Exercise Sheet 7

Aim: *Visualising of protein structures and of protein-ligand interactions, Evaluation of homology models*

Protein structure: Homology modelling

For the interactive material for this exercise follow this link:

https://www-cbi.cs.uni-saarland.de/wp-content/uploads/Softwarewerkzeuge_Teil_2/start3a.html

Follow the Link 1. Cytochrom 109D1 aus *Sorangium cellulosum*

(1) Identify the corresponding *accession code* of this protein (www.uniprot.org)
(2) Is there a readymade homology model for this protein in the SWISS-Model Repository (http://swissmodel.expasy.org)? Simply enter the accession code (in the tab Repository → Search). If yes, based on which pdb file?
(3) Save the homology model (of SWISS-Model) as well as the corresponding template structure (via template link [RCSB]). Superimpose both using a visualization program (VMD,Chimera,…) onto each other. Assign different colors to both structures and chose "cartoon" as drawing method. Which chain of the template matches onto the model?
(4) From which organism does the template structure originates?
(5) In which regions do the largest deviations occur?
(6) Compare these regions with the sequence alignment between model and template that has been generated by SWISS-MODEL.
(7) What is the coordination number of the iron atom of the Hem group (HEM)?
(8) Which molecule could occupy the free coordination site at the iron (recall the function of this cytochrome)

Accomplishing the project:

Read the description and questions first.
Identify the wanted *accession number(s)* of the protein(s).
Search for available templates in SWISS-MODEL (button → Template Identification).
Chose a suitable one for the generation of the homology model.
Exlain the reasons for your choice of template (sequence identity, resolution, gaps)
Superimpose homology model and template onto each other.
Hint: Use "cartoon" as graphical representation.
In which regions do the largest deviations occur?

Compare these regions with the sequence alignment between model and template that has been generated by SWISS-MODEL.
Rate the quality of the obtained model.
Please also pay attention to the questions given in the respective project.