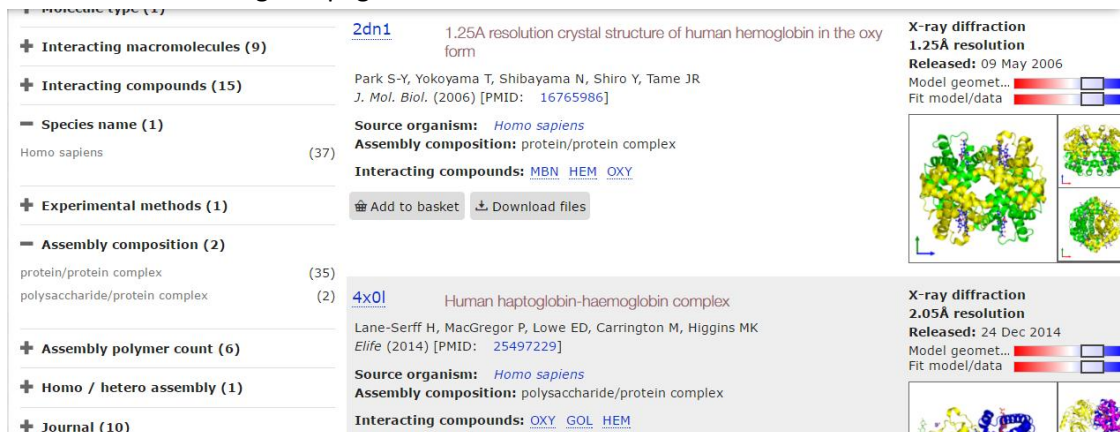# WP2 – Using the PDBe website

Name:

Date:

First, access the PDBe databank at www.ebi.ac.uk/pdbe/. From here you can search for over 100,000 structures.

1. Search for 'Hemoglobin'. How many different entries are found?

2. Why are there so many different entries found, and not just one universal structure of hemoglobin?

3. Along the left-hand pane of the page, you will be able to refine the number of results down depending on what type of molecule you want to look at. One of these allows you to refine by 'Experimental methods'. If you click on this section, you will be able to see some of the different ways that me can determine the structure of a protein. Why do you think that it is important to be able to search for structures which have been determined by different methods?

4. Two of the most important ways to refine a search are using 'Interacting compounds' and 'Species name'. Using these, refine your search to samples of human hemoglobin bound to O_2. How many entries are there?

You should be looking at a page similar to this:

It is worth noting that the database will naturally order the results by their quality, so that the highest quality result is first. This is done by looking at the resolution of the data, and the accuracy of it.

Click on the first entry, 2dn1. This should open the following page:

This will show all the information about this entry. You can access different sections using the 'Quick links' tab on the right-hand side. One of the more useful parts on the main page is the 'Ligands and Environments' section. This shows the molecules which interact with the main protein.

5. <u>What are the three ligands which interact in this protein? And why do you think the final ligand has been detected in the sample?</u>

3D VISUALISATION

To view the structure in 3D, open up the '3D Visualisation tool on the right-hand side. This should open a viewer like this:

Heterogroups – these are groups attached to the protein such as ligands.

Shows the water groups around a protein. This is important for hydrogen bonding, but for the most part can be ignored. You can hide these by clicking on the eye icon.

This is a fully 3D viewing tool which you can now use to investigate proteins. There are a few things to note:

Firstly, each structure is shown as an 'Asymmetric unit', this means that it shows you the smallest part of the structure which you cannot break down by symmetry. Most of these structures are analysed as crystals of repeated units. The asymmetric unit just means that this is taken into account. In this case, hemoglobin actually exists as a tetramer – it has 4 chains. But this model only shows two of them (pink and blue), as the tetramer can be seen by repeating the unit shown.

Along the right-hand side there are few different options to help you view the structure. One of the most useful is the Visual Type option, which allows you to select how the molecules are displayed.

1. Try out some of the different types of Polymer Visuals, giving a brief comment on why each may be useful.

As a 3D viewer, you can move this model around using your mouse. It is possible to focus on a specific section by clicking on it. When you do this, you will see blobs of blue, green and red appear around your selection. These represent the electron density of the structure and can be ignored by hiding the three density sections on the right-hand pane.

Produced by Adam Stubbs at Newcastle University as part of a summer outreach project.

Load up the entry 4ins. This will be a structure of insulin from a pig. The Protein Overview page that you see when you click onto an entry is full of information. By using the Overview of 4ins find out:

1. The scientific name of the pig species which this sample is from

2. The year that this structure was first published. Not that this is not the same as the year the structure was released. You should look for its journal article which will look like:
   J. Mol. Biol. **136** 103-28 (1980)
   Why is it important to know when this structure was first published?

3. The biochemical function of the protein

4. The cellular component – is it found on the inside or outside of the cell?

5. The type and number of bound ligands

6. The number of distinct macromolecules (large molecules making up the overall structure).