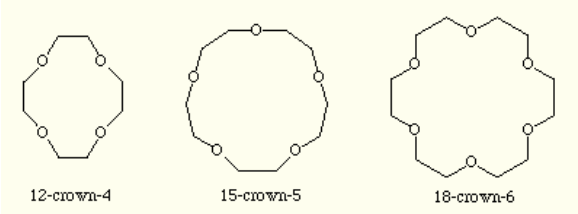
060201 Quiz 3 Morphology of Complex Materials (*10 points each part*)

1) In class we discussed three types or classes of quaternary structure in proteins depending on the composition of the quaternary structure.
a) ;b) ;c) Describe these three types of protein quaternary structure and give an example of each. (Give as much detail as you feel comfortable with but spend no more than 5 minutes on each, a paragraph).
d) Crown ethers are organic chemicals used to chelate a metal ion (coordinate the metal ion to make it soluble in hydrophobic environments for instance. The metal ion goes in the center of the crown ether ring. Crown ethers can be integral components of hybrid catalysts for instance.



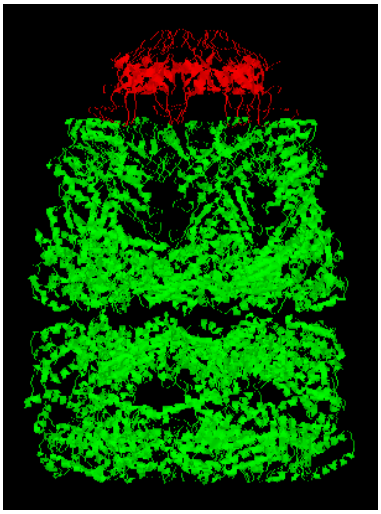
Hemoglobin contains organic molecules that have similarities to crown ethers. Give the name of the class of molecules (rings) that these molecules belong to and explain the importance of these molecules to the function of hemoglobin.

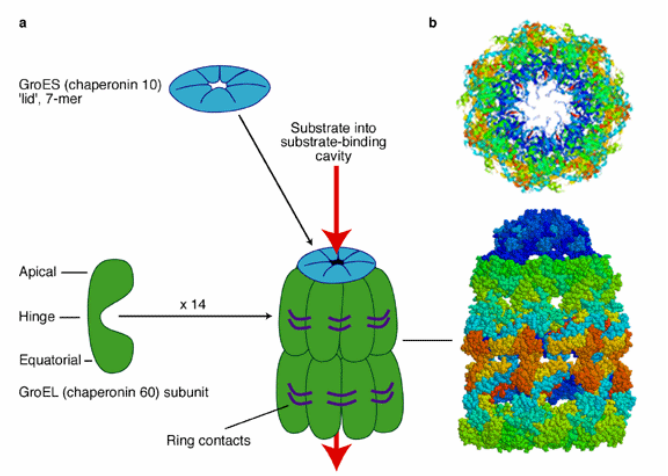
2) In class we compared protein and polymer hierarchies.
a) Polymers display short range and long range interactions. Explain what distinguishes short and long range interactions.
b) Give analogies in proteins for short and long range interactions in synthetic polymers.
c) If quaternary structure is view as a structure resulting from the interaction of multiple protein molecules, what topic in polymers relates to quarternary structure in proteins?
d) Explain why the average vector, $\langle \mathbf{r}_{i+1} \rangle_{Gaussian} = 0$, reflecting the average direction and magnitude of a step from a fixed chain step, "i", for a Gaussian (random walk) chain; while $\langle \mathbf{r}_{i+1} \rangle_{SRI}$ has a finite value, reflecting the average direction and magnirute of a step from a fixed chain step, "i", for a chain with short range interactions. How do short range interactions affect persistence length?
e) Explain how restrictions on bond rotation (rotational isomeric state theory) could lead to a larger persistence length in synthetic polymers (using your answer to part d).
f) Describe the similarities and differences between a beta sheet and the planar zig-zag conformation of polyethylene.

***ANSWERS:* 060201 Quiz 3 Morphology of Complex Materials**

1) a) Three types of quaternary structure:

Quaternary structures composed of multiple polypeptide chains such as Chaperonin. This is composed of two units a small unit (top) and a large unit (bottom), GroES (7 protein cap) and GroEL (14 protein tube in 2 rings of 7 large proteins)





Structure of chaperonin 10 and chaperonin 60
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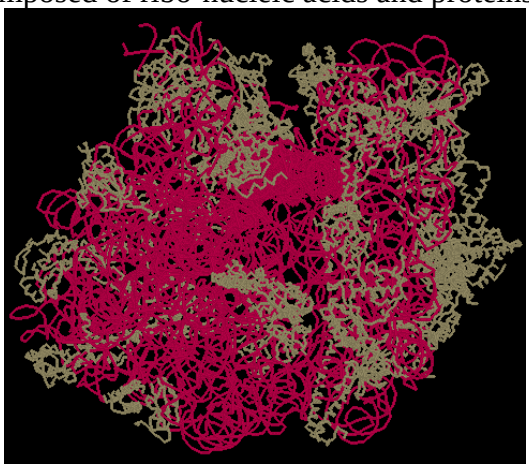
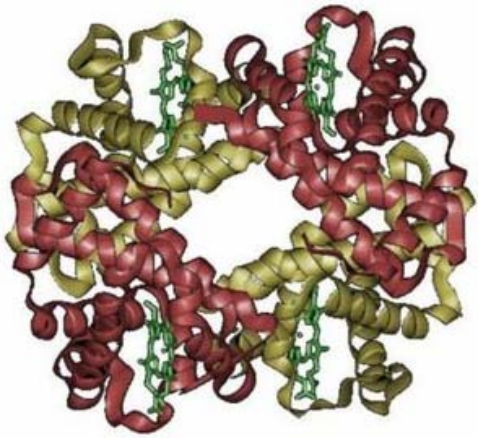
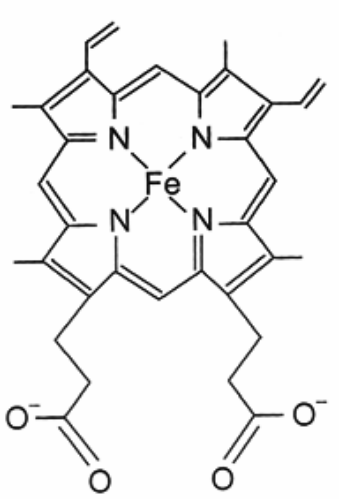
b) Quaternary structures composed of ribo-nucleic acids and proteins such as the ribosome.



The ribosome model above shows RNA molecules in red or dark and proteins in grey.

c) Quaternary structures composed of proteins and metal ions such as hemoglobin that contains the heme chelating-agent and iron. Hemoglobin is composed of 2 pairs of identical proteins, α and β, as shown below and 4 heme-molecules with 4 iron ions.





d) The heme molecule contains a porphyrin ring that chelates iron (above). The porphyrin ring locks iron in hemoglobin. Iron bonds reversibly with oxygen and carbon dioxide depending on the local and relative partial pressures of these two gasses. In high oxygen partial pressure at the lungs carbon dioxide is released an oxygen bonded. At the cell with high carbon dioxide and low oxygen, oxygen is released and carbon dioxide is bonded.

2) a) If a linear polymer chain is indexed from 1 to N then interactions between two units of similar or neighboring index are called short range interactions. Interactions between two subunits (mers) of widely different index are called long range interactions. Short range interactions occur between units that have a memory of each others direction and because of this lead to larger persistence length. Long range interactions lead to global changes in chain scaling.

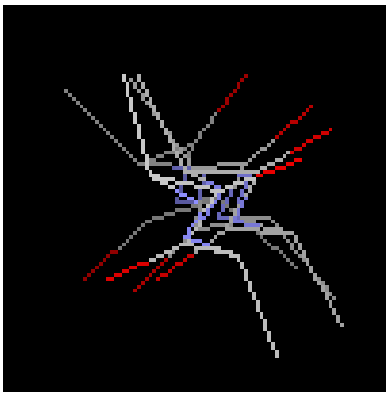
b) An alpha helix involves hydrogen bonding between peptide units of similar index and the result is a large rod like unit, the helix. The alpha helix is analogous to short range interactions. Disulfide bonds between cystine units of widely different index are analogous to long range interactions leading to changes in the global structure.

c) Quaternary structure in polymers could relate to coil overlap in semi-dilute and concentrated solutions. Coil scaling transitions at close to the overlap size might be considered a type of disordered quaternary structure. You might also consider crystalline lamellae as a kind of quaternary structure.

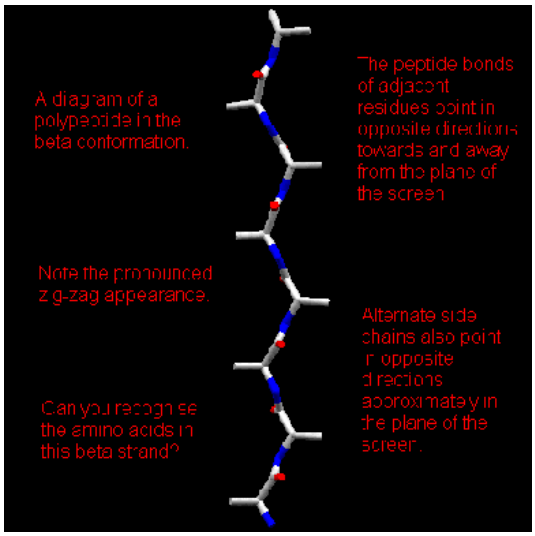
d) $\langle \mathbf{r}_{i+1} \rangle_{Gaussian} = 0$ since there is no memory of the direction $\mathbf{r}_i$ in the choice of direction $\mathbf{r}_{i+1}$ for a totally random walk. The average value of a random vector is 0. If the backward step is not allowed then $(z-1) \langle \mathbf{r}_{i+1} \rangle_{SRI} = \langle \mathbf{r}_{i+1} \rangle_{Gaussian} + \mathbf{r}_i$. So, $\langle \mathbf{r}_{i+1} \rangle_{SRI} = \mathbf{r}_i/(z-1)$, where z is the coordination number. The correlation between site "i" and site "i+1" leads to an increase in the persistence length, $b^2_{SRI} = zb^2_{Gaussian}/(z-2)$.

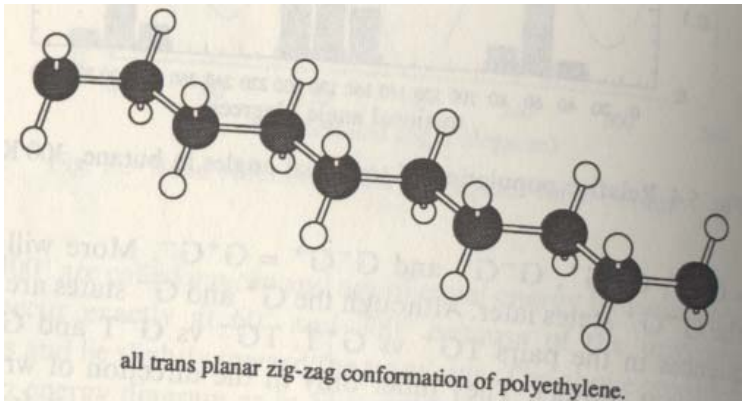
e) For a freely rotating chain z is larger than for a chain with restrictions on bond rotation. Similarly, for a chain with fixed bond angles z is smaller than a chain with free angle bonds. The reduction in z towards 2 leads to a larger persistence length, b.

f)



Beta Strand





Both the beta-strand and the planar zig-zag are similar conformations. The beta strand is not planar but is as close to planar as is possible in the polypeptide chain. Beta strands can hydrogen bond with other beta strands to form a beta sheet and the planar zig-zig zag can crystallize in polyethylene forming an orthorhombic unit cell that is similar to the anti-parallel bonding of beta-strands.

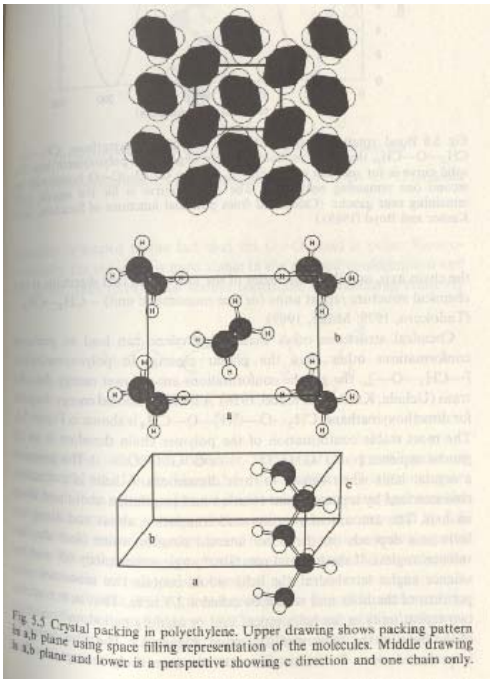


Fig. 3.5 Crystal packing in polyethylene. Upper drawing shows packing pattern in a,b plane using space filling representation of the molecules. Middle drawing is a,b plane and lower is a perspective showing c direction and one chain only.