

## Haemoglobin

**PDB 2HHB**

### Function of haemoglobin

The Protein Databank (PDB) has a good description of the function of haemoglobin, available at <http://pdb101.rcsb.org/motm/41>. Using this information and/or other resources of your choice, answer the following questions:

*In which tissue is haemoglobin found? In which cells?*

*What is its function?*

*What do the 'oxy-' and 'deoxy-' prefixes mean when referring to oxyhaemoglobin and deoxyhaemoglobin, respectively?*

### Structure of deoxyhaemoglobin

Open the EzMol start page (<http://www.sbg.bio.ic.ac.uk/~ezmol/index.html>). To visualise the structure of deoxyhaemoglobin, load PDB 2HHB.

*What organism is the protein from?*

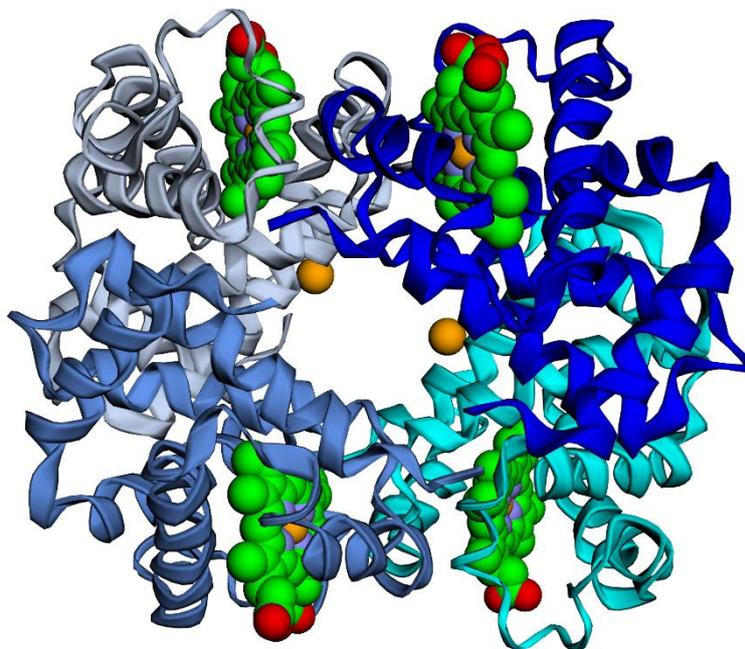
*What is the resolution of the structure? Explain briefly the concept of resolution in protein structure.*

Describe the quaternary structure of haemoglobin by answering the following questions:

*How many chains are there in the protein? What are the names of those chains?*

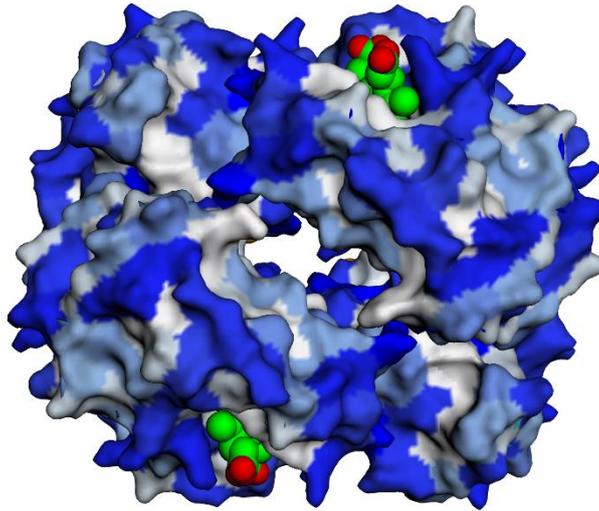
*What is the cofactor of haemoglobin? What metal ion does it contain? (You may use other online resources to find this information).*

Colour the different chains of haemoglobin and produce a figure highlighting each chain and the position of each cofactor, as in Figure 1.



**Figure 1** | The four chains of deoxyhaemoglobin, each in a different shade of blue. The haem cofactors are shown as spheres.

Colour the surface of the protein according to hydrophobicity, using a colour scheme that conveys the information clearly, such as in Figure 2.



**Figure 2** | Deoxyhaemoglobin shown as a surface coloured according to local hydrophobicity. White: high hydrophobicity; light blue: intermediate hydrophobicity; dark blue: low hydrophobicity (hydrophilic patches).

*Do you think haemoglobin is found in a hydrophobic or hydrophilic environment?*

Describe the secondary structure of deoxyhaemoglobin by answering the following questions:

*What secondary structure elements are present in the protein?*

*How many  $\alpha$ -helices are present in the  $\alpha$ - and  $\beta$ -chains? How many coil regions?*

*What interactions stabilise secondary structure elements?*

Generate a figure highlighting the secondary structure elements of an  $\alpha$ -chain and a  $\beta$ -chain. To do so, hide the other  $\alpha$  and  $\beta$ -chains and use different colours for each type of secondary structure.

You can move on to the more advanced worksheet on oxygen binding to haemoglobin. You are advised to keep a tab open with PDB 2HHB as you will need to compare oxyhaemoglobin with the deoxyhaemoglobin structure you have just studied.