DNA structure

PDB 1BNA

Open the EzMol start page (http://www.sbg.bio.ic.ac.uk/~ezmol/index.html). Load PDB 1BNA, containing a fragment of DNA.

DNA structure

What is the resolution of the structure? Briefly define the term resolution.
The structure has a resolution of 1.90Å, which means that two atoms that are at least 1.90Å away from each other can be distinguished, but two atoms closer than 1.90Å will be seen as one 'blob'.

What are the two DNA 'chains' called?
Those 'chains' are in fact called **strands***.*

Why is the structure of DNA described as a double helix*?*
The two strands are wound about the same axis, forming a helical structure.

Display the molecule as sticks, with stick heteroatoms coloured by element.

Produce a figure showing a single nucleotide. You can hide unwanted residues by selecting the eraser in 'Step 5 – Add, colour or hide side-chains'. Specify the name of the nucleotide you have chosen and label the following: base (with its name), deoxyribose, phosphate. Do not use the first nucleotide in the sequence (at the 5'-end) as it lacks a phosphate (explained later in this worksheet).

Display the entire DNA molecule as sticks again. Examine the bases.

What atoms are DNA bases made of? (You can check the colour scheme for atom colouring by hovering over the question mark under the table in 'Step 2 – Chain style').
DNA bases comprise carbon, oxygen, nitrogen and hydrogen.

Base pairing

DNA bases can be separated into two categories based on their structure: purines have a double-ring structure while pyrimidines only have one ring.

Describe the base-pairing pattern of DNA (i.e. do pyrimidines only pair up with other pyrimidines, for instance)?
A pyrimidine (single ring) only pairs up with a purine (double ring), and vice versa.

Each nucleotide (or letter in the sequence) only forms pairs with another specific nucleotide. This is called Watson-Crick base pairing.

What are the nucleotide pairs in Watson-Crick base-pairing? You may want to colour different nucleotides with different colours or to display labels in order to make it clearer.
A pairs with T and C pairs with G.

Which part of the nucleotide (base, deoxyribose or phosphate group) is responsible for the specificity of Watson-Crick base-pairing?
The base is responsible for the specificity of Watson-Crick base-pairing, as it is the only variable element in nucleotides (they all have the same deoxyribose and phosphate).

What interactions are responsible for Watson-Crick base-pairing?
Hydrogen bonds are responsible for Watson-Crick base pairing.

DNA backbone & directionality

DNA is ***directional***, i.e. it is read from one end to the other. The directionality of DNA is important as the sequence ATG will not 'mean' the same as GTA. The direction is defined based on the chemical structure of DNA, and in particular the deoxyribose. The carbon atoms of a deoxyribose molecule are numbered in Figure 5.

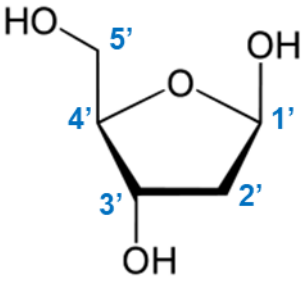

Figure 5 | Deoxyribose molecule with its carbon atoms numbered (blue).

Which carbon from deoxyribose is covalently attached to the base in a nucleotide?
Carbon 1’.

Which carbon is covalently attached to the phosphate group in a nucleotide?
Carbon 5’.

Which carbon is covalently attached to the phosphate group of the next residue in DNA?
Carbon 3’.

You may want to refer back to your first figure to distinguish between the phosphate group of a given residue and the one from the next residue.

Identify the 5'-end and the 3'-end of a strand. When studying DNA in the lab, it is common to remove the phosphate group at the 5'-end. For this reason, the structure in PDB 1BNA (as many other structures) lacks that 5'-phosphate on either strand.

Justify the names 5’-end and 3’-end based on the chemical structure of DNA.
The 5’-end is the end where there is no nucleotide attached to the phosphate at the 5’ position in the ribose.
The 3’-end is the end where there is no nucleotide attached to the 3’ position of the ribose.

Identify the two ends of the other DNA strand.

Are the two DNA strands parallel (i.e. their ends are aligned) or antiparallel (i.e. their ends do not align)?
The two strands are antiparallel: the 5’-end of each strand aligns with the 3’-end of the other.

What is the charge of the DNA backbone? What gives it that charge?
The DNA backbone is negatively charged, due to the negatively charged phosphate groups.