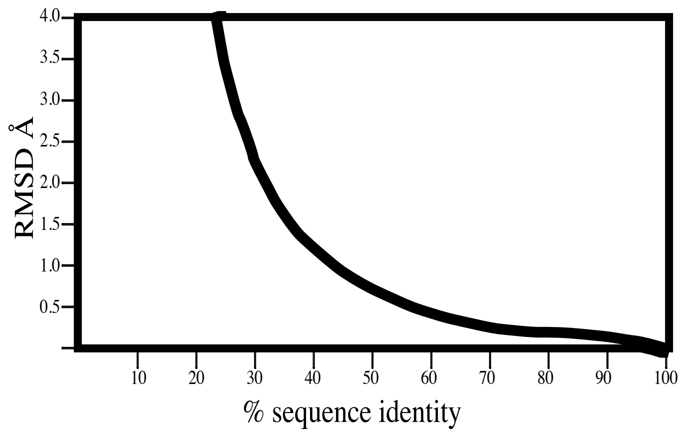
PSD -- Fall 2020 -- Homework 3

due monday Nov 30, 2020

http://www.bioinfo.rpi.edu/bystrc/courses/bcbp4870/homework.html

(1) **Molecular replacement situation -- how does coordinate error relate to phase error?**

You have collected data for a protein that has a homolog of known structure, and you want to use the homolog coordinates to calculate phases, using molecular replacement. Below is a plot showing root-mean-squared deviation(RMSD) as a function of sequence identity, where sequence identity is a measure of the amino acid sequence similarity between homologs.



(a) Calculate the expected RMS phase error for homologs with 30%, 50% and 90%-identity, based on the expected coordinate error (see graph) and 3.0Å resolution.

30%___________

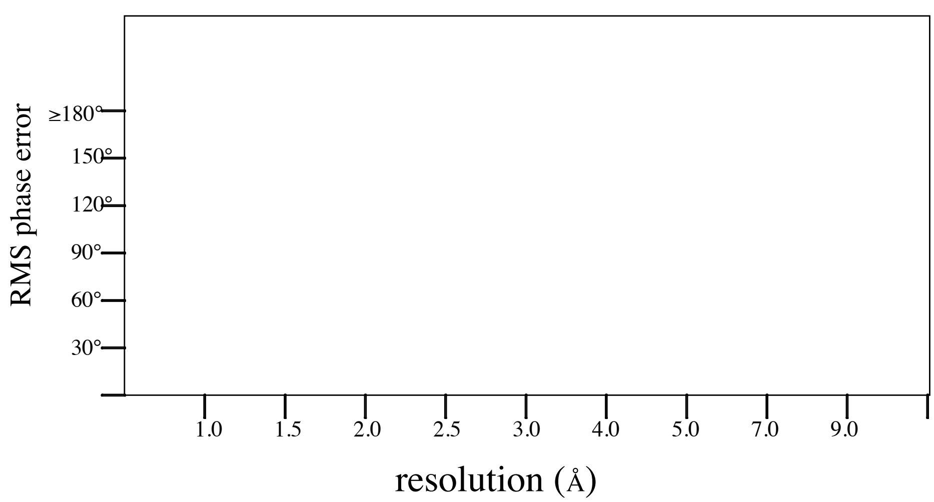
50%___________

90%___________

(b) Plot phase error as a function of resolution in the box below. One plot each of the answers in (a).

(c) What is the minimum % identity needed to phase 3.0Å data with <90° phase error?

____



(2) R-factor calculation.

Calculate the F_c data set, just three reflections, using the model listed below, just three atoms. The space group is P1, no symmetry.

For the scattering factor for all three atoms use 1.0 at **all** resolutions.
Use global scaling. Calculate the R-factor.
Show work by filling in the blanks.

Fractional coordinates:
r_1 = (0.200, 0.100, 0.134)
r_2 = (0.150, 0.350, 0.250)
r_3 = (0.250, 0.000, 0.100)

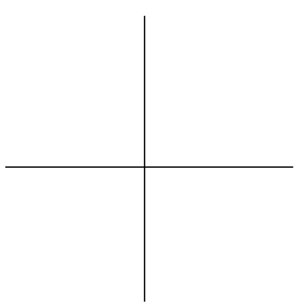
Observed amplitudes F_o:
F_o(2 3 1) = 28.
F_o(1 2 3) = 30.
F_o(-1 4 1) = 15.

atoms (fractional coordinates)

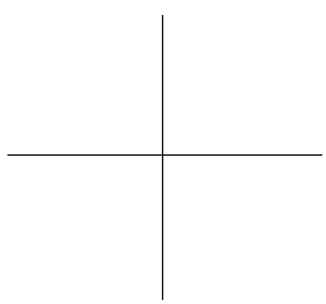
miller indeces

phases per atom (in degrees)	r1 (0.200, 0.100, 0.134)	r2 (0.150, 0.350, 0.250)	r3 (0.250, 0.000, 0.100)
2 3 1			
1 2 3			
-1 4 1			

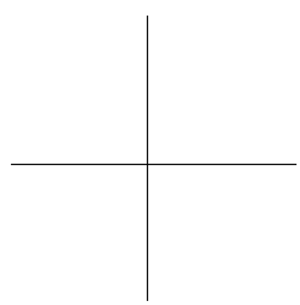
Sum unit waves to get each of the three Fc's, or sum waves as cosines and sines.



2 3 1



1 2 3



-1 4 1

Resulting F_c amplitudes and phases (degrees).

$F_c(2\ 3\ 1)$ = ________ __________

$F_c(1\ 2\ 3)$ = ________ __________

$F_c(-1\ 4\ 1)$ = ________ __________

Scale factor:
w = ____________

Scaled amplitudes and differences.
$wF_c(2\ 3\ 1)$ = ________ | $F_o(2\ 3\ 1) - wF_c(2\ 3\ 1)$ | = _____________
$wF_c(1\ 2\ 3)$ = ________ | $F_o(1\ 2\ 3) - wF_c(1\ 2\ 3)$ | = _____________
$wF_c(-1\ 4\ 1)$ = ________ | $F_o(-1\ 4\ 1) - wF_c(-1\ 4\ 1)$ | = _____________

Sum : ___________ Sum of absolute differences: _______________

R-factor = _________