

point A is N_i

point B is Ca_i

point C is C_i

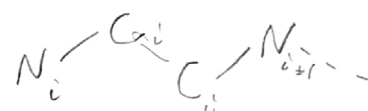
point D is N_{i+1}

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 (ϕ, θ, χ) 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_α atoms being in the wrong spot.

ATOM N	1	N	ALA	A	1	0.466	1.210	0.000	1.00	39.26
ATOM C	2	CA	ALA	A	1	-1.500	0.000	0.000	1.00	37.65
ATOM C	3	C	ALA	A	1	0.000	0.000	0.000	1.00	40.25
ATOM N END	4	N	ALA	A	2	0.634	-0.800	-1.098	1.00	41.55

