

1. (12 points)

a) and b) The following were good possibilities for interactions with the Asp and Ser side chains:
Asp: Lys⁺ or Arg⁺ (charge interaction) or any polar amino acid (D-H, H-bond interaction).

[2 pts for each correct structure; 1 pt for name; 1 pt for interaction]

Ser: Most polar (incl charged) amino acids could donate (D-H) or accept (A) H-bonds.

For both Asp & Ser, a nonpolar R-group could also be drawn (van der Waals interaction).

c) Details differ depending on the two interactions depicted; the order of strength is: [2 pts]

Charge > H-bond > van der Waals

d) 1) None of the interactions shown could affect primary structure. [0.5 pts each]

2) Most would not contribute much to secondary structure.

3) and 4) R-group interactions are the most significant factors for both tertiary and quaternary structure. [0.5 pts each]

2.

a) $DS = DH/Tm$

$$T4L (WT) = 497/(273 + 53.5) = 1.53 \text{ kJ/mol-K}$$

$$T4L (Leu118Ala) = 316/(273 + 39.6) = 1.01 \text{ kJ/mol-K}$$

b) At 46°C, $DG = DH - TDS = DH - (273 + 46)DS$ (unfolding)

$$T4L (WT) = 8.87 \text{ kJ/mol}$$

$$T4L (Leu118Ala) = -6.46 \text{ kJ/mol}$$

$$DG_{WT} - DG_{mutant} = DDG \text{ (unfolding)} = 15.33 \text{ kJ/mol}$$

c) At 27°C, $DG = DH - 300*DS$ (unfolding)

$$T4L (WT) = 37.92 \text{ kJ/mol}$$

$$T4L (Leu118Ala) = 12.72 \text{ kJ/mol}$$

$$DG_{WT} - DG_{mutant} = DDG \text{ (unfolding)} = 25.2 \text{ kJ/mol}$$

$$K_{eq} = \exp(-DG/RT) \quad F_u = K_{eq}/(1+K_{eq})$$

$$T4L (WT) = 2.40*10^{-8} \quad 2.4*10^{-7}$$

$$T4L (Leu118Ala) = 6.05*10^{-3} \quad 6.01*10^{-3}$$

$$d) \text{ Fraction lost} = DDG/DG_{WT} = 0.66$$