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Final Exam

1. 1. Structure math

eix =cosx +isinx

l cosx + isinx l = sqrt ((cosx+ isinx) (cosx – isinx))

l cosx + isinx l = sqrt ((cos2x- i2sin2x)) , i2 = -1

l cosx + isinx l =sqrt (cos2x+ sin2x) , cos2x + sin2x= 1

l cosx + isinx l = sqrt (1)

l cosx + isinx l = 1

eix =1

b. z= a +ib

l eiz l= e-b

l ei(a+ ib)l = e-b

l eia+ i2 b l = e-b , i2= -1

l eia –bl = e-b

leia * e-b l= e-b

1* e-b = e-b

2. orthothrombic

a.18 P21212 Harker Sections

b.z axis, x and y axis

c. 2X 2Y 0 (x, y, z)- (-x, -y, z) = x- -x, y- -y z-z = (2z, 2y, 0)

1/2 2Y+1/2 2Z (x,y,z)- (x +1/2,- y+ 1/2, -z)= ((x- (x+1/2)),(y – (-y+1/2)), z- -z = (1/2, 2y+1/2, 2z)

2X+1/2 1/2 2Z = (x,y,z)- (-x +1/2, y+1/2, -z) = ((x- -x),(y – (y+1/2)),(z- -z) = (2x, ½, 2z)

3. ,

a- lactalbumin is a protein whose structure has been determined by both NMR and X-ray crystallography. During X ray Crystallography the protein is purified and crystallized, then subjected to an intense beam of X-rays (Chandra, Brew, and Acharya) . The protein in the crystal diffracts the x-ray beam and this diffraction is analyzed to determine the distribution of electrons in the protein (Chandra, Brew, and Acharya). The distribution of electrons in the protein allows us to determine the location of each atom within the molecule. X ray crystallography shows each atom in a protein with additional information. X ray crystallography is better on rigid proteins that form ordered crystals. NMR on the other hand can also provide information on proteins in solution and can provide structures for flexible and dynamic proteins.

A-Lactalbumin is a protein that is expressed only in the lactating mammary gland and is secreted in the why fraction of milk(Chandra, Brew, and Acharya). The x ray crustal structure and the NMR structure shows that a unique Mn 2+ binding site is located close to the N terminus of the protein(Demarest, Hua, and Raleigh). .

Based on these methods we are able to find out information about the structure of this protein. It adopts different conformations in the crystal structure at different pH. In the ph 6.5 the crystal structure shows that residues 101-105 are in an irregular turn like conformation and residues 106-11 form an a helix(Demarest, Hua, and Raleigh). At a ph of4.2 residues 101-105 form and alpha helix and residues 106-111 form a loop like structure(Demarest, Hua, and Raleigh).

The overall structure of a-lacalbumin was consistent between NMR and X-ray crystallography.

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Demarest, Stephen, Yuxin Hua, and Daniel Raleigh. "Local Interactions Drive the Formation of Nonnative Structure in the Denatured State of Human a Lactalbumin: a High Resoltuion Structural Characterization of a Peptide Model in Aqueos Solution." n. page. Web. 28 Jul. 2012. <http://pubs.acs.org/doi/full/10.1021/bi990320z>.

Chandra, Naveen, Keith Brew, and Ravi Acharya. "Structural Evidence for the Presence of a Secondary Calcium Binding Site in Human a-Lacalbumin." n. page. Web. 31 Jul. 2012. <http://pubs.acs.org/doi/full/10.1021/bi97300t>.

4. Experimental phasing and molecular replacement are two methods used to determine the structure of a protein. There are both advantages and disadvantages to each method.

Molecular replacement is the method used to derive information about the unknown structure of a protein from a partially known existing model. In this case we would use protein M, whose sequence is 58% identical to that of protein N as the existing known model. It also provides an initial starting model for refinement. An advantage of Molecular replacement is the large number of

structures of proteins available in the PDB database. With all of these structures available there is a good chance that there will be at least a partial match that you will be able to use. A disadvantage of this method is that you can only use it when you have a good model available for use, unlike experimental phasing where you start from scratch. By depending upon, and using the structure of a similar protein to determine your structure there can be some bias.

In experimental phasing you introduce heavy atoms into the structure, and these atoms create scattering in the crystal structure. Ad advantage that I previously listed was that there is no model bias and instead you start from scratch. A disadvantage that is present when using MI, is that the heavy atoms affect the crystal formation and unti cell dimensions. However sometimes there is a lack of isomorphism which means there is a change in the unit cell or space groups. Another con in MIR is that you need lots of crystals and it is time consuming. However, these disadvantages are not present in MAD. With this method you only need a single crystal and there is no lack of isomorphism. Some disadvantages of using MAD is that you are depending on the accurate measurement of very small differences in intensities and you need enough heavy atoms present to get a signal.

As you can see there are both advantages and disadvantages in experimental phasing and molecular replacement. Each of these is an adequate method to determine the structure of a protein.

5. If one amino acid's side chain was completely mispositioned I would expect that there would be a large number of structure amplitudes that would be slightly wrong rather than a small number be completely wrong and the others remain correct. The structure amplitude is a magnitude of the structure factor. The structure factor describes the amplitude and phase of a wave defracted from a crystal lattice. The sum is over all of the atoms in a unit cell, and therefore I believe that is will be a wide spread slight change in all of the structure amplitudes.

I would expect to identify this error in the structure refinement process. This process minimizes the difference between the calculation and experimental results. Because they would not match, you seek to change until there is a reasonable fit. You need an R factor, which is the average fractional error in the calculated amplitude compared to the experimentally observed amplitude.

6.

7.

What is the repeat distance?- 232 nm

Where does it come from?- This is the fundamental long spacing repeat.

If a muscle was contracting, the length would be shorter. When the actin and myosin heads instead the length of a muscle cell shortens.

How might the diffraction pattern look different if it was from a contracting muscel When a muscle contracts, the sarcomere shortens. Because of this contraction and the shortening of the sarcomere the diffraction pattern will show an increase in the lattice spacing.

binding site is located close to the N terminus of the protein () ( ). There are no real discrepancies between the two different structures of the protein.

8.

9.