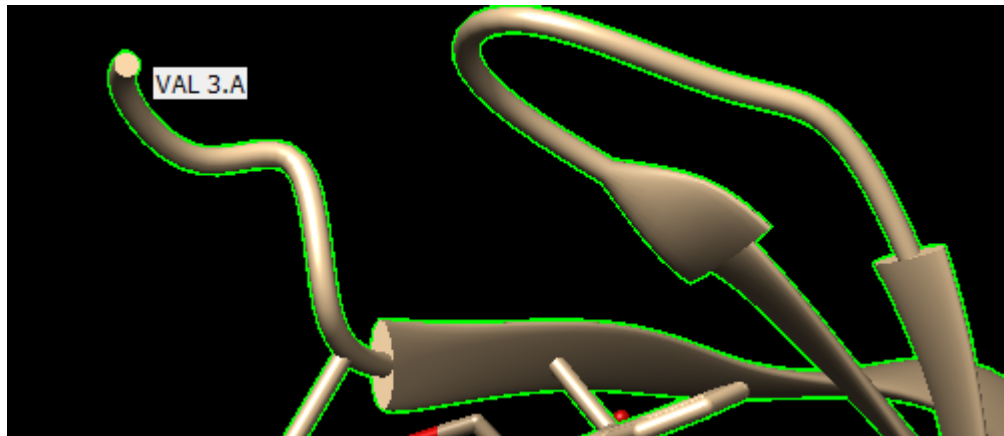


Task 1

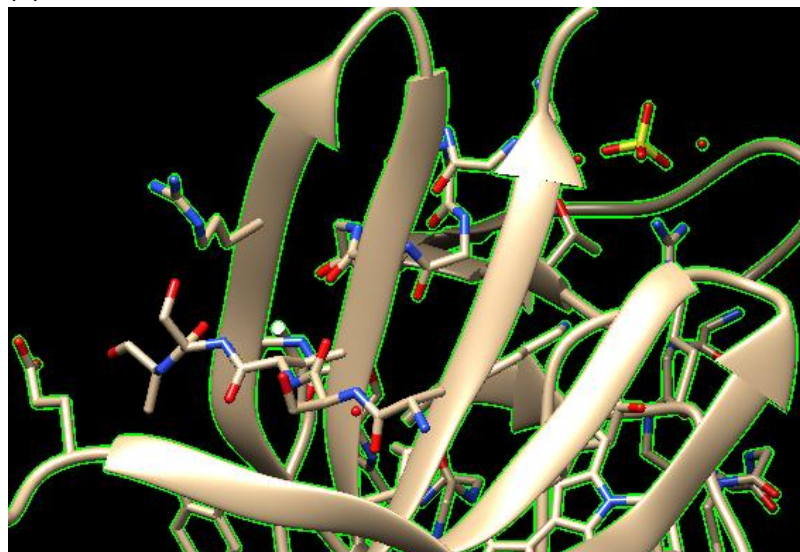
- 1) What is the name of the first amino acid (from the N-terminal) you see on the structure? What is the first secondary structure element (other than coil and turn) at the N-terminal of the protein sequence, a helix or a beta-strand? In order to see the molecule better, you need to use simplified representation of the molecule, for example, use backbone only and ribbon, or even with different colors.

- Valine (VAL 3.A)
- beta-strand



- 2) Which of the following best describes the largest beta-sheet in chain A:
(a). 4-stranded; (b). 5-stranded; (c). 6-stranded; (d). 7-stranded

- (b) 5-stranded

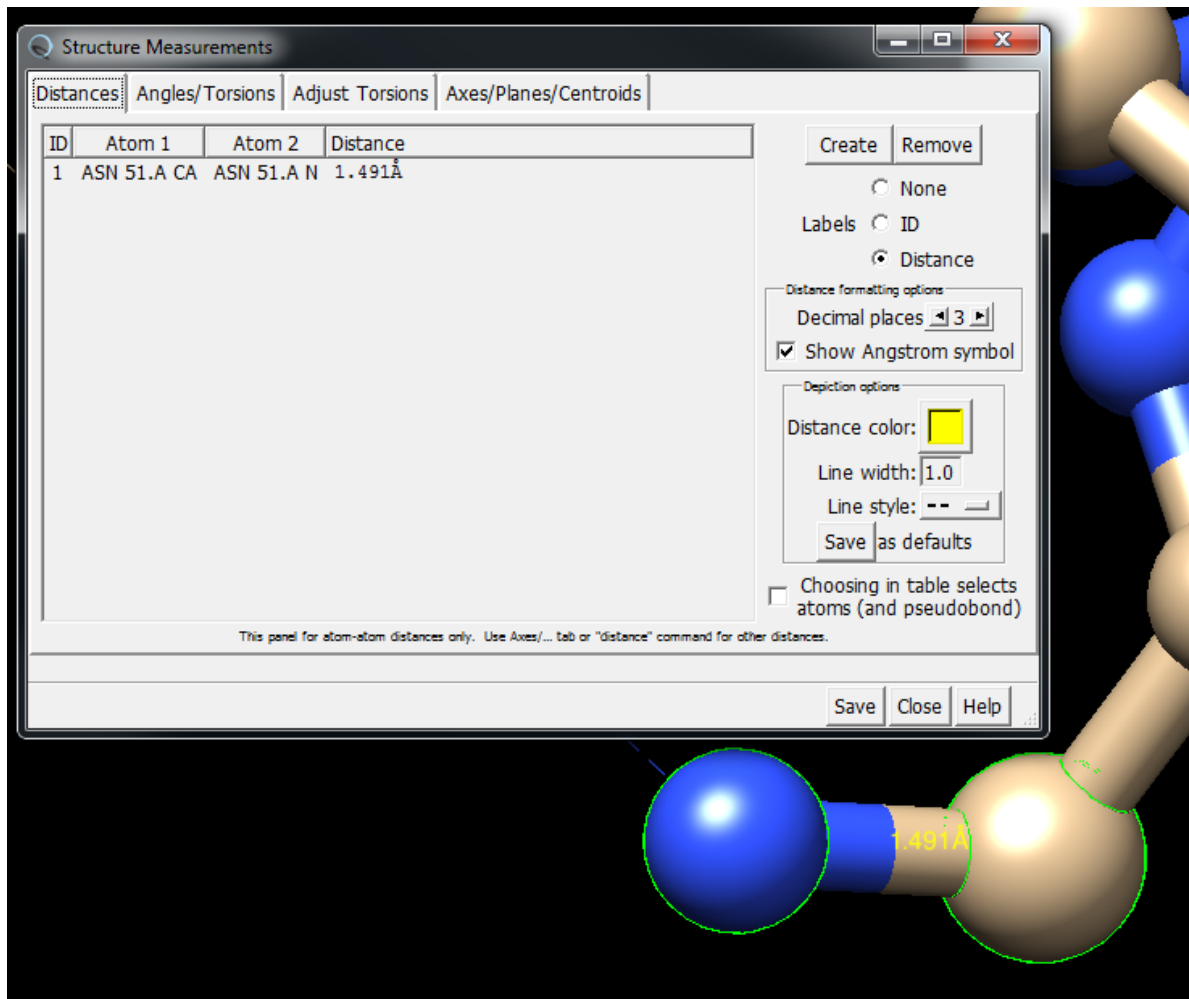


- 3) Is amino acid PRO103 in chain A on a helix, beta-strand or a coil?
- PRO103 is on the alpha helix in chain A.
- 4) You can choose to see the ribbon view or the backbone atoms or all atoms by going to "Actions - Atoms/Bonds" in the upper menu. To measure the distance between two atoms, you need to select two atoms using "control" key for the first atom, and "control+shift" keys for the second atom. Then go to "Tools - Structure Analysis - Distances" in the upper menu to measure the distance.

Measure the following bond lengths/distances and give the index of the atoms you used to measure:

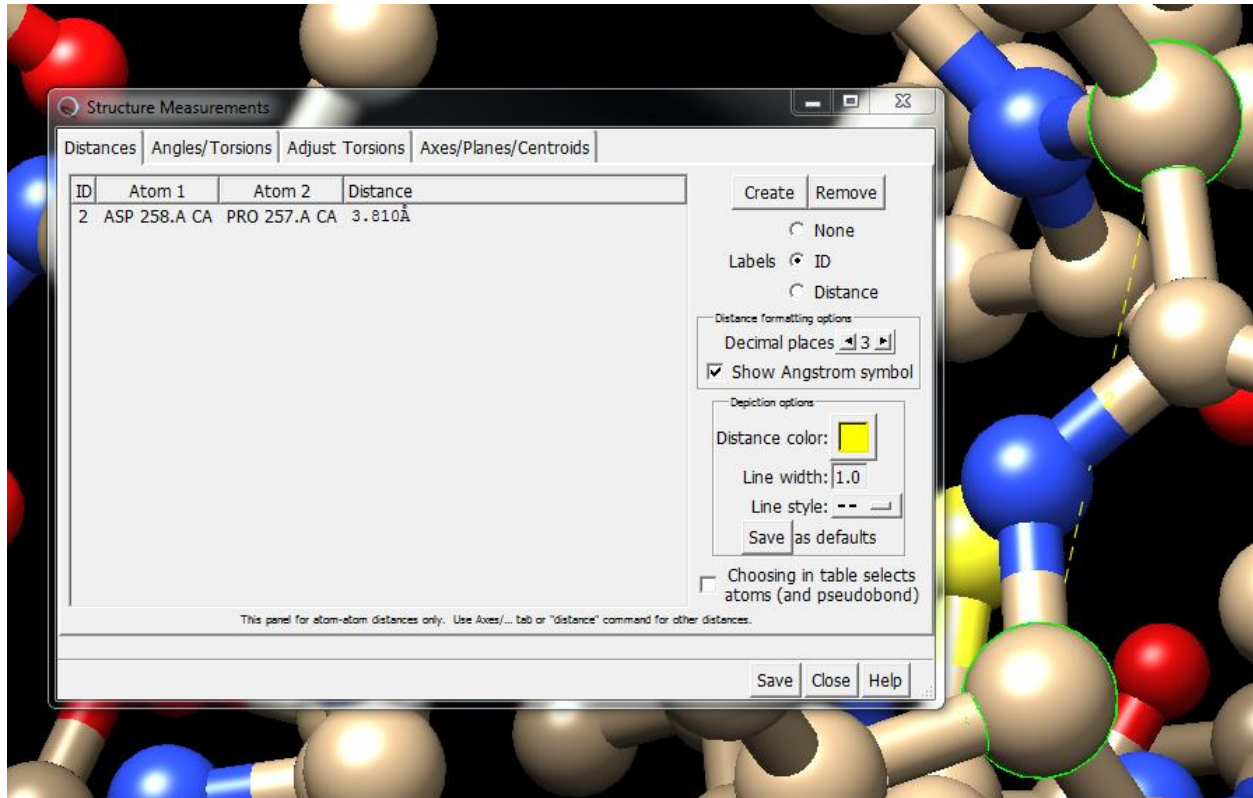
(a). The bond formed by the N and Ca atoms on the backbone;

- ASN 51.A CA(Asparagine)
- ASN 51.A N(Asparagine)
- Distance : 1.491Å



(b). The distance between two adjacent Ca atoms in a helix. Two Ca atoms are considered adjacent if they are from two consecutive amino acids in the chain.

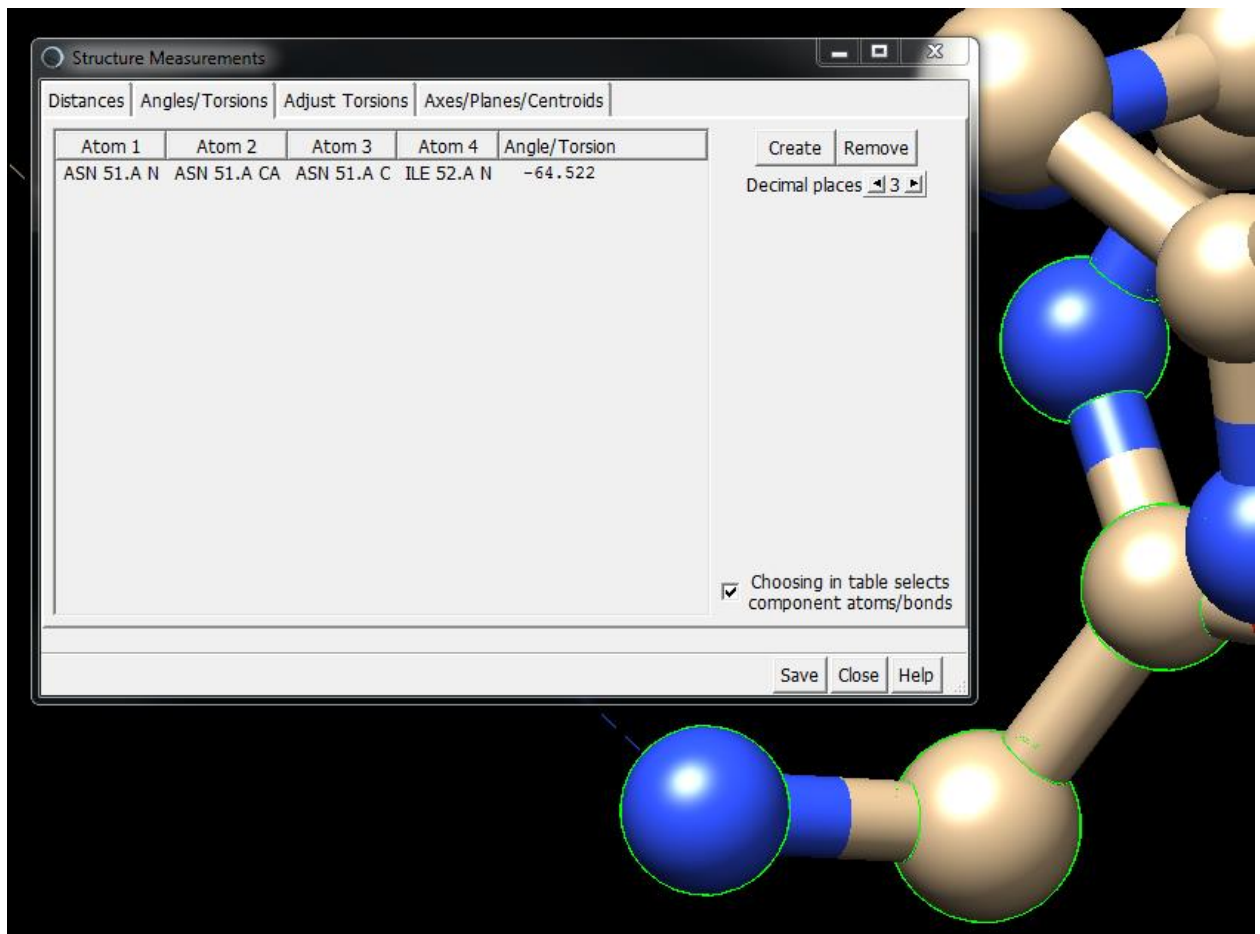
- ASP 258.A CA (Aspartic acid)
- PRO 257.A CA (Proline)
- Distance : 3.810Å



Similarly to measuring the bond length, we can measure the bond angle and torsion angle in Chimera. To measure the torsion angle, you need four atoms. Go to "Tools - Structure Analysis - Angle/torsion". You can select four atoms the same way when you select two atoms in the above question. click the "create" button in the Angle/Torsion window.

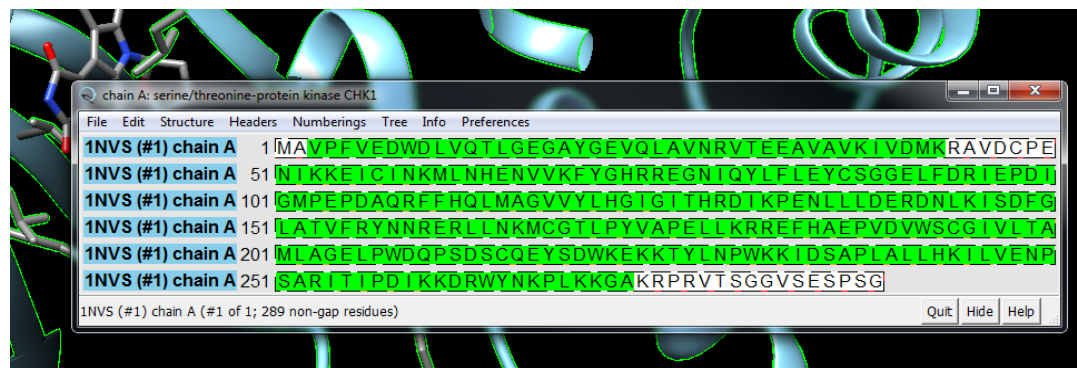
(c). Measure the torsion angle formed by the backbone consecutive atoms: N, Ca, C, N. Write the label of the four atoms and the torsion angle formed.

- ASN 51.A N(Asparagine)
- ASN 51.A CA(Asparagine)
- ASN 51.A C(Asparagine)
- ILE 52.A N(Isoleucine)
- Tortion/Angle : -64.522

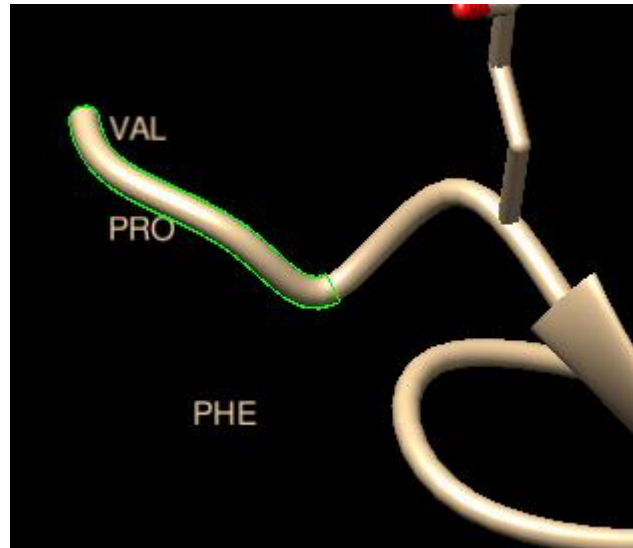


5) What is the amino acid sequence of this protein? What are the first three amino acids at the N-terminal of the chain? What are the three amino acids at the C-terminal of the chain? You may want to use the sequence view under "Tools".

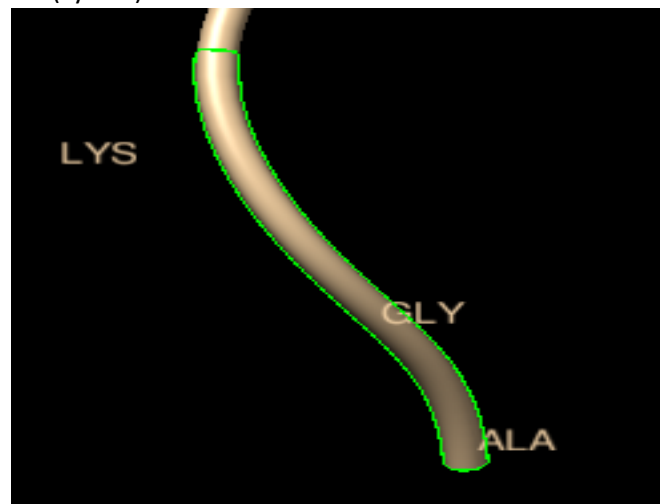
- The amino acid sequence of this protein is
 - i. VPFVEDWDLVQTLGEGAYGEVQLAVNRVTEEAVAVKIVDMKRAVDCPENIKKEICINKML
 NHENVVKFYGHRREGNIQYLFLEYCSGGELFDRIEPDIGHMPEPDAQRFHQLMAGVVYLH
 GIGITHRDIKPENLLLDERDNLKISDFGLATVFRYNNRERLLNKMCGTLPYVAPELLKRREFH
 AEPVDVWSCGIVLTAMLAGELPWDQPSDSCQEYSDWKEKKTYLNPWKKIDSAPLALLHKI
 LVENPSARITIPDIKKDRWYNKPLKKGAKRPRVTSGGVSESPSG



- The first three amino acids at the N-terminal are
 - i. VAL (Valine)
 - ii. PRO(Proline)
 - iii. PHE(Phenylalanine)



- The three amino acids at the C-terminal are
 - i. ALA(Alanine)
 - ii. GLY(Glycine)
 - iii. LYS(Lysine)

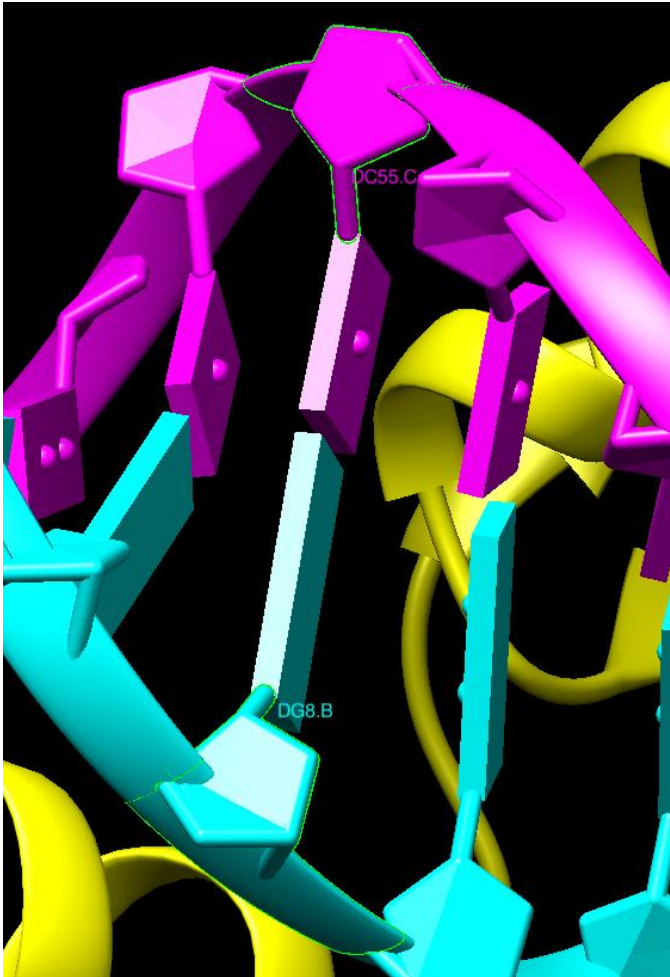


Task 2

- 1) Please give the names of at least two possible pairing nucleotides using your judgment and explain why.

For example: You can say B chain A with id 10 pairing with C chain G with id 60. (or use A10.B - G60.C to represent).

- DC55.C bonded with DG8.B

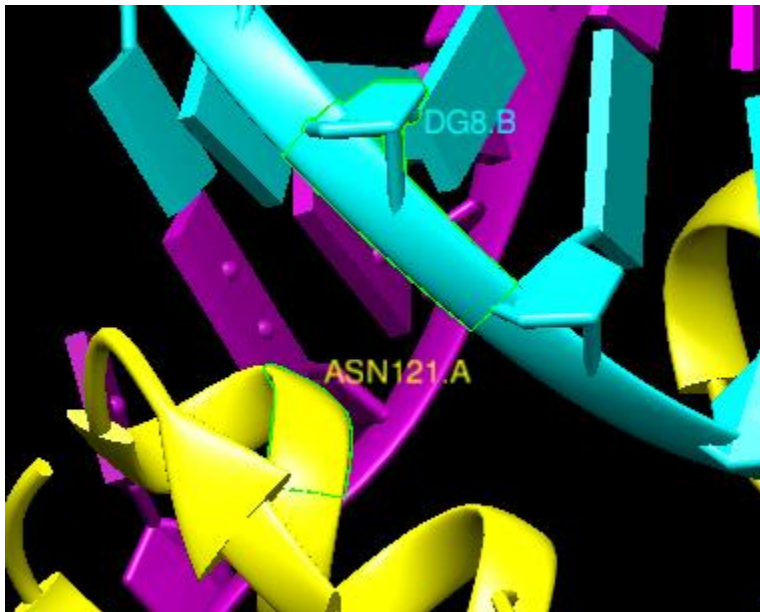


- DC 56.C bonded with DG 7.G

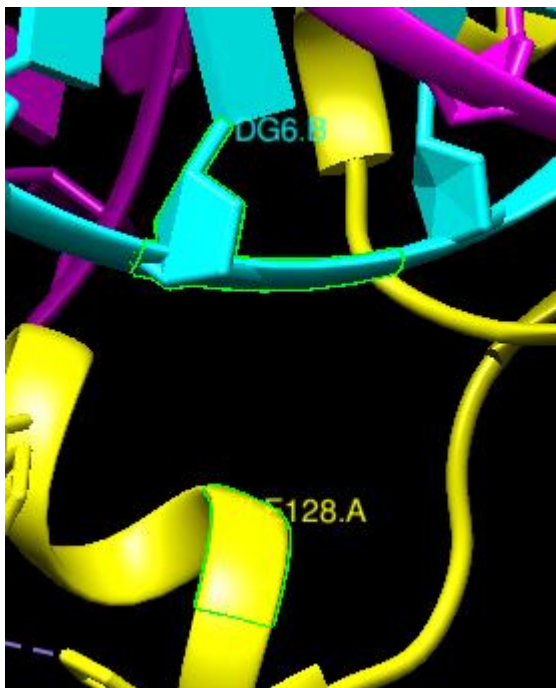


2) Give the name and the sequence ID of at least two possible amino acids on the protein which interact with DNA. Use your own judgment and explain why you think so.

- Asparagine Molecule
- Sequence Id is ASN 121.A-DG8.B



- Isoleucine Molecule
- ILE 128.A-DG6.B



3) What is the first amino acid you see on the protein and what is the last amino acid on the protein?

- The first amino acid is ARG 103.A(Arginine)
- The last amino acid is LEU 186.A(Leucine)