

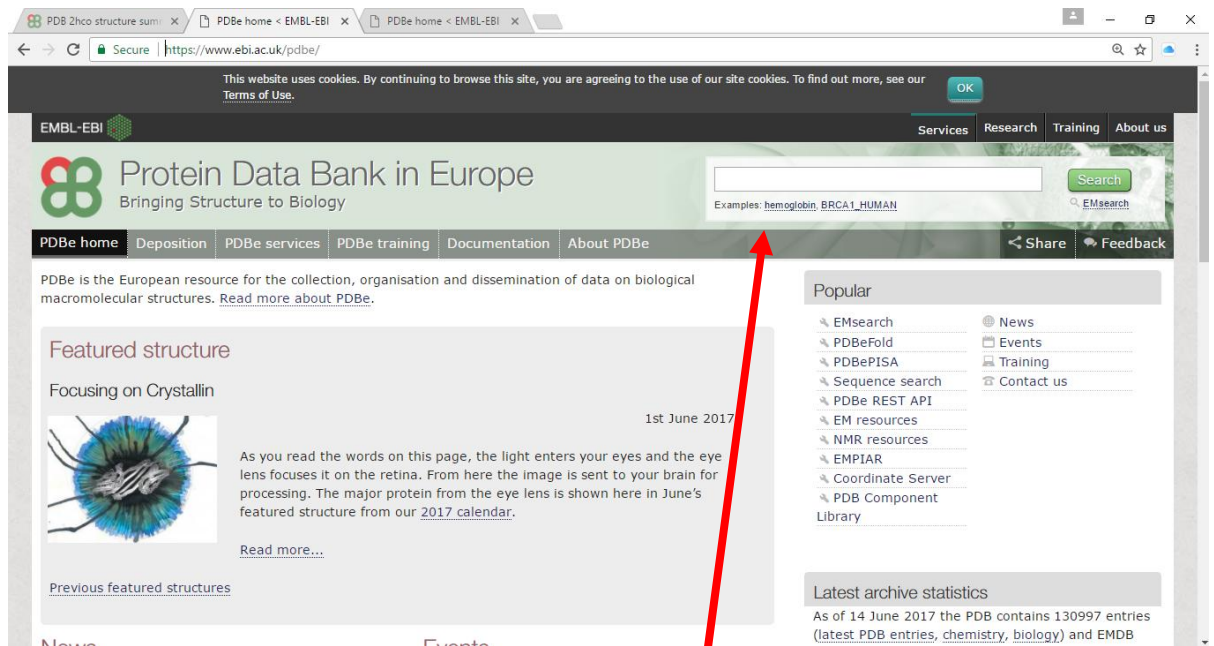
# TP1 - Using the PDBe website

The PDBe website is an archive of over 100,000 proteins and macromolecules which have been sequenced and analysed. Proteins can be very large, or relatively small molecules, and they can appear to be structurally complicated. However, the PDBe website offers a simple and high quality way to visualise these proteins and understand how their 3D structure effects their function.

Often proteins are shown in 2D diagrams in textbooks. Although this can be a good way to understand the basic principles, proteins truly come alive when seen in 3D. This is because proteins are naturally 3D structures, and seeing how they arrange and interact in 3D gives a more realistic viewpoint, and fascinating insight into protein biochemistry.

Using the PDBe you can search for a known protein to explore further, such as insulin or haemoglobin, or take a look at the **QuiPs** (Quite Interesting Protein Structures) archive available at [www.ebi.ac.uk/pdbe/quiPs](http://www.ebi.ac.uk/pdbe/quiPs). You can search for entries released this very week or ones solved in the 1970's. If you're interested in how proteins relate to **DNA** or which **ligands** bind to which proteins, there will be a structure for you to explore! The hard part is narrowing down your options and choosing just one of the interesting structures to investigate.

1. First, access the PDBe databank at [www.ebi.ac.uk/pdbe/](http://www.ebi.ac.uk/pdbe/), this should open a webpage like this:

A screenshot of the PDBe website homepage. The browser address bar shows 'https://www.ebi.ac.uk/pdbe/'. The page features a search bar at the top right with a 'Search' button and examples: 'hemoglobin', 'BRCA1\_HUMAN'. Below the search bar is a navigation menu with 'PDBe home', 'Deposition', 'PDBe services', 'PDBe training', 'Documentation', and 'About PDBe'. The main content area includes a 'Featured structure' section titled 'Focusing on Crystallin' with a date of '1st June 2017' and a description of the eye lens protein. A red arrow points from the search bar to the 'EMsearch' link in the 'Popular' sidebar on the right. The sidebar also contains links for 'News', 'Events', 'Training', and 'Contact us'. At the bottom, there is a 'Latest archive statistics' section stating 'As of 14 June 2017 the PDB contains 130997 entries (latest PDB entries, chemistry, biology) and EMDB'.

From here you can search for specific proteins using the search bar on the top right of the page. You can search for the molecule by name, its unique 4-character code, or other details, such as its author, or molecular family.

As an example, search for the human PYY peptide, code 2dez.

Once you've searched for 2dez, click on the entry to open its homepage, as shown.

Select '3D Visualisation' to bring up the online viewer.

Select 'Molecule details' to bring up details of the primary structure of each polypeptide chain.

This is the Molecule details page. It shows the primary structure of the polypeptide, and has a small visualisation of the protein's structure. Hovering over a section of the protein will highlight the amino acid which corresponds to that part in the chain.

When selecting the 3D Visualisation, the protein is rendered in 3D and can be manipulated by clicking and dragging your mouse across the screen. The protein can be viewed in different ways using the 'Polymer Visual' tab. Toggle through the different options to see how each view differs.

'Colouring' helps to distinguish parts of the protein such as different amino acids in a sequence. For larger structures, you can differentiate by each polypeptide chain, such as with haemoglobin.