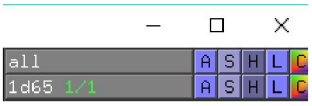
Name:
Date:

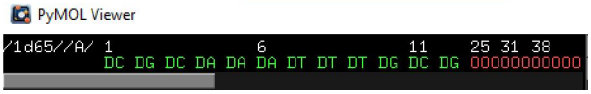
WA7 – DNA Structure

In this activity, you will be exploring the structure of DNA nucleotides – these are the building block monomers which polymerise to make DNA molecules.

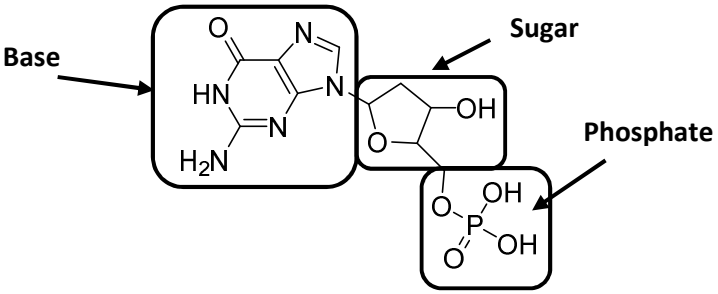
Open up PyMOL and enter '**fetch 1d65**' into the viewer. Using the right-hand pane, select the command **all > S > as > sticks**. This will show the DNA strand in the stick view. Now select **all > S > valence**. This will distinguish single and double bonds.



In the bottom right-hand of the screen, there is another **S** button – click on it. This one shows the list of individual nucleotides which make up the DNA segment shown. Now select the second pair of letter **DG**, on the top of the screen. Click the command **(sele) > H > unselected**. This will now only show one of the nucleotides. To centre this in the viewer, select **(sele) > A > centre**. The nucleotide can be zoomed in on using the right mouse button. Finally, tap **(sele) > L > element symbol**, and then **deselect (sele)** to show each atom labelled as its element.



1. Nucleotides are composed of a phosphate group, a deoxyribose sugar (pentose – 5 carbon), and a varying base. Draw the skeletal structure of the nucleotide that you are currently looking at on PyMOL, drawing boxes around each group to label them.
   Hydrogen atoms are not shown – assume that any unfilled atoms have hydrogen atoms bound. Note that the phosphate group has two P-O single bonds, not one as shown.



2. Nucleotides can have one of four different bases: adenine (A), cytosine (C), guanine (G), or thymine (T). In PyMOL, the pairs of letters shown at the top represent different nucleotides, with the second letter of the pair corresponding to the base. The nucleotide that you have just drawn has the base G – guanine. By repeating the process above, view and draw the structures of all four of the DNA bases, representing the rest of the nucleotide with the label R.

Produced by Alexandru Ulianov at Emmanuel College as part of an extracurricular project.
Edited by Adam Stubbs at Newcastle University as part of a summer outreach project.

Adenine	Cytosine	Guanine	Thymine

3. Now select two adjacent nucleotides at the same time, such as the first two nucleotides of DC and DG, and hide the rest of the DNA using the same process as before. How do the nucleotides bond together? Which groups does the bond form between?
   The nucleotides bond though the **sugar** of one, and the **phosphate** group of another.

4. The bond formed is called a phosphodiester bond. What type of bond is this?
   a. **Covalent** ✓
   b. Hydrogen
   c. Ionic
   d. Disulfide.

5. Now enter the command '**select chain a**' in the command box. Then, **select (sele)** on the right-hand pane, and use the command **(sele) > S > as > sticks**. This will show one long polynucleotide chain. Describe the general shape of the chain.
   The chain exists in a **helix**. The nucleotides in the polynucleotide chain twist around into the helix shape.

6. Now we will see how polynucleotide strands join together, to form a double helix structure. **Deselect everything**, by making sure that the (sele) button is unselected, and the nucleotide list at the top of the screen hasn't been highlighted. Select the first nucleotide, **DC**, and the very last one at the end of the bar, **DG**. Use the command **(sele) > S > as > sticks**, followed by **(sele) > H > unselected**. This will show a pair of nucleotides next to each other. Observe how the two nucleotides line up alongside each other. Use the command **(sele) > A > find > polar contacts > within selection**, this will show any polar interactions between the two nucleotides. Predict which type of polar interaction is occurring between the nucleotides here.
   Hydrogen bonding.

7. Now visualise the full double helix structure using the command **1d65 > S > as > sticks**, and **1d65 > A > orient**.
   The bases are the parts of DNA which vary, and which ultimately carry the genetic code. Explain the purpose of the sugar and phosphate groups.
   The sugar and phosphate groups combine to form a **sugar-phosphate backbone**. This **holds the DNA bases in place**, in the **correct sequence**.

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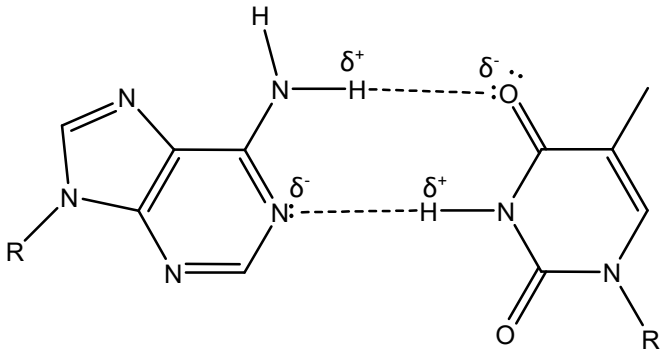
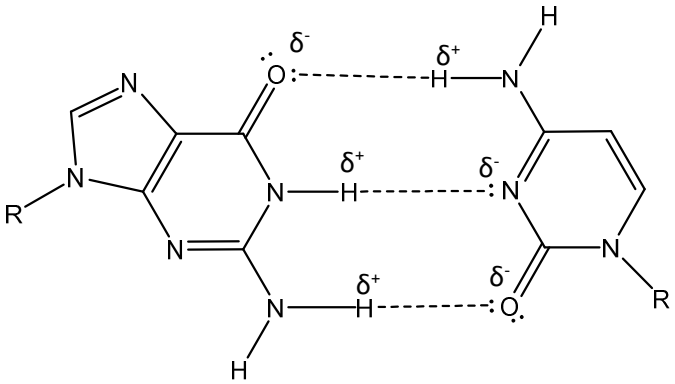
8. The base adenine bonds exclusively to thymine. And the base cytosine bonds exclusively to guanine. Using the structures of the bases that you drew before, show the bonding between each of the base pairs, including all partial charges and lone pairs of electrons which are involved.

Adenine



Thymine

Guanine



Cytosine