

WA8 – DNA Base Pairing

Name:
Date:

Using PyMOL, load the entry **1enn**, by entering the command **'fetch 1enn'**. This is a short section of DNA. Represent this as a cartoon and hide the solvent by using the command chain

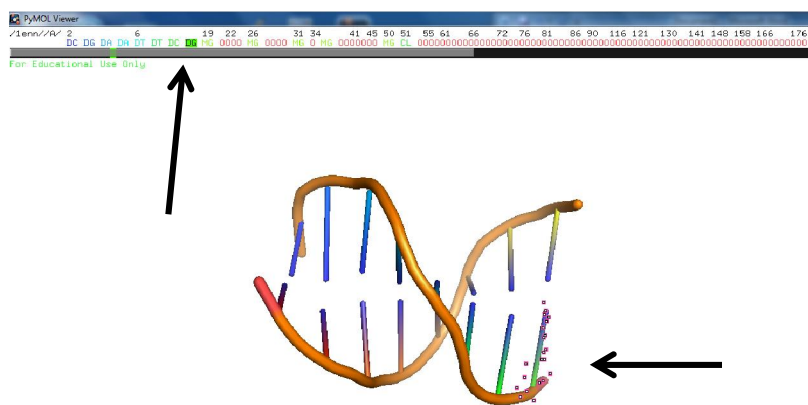
A>preset>pretty.

Load up the residue bar, using the **S** button on the **bottom right** of the screen. To make the DNA structure easier to visualise, select the two residues on the ends, which are not paired up. These should be highlighted in the residue bar as **/A/1** and **/B/10**.

Now, by entering the command **remove sele** into the command bar, delete the residues. Now you should now see a simple double helix.



1. Each of the 'sticks' in the double helix is a DNA base. By going along each DNA chain in turn, write down the sequence of bases which make up this DNA double helix. To do this, click on one of the bases on one chain, on one end of the molecule. Then, by scrolling along the residue bar at the top, note down the second letter which has been highlighted. The first letter will be D, showing that it is a DNA base.



Now, by moving along the helix, select each base in sequence, and note down the base sequence below until you have reached the end of the chain. Once you have sequenced one chain, do the same for the other chain, starting from the base which is paired to your first one – this makes sure that the DNA bases are paired correctly.

Chain 1 sequence	C	G	A	A	T	T	C	G
Chain 2 sequence	G	C	T	T	A	A	G	C

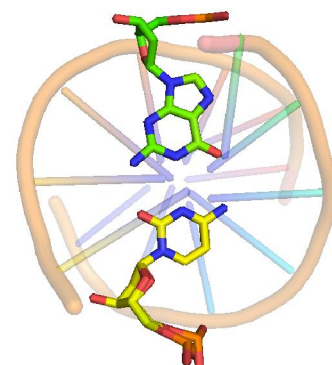
These can be read forwards or backwards, the important part is that the order is right, and the bases are paired up correctly.

2. What do you notice about the base pairing along the double helix?
A is paired to T, and C is paired to G exclusively.
3. Select the two bases in the complementary base pair at the one end of the helix. Using the command **(sele)>S>as>sticks**, view the base pair in its stick structure. What are the main advantages and disadvantages of representing the bases as cartoons vs sticks?

Cartoon		Stick	
Advantages	Disadvantages	Advantages	Disadvantages
Simple – can see overall structure	Simple – cannot see nucleotide structures	Can see individual nucleotides	Very cluttered representation
Easy to spot ligands and other molecules	Cannot tell which base is which	Can distinguish bases	Impractical for very large structures
	Suggests all bases are the same size	Can see bonding clearly	

4. Using the command **(sele)>A>find>polar contacts>within selection**. Note that this will only work if the two bases have been selected previously. Using this, what type of interaction is holding the bases, and therefore the two helices, together?

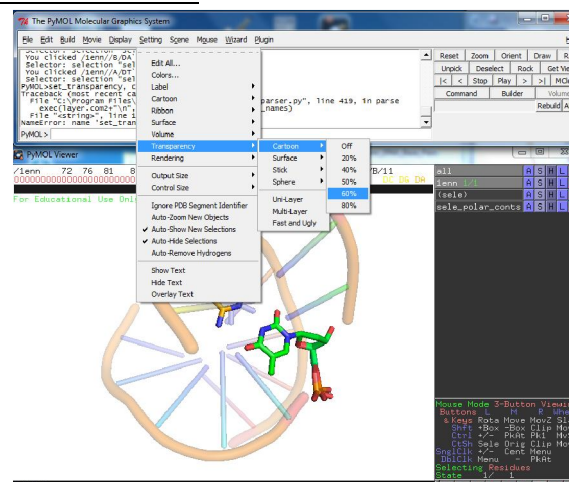
A **polar contact**, in fact it is **hydrogen bonding** which connects the two bases, and links the two strands of polynucleotides.



5. Deselect the base pair and then select a base pair which contains A and T.

Using the same series of commands as above, show the structure in its stick form with polar contacts shown. It may help to make the cartoon representation more transparent, using the settings window as shown below. You can remove the transparency by using the same process and selecting 'Off'. How many interactions hold this base pair together?

There are two **hydrogen bonds** between the A=T pair.



6. What else is visible in the stick representation of the nucleotide residues that you have selected?

A **deoxyribose sugar** and a **phosphate group**.