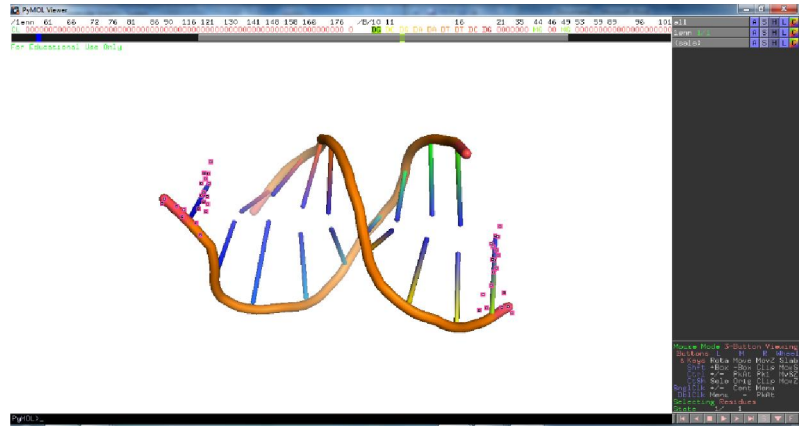


Name:  
Date:

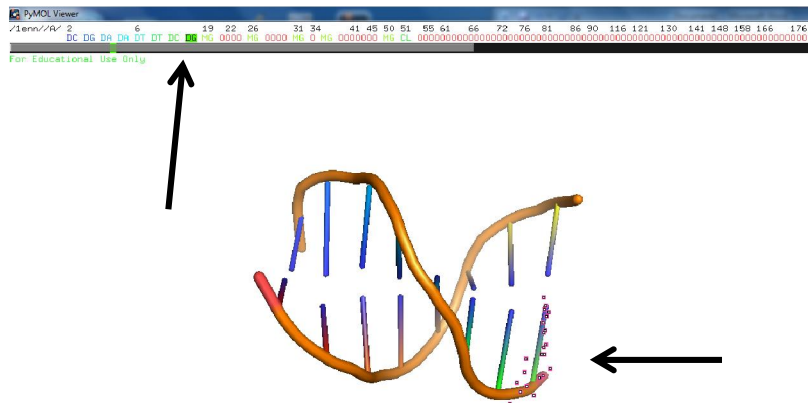
# WA8 – DNA Base Pairing

Using PyMOL, load the entry **1enn**, by entering the command **'fetch 1enn'**. This is a sort 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.



- 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.

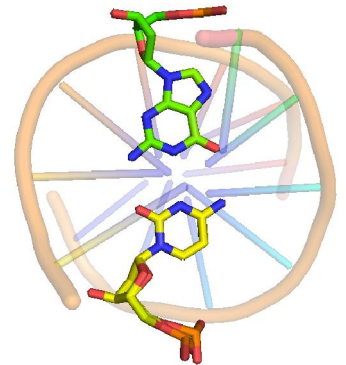


Now, by moving along the helix, select each base in sequence, and note down the base sequence below until you have reached the end of the chain. Once you have sequenced one chain, do the same for the other chain, starting from the base which is paired to your first one – this makes sure that the DNA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

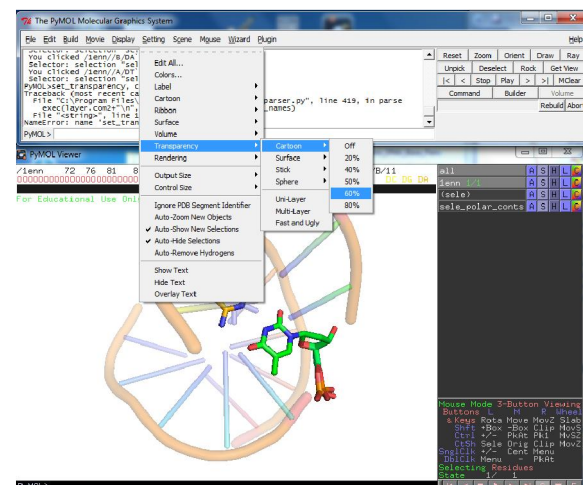
Chain 1 sequence								
Chain 2 sequence								

2. What do you notice about the base pairing along the double helix?
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?

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?



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?



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