Structure of DNA [pln39]

Deoxyribonucleic acid (DNA) consists of two biopolymer strands cross-linked into a double helix.

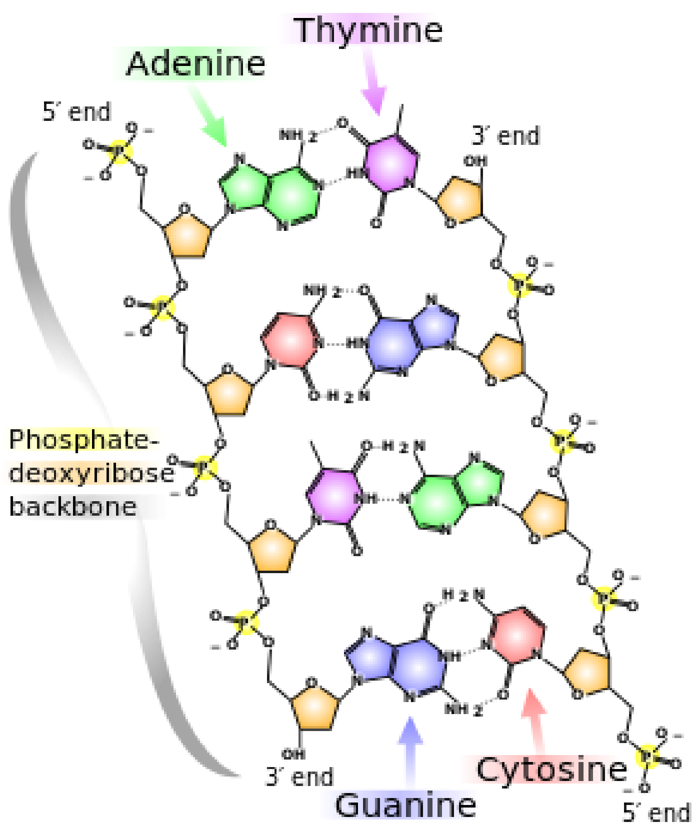
Each strand is a polynucleotide.

Composition of nucleotide:

- nucleobase: guanine (G), adenine (A), thymine (T), cytosine (C),
- deoxyribose: monosaccharide sugar,
- phosphate group.

The backbone of a strand is formed by covalent bonds between sugar and phosphate in an alternating sequence with distinct ends:

- 5′: terminal phosphate,
- 3′: terminal hydroxyl group of sugar.



[image from Wikipedia]

Double-stranded (ds) DNA cross-linked by H-bonds between bases of opposite strands. Only two kinds of base pairs are realized:

- A−T (two H-bonds),
- C−G (three H-bonds).

Double helix stabilized mainly by two interactions:

- base pairing (inter-strand interaction),
- base stacking (intra-strand interaction).

Two kinds of transformation between conformations may occur under tension, torque, or environmental change:

- *order-disorder transformation* (DNA melting with strands coming apart, trurning segments of ds-DNA into segments of ss-DNA),
- *structural transformation* (e.g. B/S transition or supercoiling, where strands stay connected in dsDNA but undergo a conformational change).

Hierarchy of structures:

- *primary*: nucleotide sequence from nucleobase, deoxyribose, phosphate,
- *secondary*: double helix stabilized by base pairing and base stacking,
- *tertiary*: formation of superhelical twist, nucleosomes, chromosomes.

B-DNA

- Pitch: 34Å (distance between successive turns).
- Radius: 10Å (straight segment).
- Length per base pair: 3.3Å.
- 10.5 base pairs per turn.
- Strands have opposite terminals, $5'$ and $3'$, at each end.
- High C−G content increases stability.

S-DNA

- Conformation of ds-DNA with structure yet to be determined.
- All base pairs are intact but the base stacking is disrupted.
- Ladder-like structure with a twist.
- Length per base pair: 5.6Å.
- 37.5 base pairs per turn.

P-DNA

- Overwound B-DNA under increasing tension tends to undergo a conformational change into P-DNA. Structural transition.
- Base pairs broken and bases exposed. Phosphate backbone on the inside of helical structure.
- Length per base pair: 5.3Å.
- Helical periodicity, 2.6 bp/turn, releases torque during transition.
- Conformation named after Pauling. It shares features with Pauling's 1953 DNA model.
- Aleft-handed version of P-DNA has been named Q-DNA.

Z-DNA

- Left-handed double helix conformation similar to B-DNA.
- L-DNA is another left-handed conformation. It may contain segments of Z-DNA and segments of melted DNA.

ss-DNA

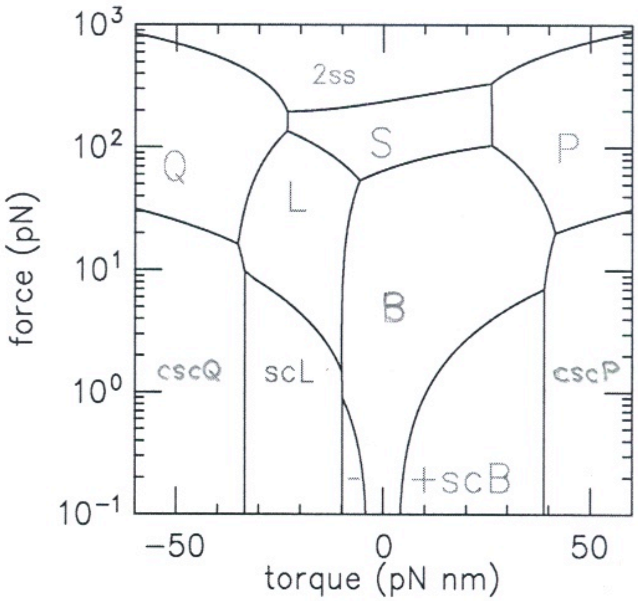
- Under mild tension, ss-DNA is about 1.7 times longer than ds-DNA in its B-DNA conformation.
- Underwound B-DNA under increasing tension tends to denature into segments of ss-DNA (melting bubbles). Order-disorder transition.
- ss-DNA is the result of DNA melting as described in [pln89].

sc-DNA

- ds-DNA with superhelical writhing (formation of plectonemes).
- Two distinct types of plectonemic supercoiling have been identified: inflated supercoils (sc) and collapsed supercoils (csc). The type realized depends on whether interactions between DNA segments that come into contact because of the looping shape are predominantly repulsive or attractive.

In experiments with individual DNA-molecules mounted in magnetic or optical tweezers and subjected to controlled tension and torque there is evidence for 'transitions'[1] between distinct conformations.

One type of modeling produces the phase diagram in the plane of control variables as shown. The 'transitions' between adjacent conformations are first-order like, for the most part.



[image from Marko and Neukirch 2013]

[1]Thermal fluctuations do not permit sharp transitions in 1D systems with short-range interactions. What is observed are really crossovers albeit relatively sharp ones. The exception is DNA melting via bubbles because the ss-DNA loops amount to a long-range interaction.

Additional points of interest:

- Persistence length of S-DNA is much longer than that of ss-DNA: $l_\mathrm{p} \simeq 10$nm versus $l_\mathrm{p} \simeq 0.7$nm. Low salt concentration destabilizes S-DNA in favor ss-DNA. Under increasing tension B-DNA tends to convert directly into ss-DNA if the DNA is AT-rich. In CG-rich DNA an increase in tension tends to transition first into S-DNA and then into ss-DNA.
- λ-DNA represents a typical genomic DNA regarding distributions of AT and CG base pairs.
- Physiological conditions for DNA means room temperature, pH 7.5, and 150mM of NaCl.