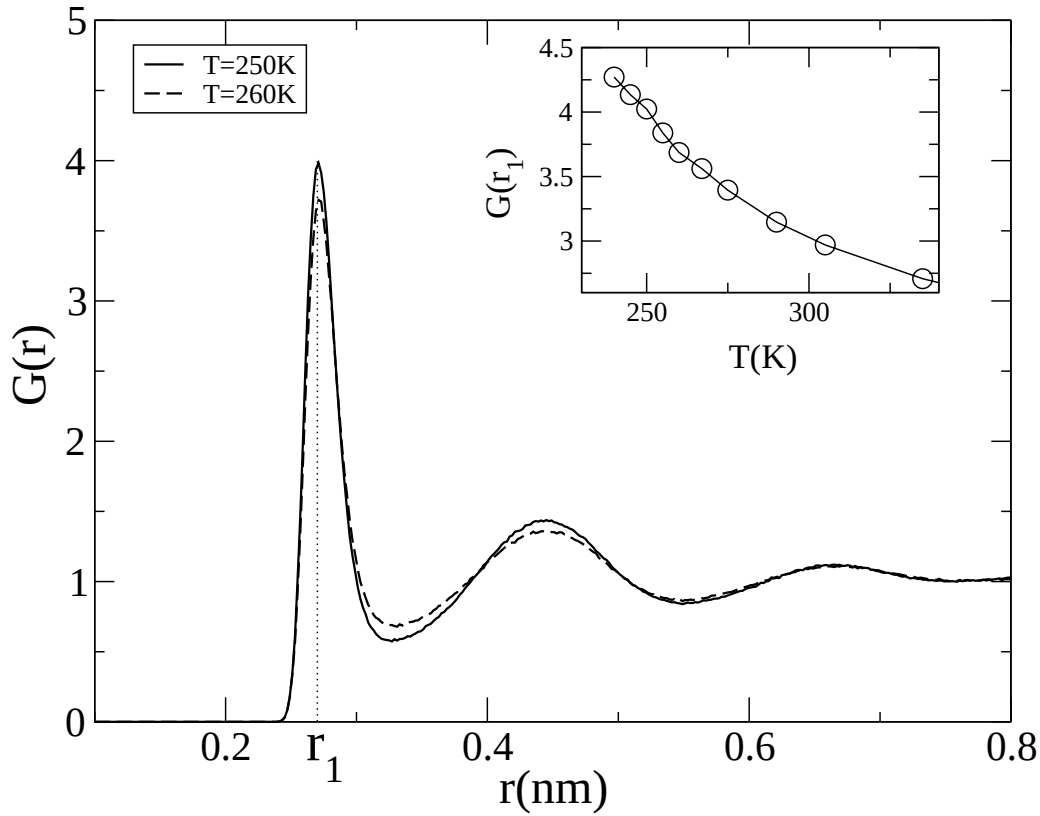




Specific Heat of whole system (water+DNA)

Diffusion constant of hydration water

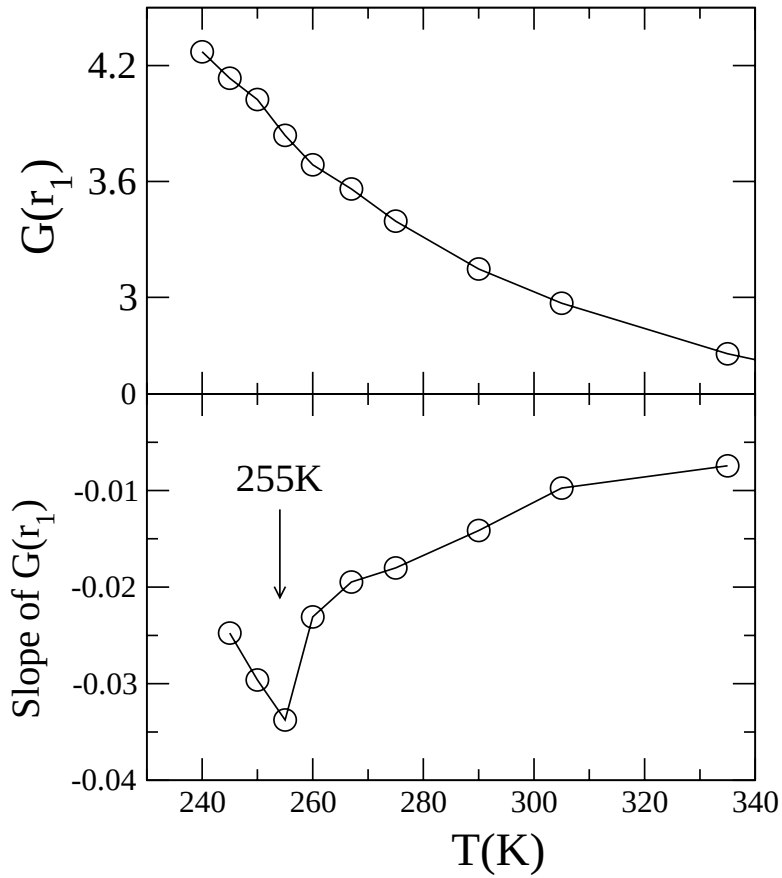
Structure change of water:



Radial distribution function

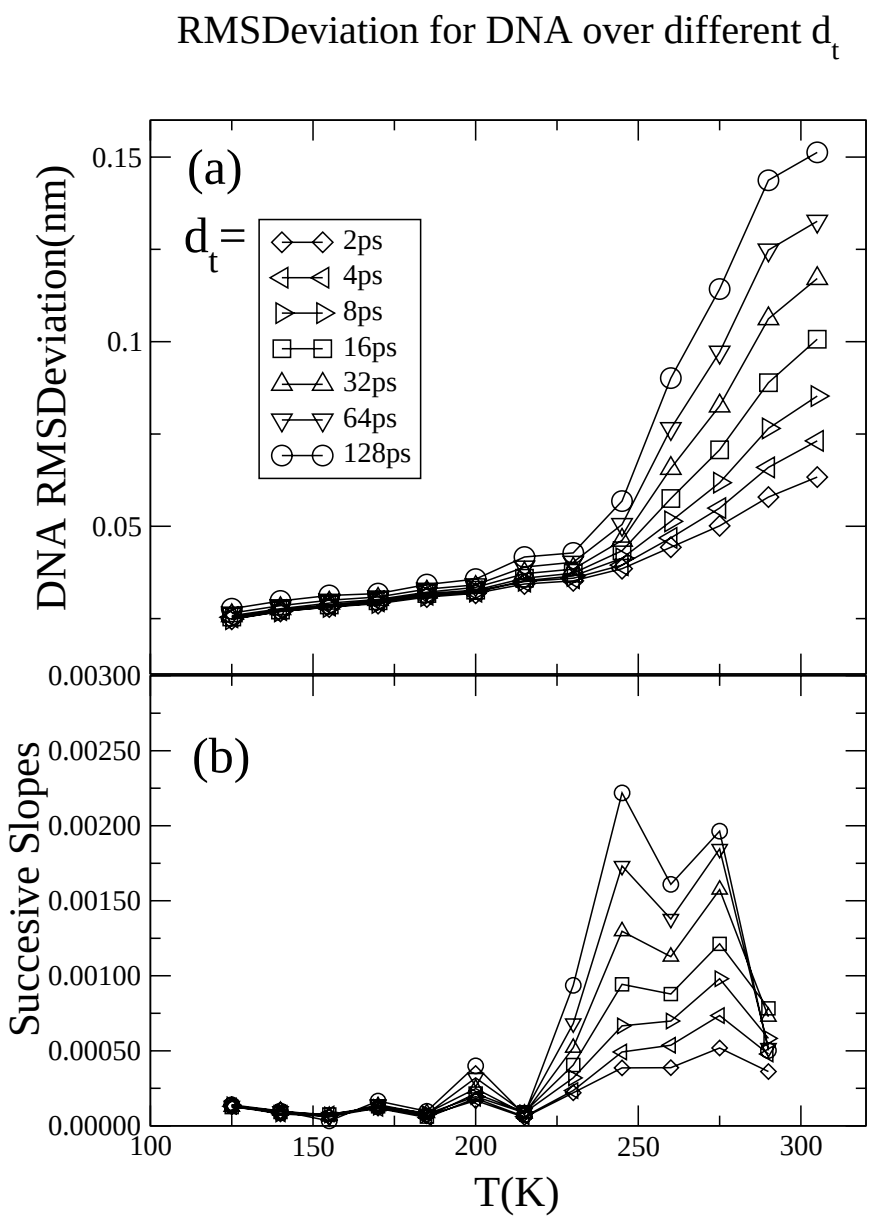
Inset: G(r) at first peak as function of T

Structure change of water:



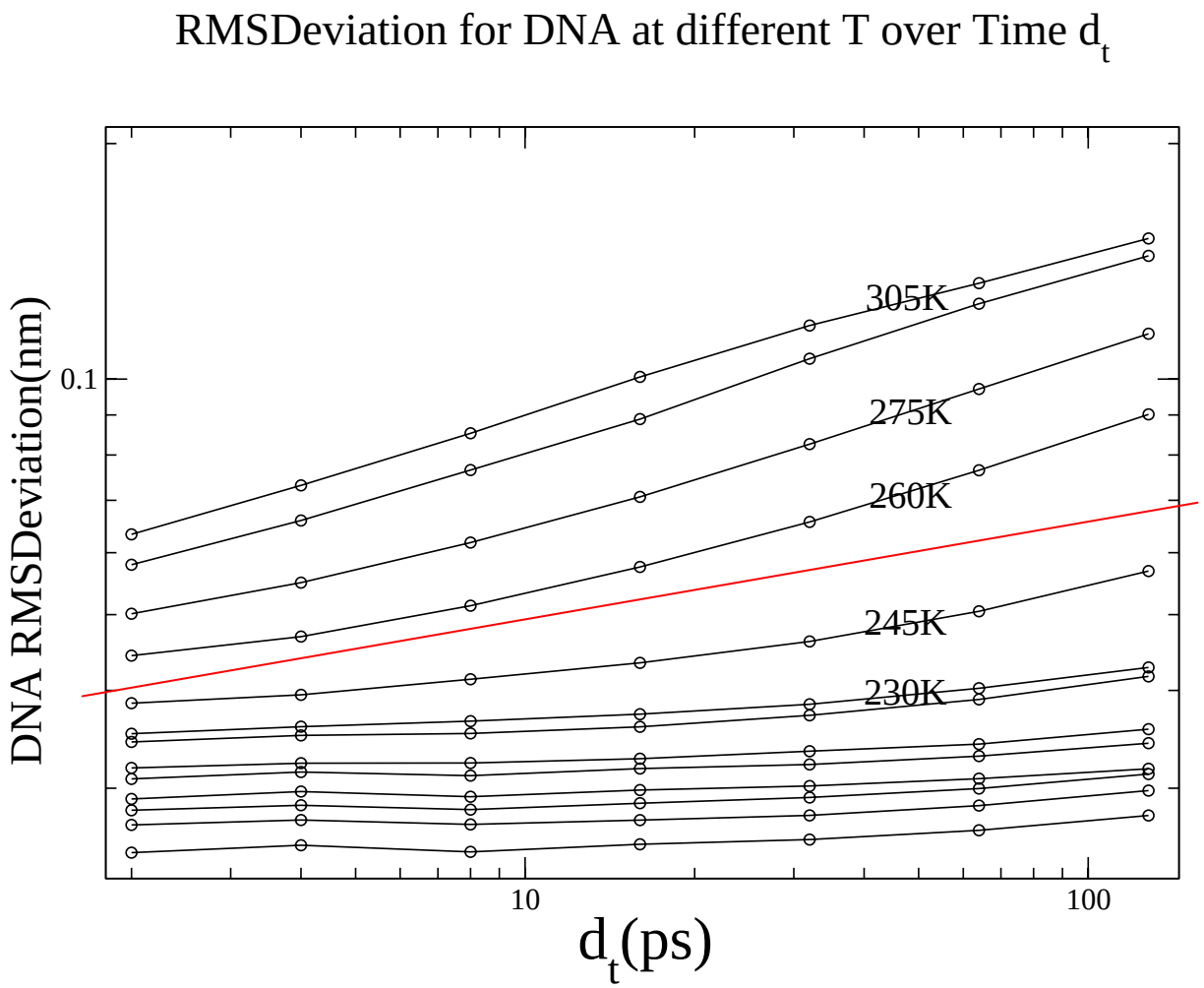
The $g(r_1)$ at first peak as function of T, and the slope as function of T

More: root mean square deviation of DNA (RMSD)



Each structure from a trajectory is compared to a reference structure *dt time ago* by least-squares fitting the structures on top of each other.

RMSD as function of time



Future work

- Boson peak
- Hydrogen bonds melting of bound water molecules on surface of DNA?
- Molecular group difference of fluctuation?

  riboses, phosphate, Guanine(G),Cytosine(C), Adenine(A), Thymine(T).