Biomolecular structures: nucleic acids and proteins

Figures from Matthews, van Holde: Biochemistry, Benjamin/Cummings. Daune: Molecular Biophysics, Oxford Univ. Press. Wikipedia.

Biomolecules

Biopolymers

Nucleic acids: phosphate group, sugar, base

Proteins: amino acids

Carbohydrates: sugar units

Lipids: head group, alifatic chain



Nucleic acids

Monomer = nucleotide phosphate group, sugar, base



RNAnucleotidesDNA(phosphate group – dissociated at physiologic conditions)

Nucleobases



Polymers



Primary structure of nucleic acids

- Sequence of nucleotides/bases in the strand
- Written as ACGTT, d(ACGTT), d(ApCpGpTpT) etc. TGCAA
- Complementarity due to base pairing
 - Usually only one strand written

Watson-Crick base pairing



- exclusively A-T and G-C (a pyrimidine with a purine)
- strong hydrogen bonds ~100 kJ/mol

(chem. bond

~400 kJ/mol)

Secondary structure of DNA

- Double strand, base pairing (Watson-Crick)



Secondary structure of DNA

- "Conservative" base pairing – use in nano-technology



Yan, ChemPhysChem 2006

Secondary structure of RNA

- various structures
- an extra OH group rich H-bonding possibilities





DNA double helix

Two distinct grooves minor x major

10 base pairs per turn3.4 nm per turn36° rotation between the pairs

→ 0.34 nm between pairs



Stacking interaction



- per base pair: ~100 kJ/mol (chem. bond ~400 kJ/mol)
 as strong as hydrogen bonds
- van der Waals interaction (dispersive forces – instantaneous dipole-induced dipole)
- key factor of the stabilization of DNA structure

A- and B-DNA



A form B form

A-DNA: 11 bases per turn, 33° rotation Z-DNA: left-handed, different steps

Replication

Duplication of a DNA molecule



of information from DNA to mRNA (messenger RNA)



Denaturation



Replication DNA Transcription PNA RNA Translation Protein

From DNA to a protein

mRNA: messenger RNA

carrier of information stored in DNA for protein synthesis

tRNA: transfer RNA

transporter of an amino acid in the translation

central dogma of molecular biology

From DNA to a protein



Gene: a locatable region of genomic sequence





Proteins



- Primary structure sequence of amino acids
- Secondary structure helix, sheet, turn
- Tertiary structure 3D ordering of 2°-structure-elements

20 amino acids



Amino acids as building stones



Condensation – peptide bond (actually amide bond)



Condensation

Polymerization



Peptide bond



~80 kJ/mol

bond ~200 kJ/mol)



C=N – partial double-bond character

barrier opposing rotation
 (single bond ~10 kJ/mol, double

 \rightarrow only rotation around the single bonds free (C–C^{α}, N–C^{α})



Conformation of peptides / proteins

single bonds C–C^{α} and N–C^{α}

Y und M – torsional angles around these bonds

Elements of secondary structure



Helices (3₁₀, alpha, pi)

Beta-sheet (parallel, anti-parallel)

Various turns etc.

Conformational space





Codons of 3 bases Redundant code





