

HW4: Chapter 4: 1, 4, 7, 10, 15, 16

①	C-N bond in peptides	1.32 Å
	Typical C-N bond length	1.49 Å
	Typical C=N bond length	1.27 Å

a) Its length suggests that the peptide bond has partial double bond character

b) The planarity suggests it has partial  $sp^2$  hybridization which means that there is no rotation around the bond

② Poly Glu:  $\alpha$  helix @ pH 3  
Random coil @ pH 7

The  $\alpha$ -helix is held together by bonds b/w the carbonyl oxygen and amide hydrogen, BUT the side chains of the amino acids project out from the helical axis.

Poly Lys: Random coil @ < pH 8.5  
 $\alpha$ -helix @ > pH 8.5

The side chain pK<sub>a</sub>s are determining the secondary structural state of each polymer by electrostatic repulsion



- 1) Asp: Exterior  
 Ile: Interior  
 Thr: Interior or Exterior  
 Ala: Interior  
 Glu: Exterior  
 Lys: Exterior

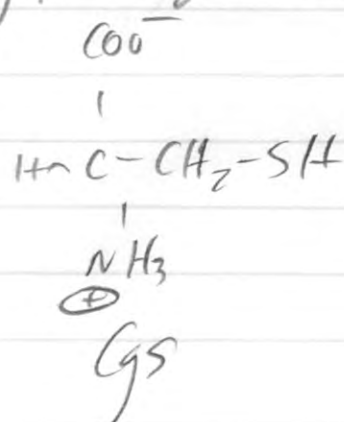
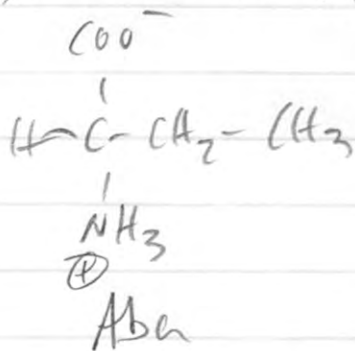
Charged residues (Asp, Lys) may also be found in salt bridges in the interior of the protein.

⑩ Protein b is entirely  $\alpha$ -helical, so it is likely found in the Ramachandran plot in (D)

Protein a is mostly  $\beta$ -sheet so its Ramachandran plot is likely (C).

⑪ you got this. No answers needed (It is NF-Kappa B or p65)

⑫ a) The Ala is roughly the same size as Gys so that is one reason why it might have worked.



The Aba would be unable to form a disulfide bond, so that is one reason it might not have worked.

b) i) Aba is chemically different from Gs with respect to polarity, so it might disrupt the "normal" hydrophobic core by folding away from solvent. Gs is hydrophobic and is solvent accessible

ii) Aba cannot form disulfide bonds and they may be needed for the protein to fold properly

iii) The cytosol is different than the buffer used, so the protein may misfold because of a solution problem

d) Disulfide bonds are not important in maintaining the structure of HIV protease

d) For situation 1: with the exception of chirality, everything else is the same if D-amino acids are used

Against situation 1: Chirality is frankly important!!! It determines the handedness of the 2<sup>o</sup> structures among other things.

For situation 2: Since the chiralities are opposite, the D-amino acid based protein should fold in the opposite manner

Against situation 2: Chirality is only one part of protein folding so the D-amino acid based protein might fold only something completely different.

Situation 3 is a catch all situation. you could use any of the above arguments for or against it.

- e) Model 1 is supported by the data
- f) Evans Blue is achiral so it doesn't matter to the enzyme (its chirality doesn't matter)
- g) No because chymotrypsin recognizes L-amino acids not D-amino acids
- h) Who knows? There is no way to predict.

