Using the PDBe database (http://www.ebi.ac.uk/pdbe/) search for the entry: 2hco, and load the 3D Visualisation. It should be a model of human carboxyhemoglobin which looks like this:

1. Which type of secondary structure can you see in this protein?

2. The protein chains are connected to a porphyrin group which, in this case, carry carbon monoxide bonded to iron. What is the name of this type of structure?

3. Using the mouse, change the view around the protein so that you get a clear image of the porphyrin ring. Just using the automatic cartoon view, why do you think that the porphyrin ring binds to the polypeptide in that specific location?

4. Now change the Polymer Visual to ‘VDW Balls’. Describe how the porphyrin group sits in relation to the overall shape of the molecule.

5. Change the Polymer Visual again to ‘Surface’, how does this differ to the VDW Balls view? Why may there be some overlap with the porphyrin ring, and how would a CO molecule enter/leave the Fe binding site on porphyrin given that there appears to be a lot of protein in the way?
6. Change the Polymer Visual back to ‘Cartoon’, to see the porphyrin ring more clearly, and click on the central atom, Fe, to bring it into focus. You should see all the neighbouring amino acid side chains come into view. Fe often exists as an octahedral complex, bound to six other atoms, but it appears that it is only bound to five, the one CO above it, and four from the porphyrin ring around it. By manipulating this view, deduce how the porphyrin group stays stable in its place. If it helps, change the magnification with the ‘FOV’ option accessible on the top right-hand side of the screen.

7. Using your knowledge of proteins, predict what would happen if some of the amino acids in the polypeptide chain were changed.

8. Explain why hemoglobin wouldn’t be able to carry a large molecule such as glucose on the iron.