1. a. $z = a + ib$; $z^* = a - ib$; $|z| = \sqrt{zz^*}$; $\cos x = a$; $\sin x = b$
   $|e^{ix}| = \sqrt{(\cos x + i \sin x)(\cos x - i \sin x)}$
   $= \sqrt{\cos^2 x + \sin^2 x + i \cos x \sin x - i \cos x \sin x}$
   $= \sqrt{\cos^2 x + \sin^2 x}$
   $= \sqrt{1}$
   $= 1$

   b. $z = a + ib$
   $e^{iz} = e^{i(a+ib)} = e^{ia-b} = e^{ia}\, e^{-b}$
   $| e^{ia}\, e^{-b} | = | e^{ia} || e^{-b} |$
   $| e^{ia} | = 1$
   $| e^{-b} | = |e|^{-b}$
   $|e| = e$
   $| e^{iz} | = e^{-b}$
2. a. orthorhombic

   b. 2-fold axis: z axis; screw axes: x and y axis

   c. $(x,y,z) - (-x + ½, y + ½, -z) = (2x, ½, 2z)$

   $(-x,-y,z) - (-x + ½, y + ½, -z) = (0, -2y + ½, 2z)$

   $(x,y,z) - (x + ½, -y + ½, -z) = (1/2, 2y + ½, 2z)$

   $(-x, -y, z) - (x + ½, -y + ½, -z) = (-2x + ½, ½, 2z)$

   I would look at $(u,v,w) = (-2x + ½, ½, 2z)$, $(1/2, 2y + ½, 2z)$, $(2x, ½, 2z)$, where we would look for strong peaks at u and $v = ½$

3. Firstly, the X-ray diffraction structure determination includes finer details such as ligands and particles binding to the protein structure. This higher level of detail allows for the observer to see how a structure interacts with particles which are in the environment. Also, the crystallographic method also gives an R-Free value which alludes to the fitness of a model to the actual structural conformation. With the X-ray diffraction, the R-free value is 0.238, which is a fairly reliable value for a structure (a good value would be 0.2 of lower). Both methods allude to the domains in the protein structure and give good information on how the secondary structure plays out. The similarity between the resolution of both methods is high; secondary structure is easily determinable with alpha helixes and beta sheets well refined in the structure. However, the resolution in a solution NMR structure determination is not applicable, whereas the resolution of the X-ray diffraction is at 2.8 angstroms, which is a relatively detailed scale. As part of the X-ray diffraction experiment, zinc was used in order to determine the similarity of structure from

cyanobacteria to plant PsbQ as stated in the study behind PDB structure 2XB3. This use of heavy atoms is an example of using experimental phasing to determine the structure of the protein.

4. a. I would say that a small number of structure amplitudes were incorrect because if one amino acid side chain were mispositioned, it would likely only affect other surrounding side chains which could interact with it via hydrogen bonds, cys bonds, etc.

b. I would look at the height and color of the bars in the coot program which speaks of the how well placed side chains and amino acids are placed in the obtained electron densities. Also, I would look at ramachandran angles and if these two cannot be resolved in a fashion which allows for a reasonable conformation, I would assume an error.

5. For molecular replacement, I would say that this would be highly advantageous. Firstly, there is already a determined structure to use as a baseline. Because the sequence is 58% identical, it is likely they are the similar in structure as about 30% identical means a very similar structure usually. However, a disadvantage is that by no means is this a guarantee that these are structurally similar proteins. Using experimental phasing using MIR and MAD (binding by heavy atoms or selenomethionine) however, would produce results which would allude to whether the structure was similar via binding of these atoms. This type of binding would give way to use of Harker sections to determine the locations of these heavy atoms. This would advantageous in determining whether the identical sequence truly makes a similar structure via similar bonding. I would say that between the two of these methods, you could truly determine whether the structure is similar along with the highly identical sequences.

6. co-ordinate frame, tip, inclination, opening, propeller, buckle, twist, roll, tilt, slide, rise, shift

7. The repeat distance is 1/38.7 nm, which is 0.0258 nm. This comes from the helical organization of the proteins. The true repeat distance or 1/R is the distance between one amino acid on a helical structure and the next helical structure which is lined up with the previous helical structure on a direct translation along the helical axis. This diffraction pattern may be a longer distance if the muscle is contracted because it would be shorter distance in reality, but in the diffraction pattern, since it is reciprocal, the distance would be longer.

8. There are several methods of computational tools which can be employed at time scales for characterizing biological structures including NMR, QM, X-ray, and electron microscopy. With X-ray crystallography and EM, the time scale associated with these is largely static. The structure is being investigated in a static state, which means that there is no time scale associated. However, with NMR, a time scale anywhere from a picoseconds to minutes can be investigated. With quantum mechanics (QM), it is a smaller resolution of time which is investigated, likely between picoseconds to a scale a thousandth that size. With electron microscopy, it is important that the sample stay static in a lower temperature environment to prevent sample degradation; it is because of this aspect of electron microscopy that it is on the timescale for static investigation.

9. The slope of ln(I(q) v. q^2 gives $R_G^2/3$ value. Using a range from the data set of cells from rows 150 to 249, the Rg value yields 4.78, which gives a q*Rg value of 1.28, just under the 1.3 value for globular protein. $R_g^2 = 3R^2 / 5$. R = 6.17 angstroms. For a prolate ellipsoid, Rg2 = R2 / 2, meaning R = sqrt (2Rg2) = 6.76 angstroms. The length would be calculated by Rg2 = L2 / 12 + R2 / 2. L = 0.069 angstroms.

I decided the range for this by experimenting with values in excel. I calculated the Rg values of certain ranges and narrowed down until acquiring a qmax*Rg value of just under 1.3.