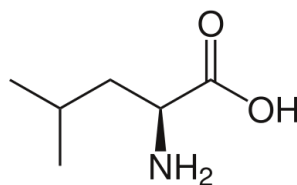


NAME:

Total: 40 points (Please answer 4 questions out of 6)

1. (10 points)



<Leucine>

(a) How many side-chain dihedral angles does the amino acid Leu possess?

(b) If a polypeptide consists of seven C $\alpha$  atoms, how many unique backbone dihedral and bond angles does it possess?

2. (10 points)

(a) What is the densest packing fraction for monodisperse hard spheres?

(b) What is the densest packing fraction for disordered collections of monodisperse hard spheres?

(c) What is the packing fraction of all-atom hard-sphere representations of residues in protein cores?

3. (10 points) Plot the purely repulsive Lennard-Jones interatomic potential  $V(r_{ij})$  as a function of the separation between atoms  $r_{ij}$ .

NAME:

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4. (10 points)

(a) What is the difference between a deterministic and stochastic model?

(b) Which term applies to Ordinary Differential Equation (ODE) models?

5. (10 points) In the context of mathematical modeling, what is an F test used for?

6. (10 points) The SIR model can be used to predict the course of an epidemic in a large population. In the model equations given below, describe the meaning of each state variable (S, I and R) and each parameter ( $\beta$  and  $\mu$ ):

$$\frac{dS}{dt} = -\beta SI$$

$$\frac{dI}{dt} = \beta SI - \mu I$$

$$\frac{dR}{dt} = \mu I$$