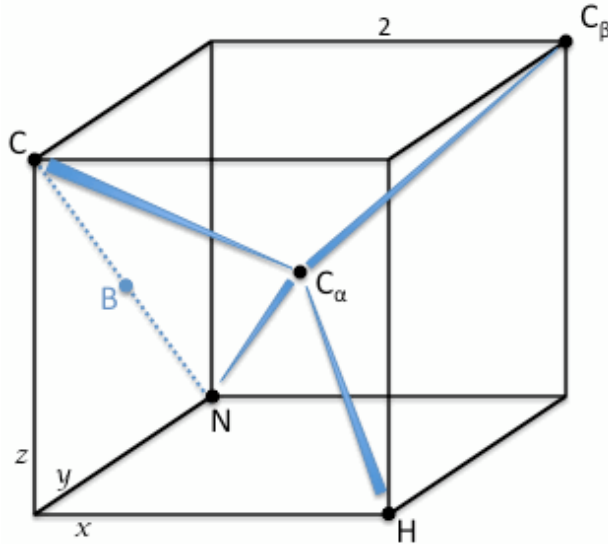


Construction of the Carbon-beta position, given N, C α and C

- Assume simple tetrahedral geometry, no chemistry
- Useful for constructing stereochemistry if the amino acid does not have a sidechain model
- Use for placing glycines (which do not have beta-carbons) in a standard orientation, for viewing the model

Place the N, H, C β and C on the corners of a cube, with C α in the middle.



Set the cube edge to 2, and the C α position at the origin. The positions of the atoms are then,

N	(-1,1,-1)
H	(1,-1,-1)
C β	(1,1,1)
C	(-1,-1,1)
C α	(0,0,0)

The tetrahedral bond angle is calculated as,

$$\theta = \arccos\left(\frac{C \cdot N}{|C||N|}\right) = \arccos\left(\frac{-1}{3}\right) = 109.47^\circ.$$

The angle $\angle \mathbf{B} \mathbf{C}_\alpha \mathbf{C}_\beta$ is calculated as,

$$\theta = \arccos\left(\frac{B \cdot C_\beta}{|B||C_\beta|}\right) = \arccos\left(\frac{(-1,0,0) \cdot (1,1,1)}{\sqrt{3}}\right) = 125.26^\circ.$$