

Homework Set 1

(#1-6 are due on Feb 26 (Monday), 2007; #7 should be done early this week so that we can use your crystals for data collection. * indicates that you should email me the coordinates, or the screen shot, of your results)

Problem 1) Complete the derivation of the 2D rotation matrix, i.e., show that $y = x' \sin\phi + y' \cos\phi$ (on lecture slide # 13). You may want to draw some additional lines to help you.

Problem 2) Vector F1 and F2 in Cartesian coordinates are (10, 5, 3) and (-9, 7, 5). Express F2-F1 in Cartesian coordinates and calculate the length of F2-F1. Also express the three vectors in cylindrical and spherical coordinates.

Problem 3) A molecule is rotated -75° around the Y-axis, express this rotation in Eulerian angles and spherical polar angles.

Problem 4) Using O. Download one of the HIV protease structures from PDB (1HWR), and display it in O. Using O to (i) measure the closest distances between the side chains of the active site ASPs to the inhibitor; (ii) mutate the active site ASPs to GLUs, see what happens. Write out the mutant structure*.

Problem 5) Using CNS. (i) Generate the structural file (.mtf) for the above HIV protease structure. (ii) Transfer coordinates into the principal axis system ("coor orient") and write out the coordinates as a new PDB file. Display it in O to see what happened to the molecule. (iii) Do an operation in CNS so that you get the two monomers in the HIV protease switching side (can you also include the inhibitor in the operation?)*. (iv) Superimpose the two monomers and obtain the r.m.s.d. for the C α atoms.

Problem 6) An atom is at position (32, 45, 21) in a unit cell of P2₁2₁2₁ symmetry with unit cell length of a = 67, b = 82, c = 45. Write the coordinate of this atom in fractional coordinates and find the positions of all the other crystallographically equivalent atoms in the unit cell. What if the space group is P2₁ with $\beta = 115^\circ$?

Problem 7) Crystallizing lysozyme according to the following protocol (courtesy of MSC):

Chemicals needed:

Sigma Lysozyme from Chicken Egg White #L-6876

Sodium Chloride

Sodium Acetate buffer

Ethylene Glycol

Sodium Azide

Distilled water

Procedure:

Prepare 75mg/ml sample of Lysozyme in 0.1 M NaAc pH 4.8 plus 0.02% (w/v) Sodium azide.

Linbro or VDX tray well solution consists of 1ml of 10% (w/v) NaCl, 0.1M NaAc pH 4.8, 0.02% (w/v) Sodium azide, and 25% (v/v) Ethylene Glycol.

On a clean silated cover slip create a drop of 6 or 7 microliters Lysozyme solution, and 4 or 3 microliters of well solution, respectfully, for a total drop size of 10 microliters.

Seal a cover slip with grease over each well.

Crystals should grow in about 1-2 days and be ready for freezing.

If crystals are smaller than desired try varying drop ratio between protein and well, or vary Lysozyme concentration between 50mg/ml and 75mg/ml.