

point A is  $N_i$

point B is  $Ca_i$

point C is  $C_i$

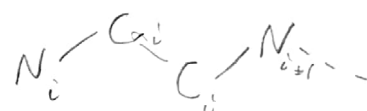
point D is  $N_{i+1}$

Morgan  
Nance

Hw #2

Q #1

point C :  $(0, 0, 0)$  by definition  
 $C_i$



point B:  $(-1.5, 0, 0)$  down x-axis by C-C bond length  
 $Ca_i$

point A:  $(-l \cos \theta, l \sin \theta, 0)$   $\theta = 115^\circ$   
 $N_i$   $(-1.3 \cdot \cos(115^\circ), 1.3 \cdot \sin(115^\circ), 0)$   
 $(0.466, 1.21, 0)$

point D:  $(-l \cos \theta, l \sin \theta \cos \phi, l \sin \theta \sin \phi)$   $l = 1.3$   
 $N_{i+1}$   $(-1.3 \cos(115^\circ), 1.3 \cdot \sin(115^\circ) \cdot \cos(-126.1^\circ), 1.3 \cdot \sin(115^\circ) \cdot \sin(-126.1^\circ))$   
 $\theta = 115^\circ$   
 $\phi = -126.1^\circ$

$$N_{i+1} = D = (0.634, -0.800, -1.098) \times M$$

but couldn't figure out M rotation matrix

Q1.b. I would translate the xyz plane to the next carbonyl carbon and recalculate the xyz coordinates for the next N atom. This would repeat using the previous residue's  $(\phi, \theta, \chi)$  coordinates to answer the next.

Q1.d. Without the M rotation matrix, the  $N_{i+1}$  is in the wrong spot. I also had a problem with the C and  $C_\alpha$  atoms being in the wrong spot.