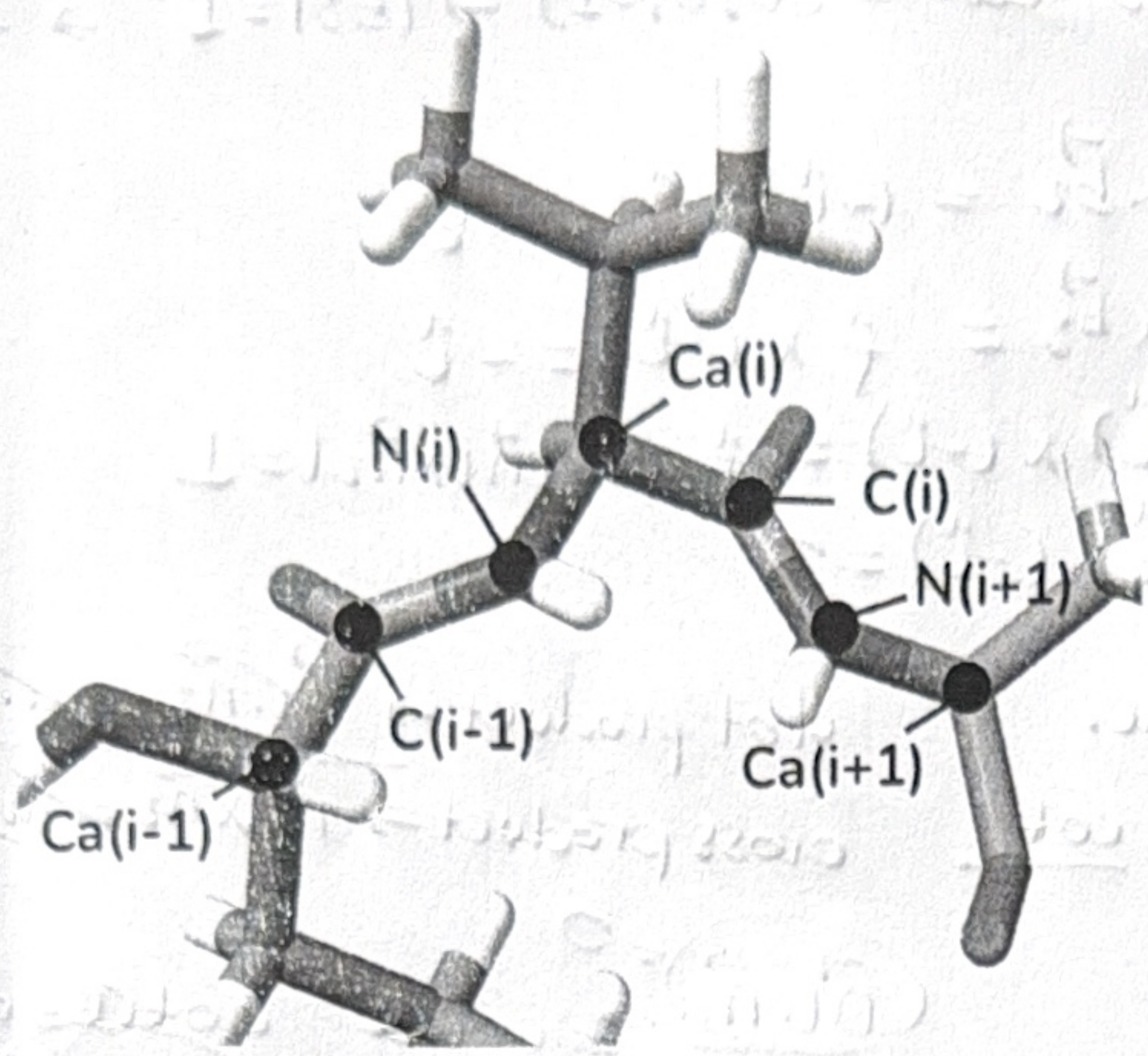
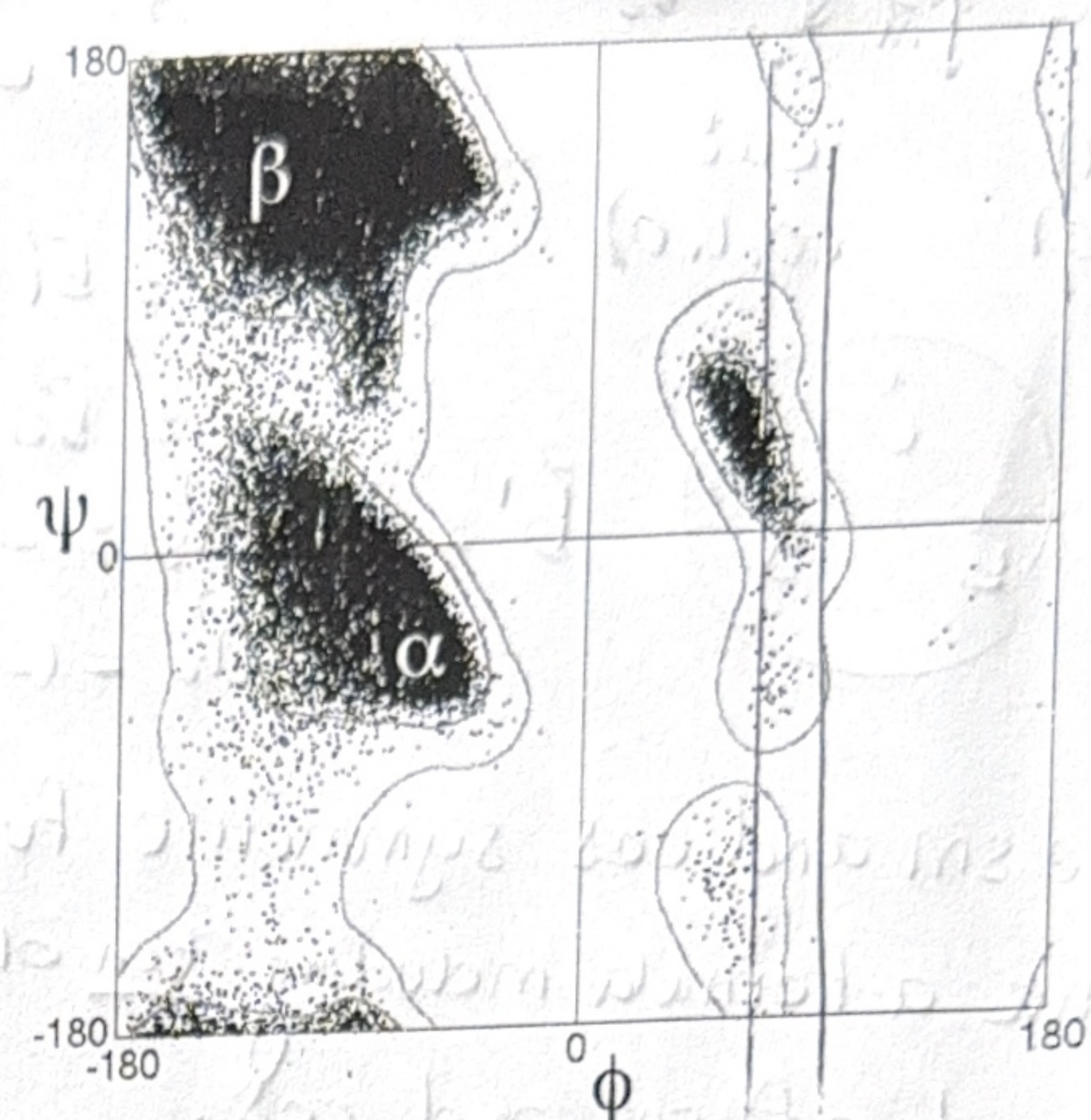


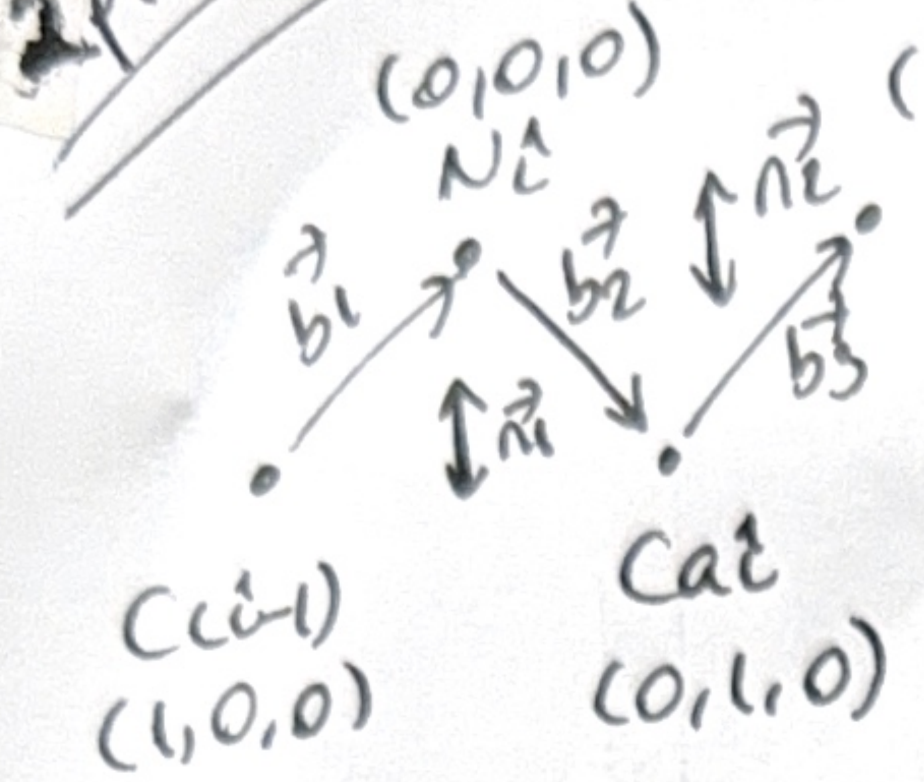


$\Phi = C_{(i-1)}, N_i, C\alpha_i, C_i$
$\Psi = N_i, C\alpha_i, C_i, N_{(i+1)}$

$C_{(i-1)} = (1,0,0)$
$N_i = (0,0,0)$
$C\alpha_i = (0,1,0)$
$C_i = (0,1,-1)$
$N_{(i+1)} = (0,1,1)$

Above the Valine (V) amino acid and the Ramachandran plot of Φ and Ψ dihedrals of this Valine are shown. Calculate the backbone dihedral angles Φ and Ψ of the V using the coordinates provided and using the Ramachandran plot, determine which secondary structure this V falls into?

2pts



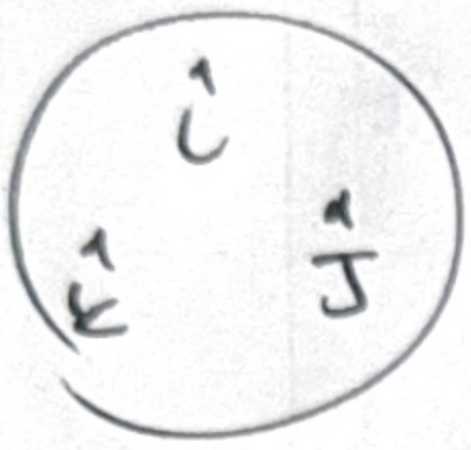
$\vec{b_1} = Ni - Ci\text{-}1 = (-1,0,0) \rightarrow |\vec{b_1}| = 1 \rightarrow -\hat{i}$

$\vec{b_2} = Cai - Ni = (0,1,0) \rightarrow |\vec{b_2}| = 1 \rightarrow \hat{j}$

$\vec{b_3} = Ci - Cai = (0,0,-1) \rightarrow |\vec{b_3}| = 1 \rightarrow -\hat{k}$

$\vec{n_1} = \vec{b_1} \times \vec{b_2} = (-\hat{i}) \times \hat{j} = -\hat{k}$

$\vec{n_2} = \vec{b_2} \times \vec{b_3} = \hat{j} \times (-\hat{k}) = -\hat{i}$



$\vec{b'} = \vec{n_1} \times \vec{n_2} = (-\hat{k}) \times (-\hat{i}) = \hat{j} \rightarrow |\vec{n_1} \times \vec{n_2}| = 1$

$\vec{n_1} \cdot \vec{n_2} = (-\hat{k}) \cdot (-\hat{i}) = 0$

Since sin and cos symmetric func. derive a formula including tan or cot instead of sin and cos.

cotθ

dot product $\rightarrow \vec{n_1} \cdot \vec{n_2} = \cancel{n_1 . n_2} \cos\theta$

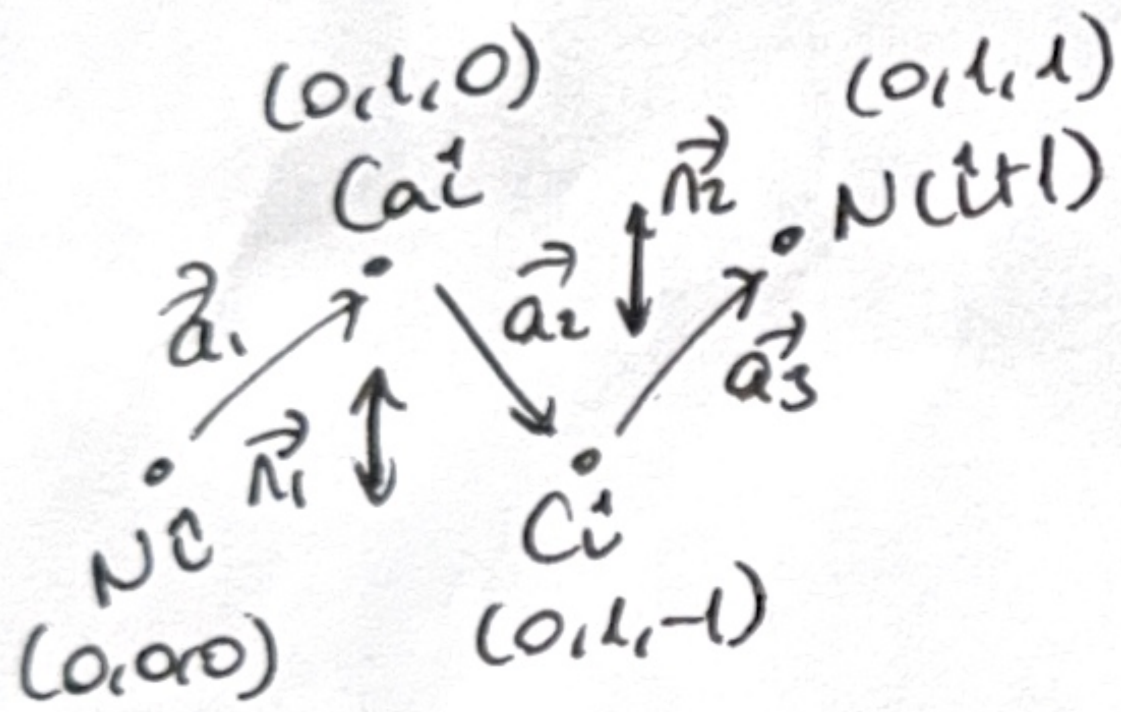
cross product $\rightarrow \vec{n_1} \times \vec{n_2} = \cancel{n_1 . n_2} \sin\theta$

$\dfrac{\overset{=0}{\vec{n_1} \cdot \vec{n_2}}}{\underset{=1}{|\vec{n_1} \times \vec{n_2}|}} = \cot\theta$ $\quad \cot\theta = 0$

$\phi = 90°$ 0.5 pts

$x = \pi/2 + k\pi,\ k \in \mathbb{Z}$

$x = \pi/2,\ 3\pi/2, \dots$



$\vec{a_1} = Cai - Ni = (0,1,0) \rightarrow |\vec{a_1}| = 1 \rightarrow \hat{j}$

$\vec{a_2} = Ci - Cai = (0,0,-1) \rightarrow |\vec{a_2}| = 1 \rightarrow -\hat{k}$

$\vec{a_3} = N(i+1) - Ci = (0,0,2) \rightarrow |\vec{a_3}| = 2 \rightarrow 2\hat{k}$

$\vec{n_1} = \vec{a_1} \times \vec{a_2} = \hat{j} \times (-\hat{k}) = -\hat{i}$

$\vec{n_2} = \vec{a_2} \times \vec{a_3} = (-\hat{k}) \times (2\hat{k}) = 0 = (0\hat{i} + 0\hat{j} + 0\hat{k})$ 1 pts

$|\vec{n_1} \times \vec{n_2}| = 0$ $\quad \tan\theta = \dfrac{0}{x} \rightarrow \vec{n_1} \cdot \vec{n_2} = 0$ $\quad \tan\theta = \dfrac{0}{0}$

θ is undefined!

cannot find the secondary structure

$\Rightarrow$ we cannot find ψ due to uncertainty, however, previously we have found $\phi = 90°$. Based on this, this Val residue cannot take place either in right-handed α-helical or β-sheet region. It can only be found around left-handed α-helical region.

0.5 pts