IIT Guwahati

Lecture 5

Course BT 631

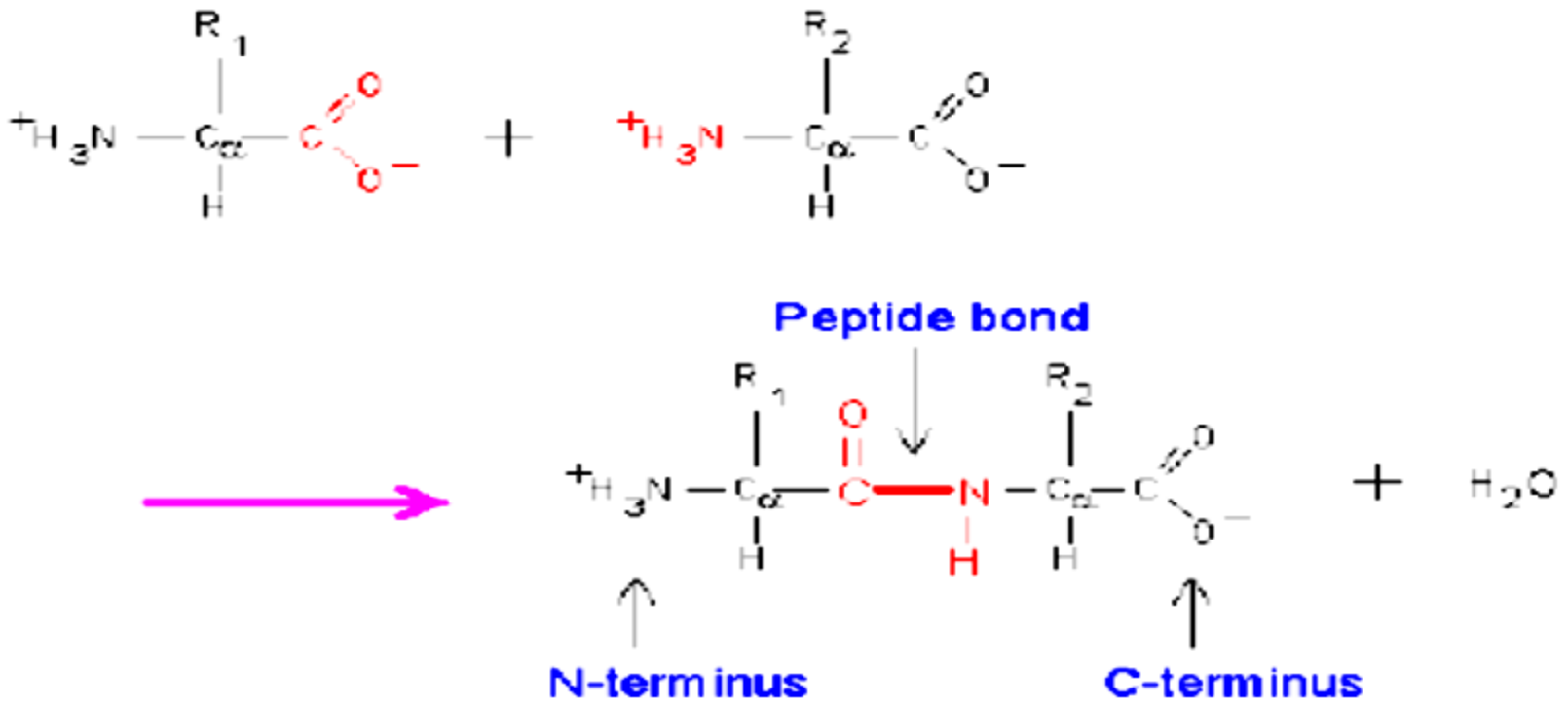
Protein Structure function and Crystallography

Prof. Arun Goyal

Dept. of Biosciences and Bioengineering

Peptide Bond

- Amino acids are linked by forming amide bond between α-carboxylic group of one amino acid and α- Amino group of other amino acid, it is called Peptide bond.
- When two amino acids are joined together by a peptide bond it is called as Dipeptide.



Formation of Peptide Bond

Types of Peptide Bond

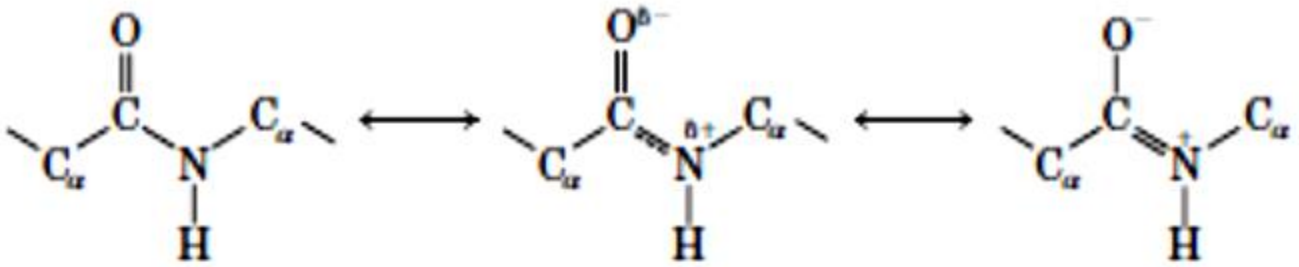
1. **Linear Peptide:** It is formed between α-Carboxylic group of one amino acid and α-Amino group of other amino acid e.g. Most of the peptide bonds
2. **Semi-cyclic Peptide Bond:** It is formed between α-Carboxylic group or α-Amino group of an amino acid and its side chain containing Amino group or carboxylic group, respectively. This type of peptide bond is known as semi-cyclic peptide bond. e.g. Bacitracin A
3. **Cyclic Peptide Bond:** It is formed between N-terminal amino group and C-terminal carboxyl group of amino acid of the same polypeptide chain. This type of peptide bond is known as cyclic peptide bond. e.g. Tyrocidine is naturally occurring cyclo-decapeptide. Gramicidin S is a decapeptide. Vallinomycin (antibiotic) is also cyclo-peptide.

Characteristics of Peptide Bond

1. **Peptide bond is rigid and planner.**
2. **Peptide bond has Partial Double Bond characteristics (Double bond is due to Resonance). On average, a peptide bond length is 1.32 Å as compared to 1.45 Å for an ordinary C-N bond. Whereas, the average bond length of a C=N double bond is 1.25 Å.**

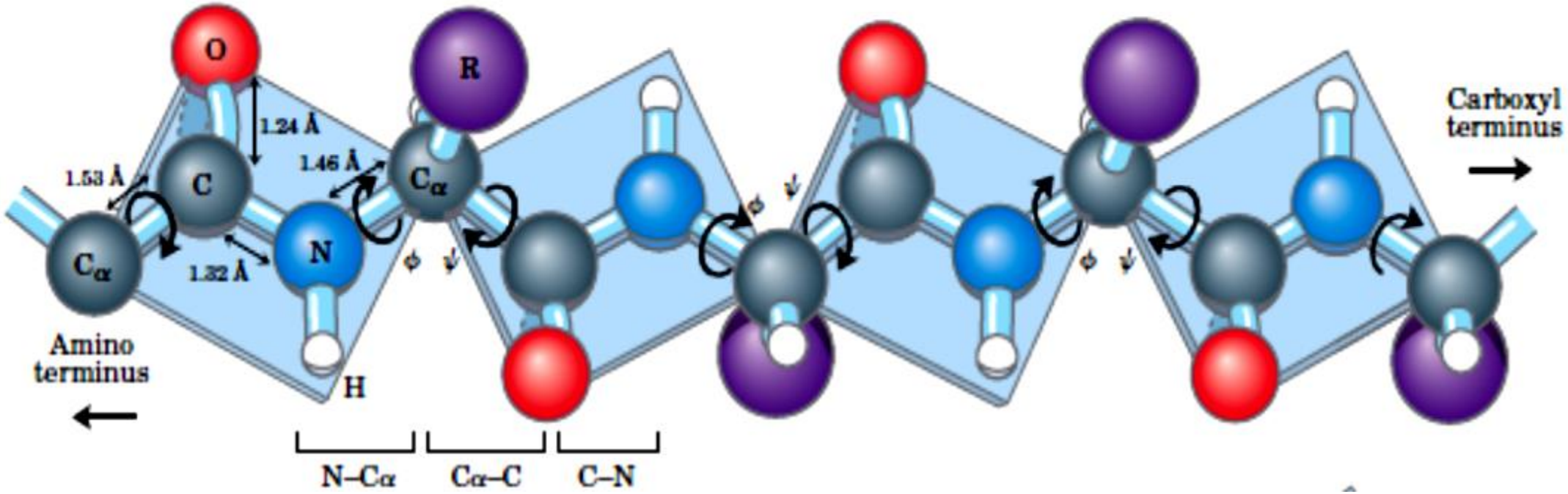
***Thus, partial double bond restricts the rotation around this bond. This leads to the six atoms being coplanar*.**

Characteristics of Peptide Bond



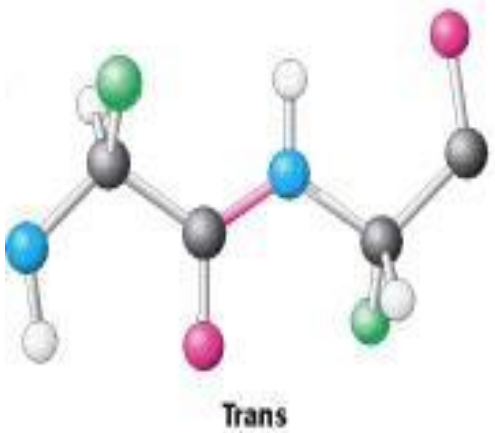
The carbonyl oxygen has a partial negative charge and the amide nitrogen a partial positive charge, setting up a small electric dipole. Virtually all peptide bonds in proteins occur in this trans configuration; an exception is noted in Figure 4–8b.

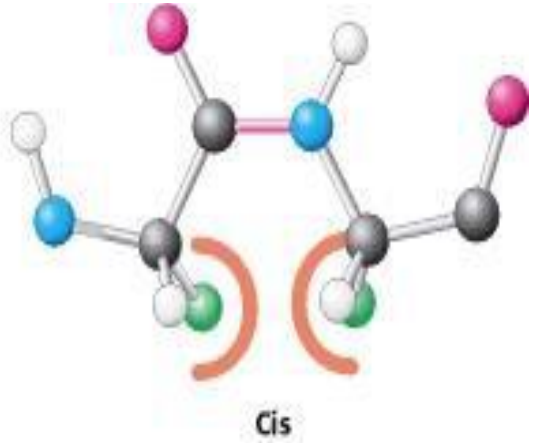
(a)

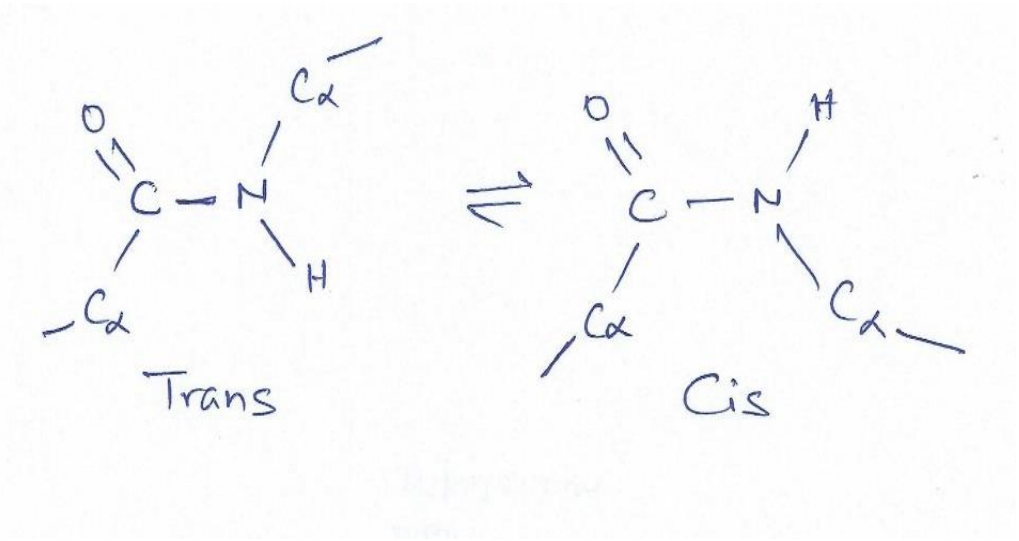


Characteristics of Peptide Bond

3. All peptide bonds are Trans in nature. Because Trans Bonds are 2 kcal more stable, with an exception of X-Proline peptide bond (Where X is any amino acid behind proline).

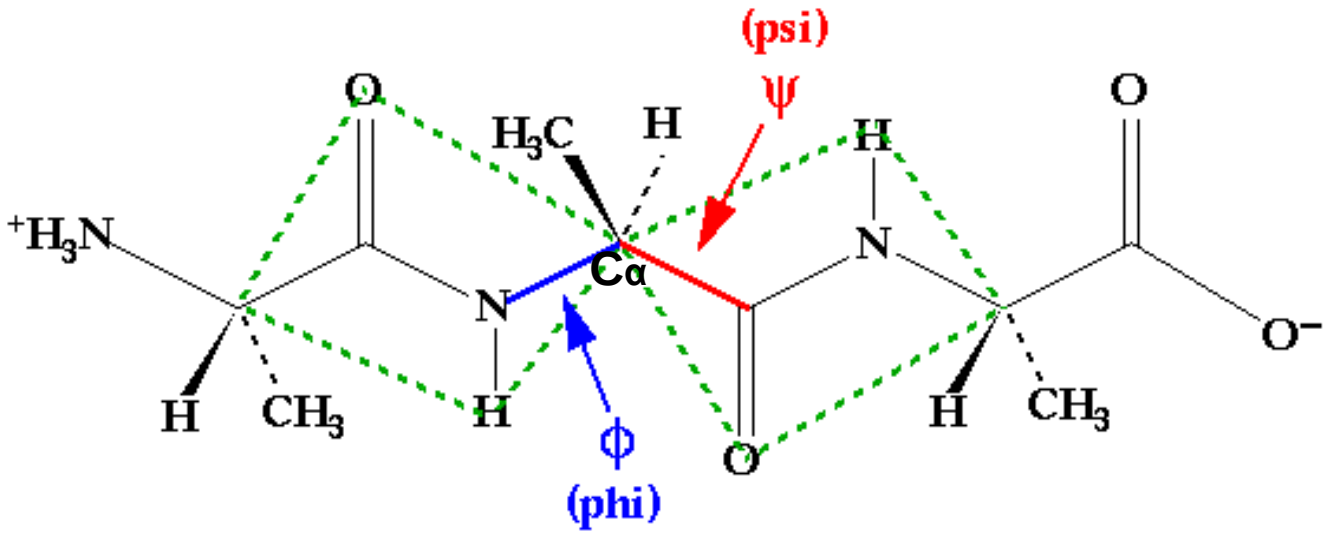


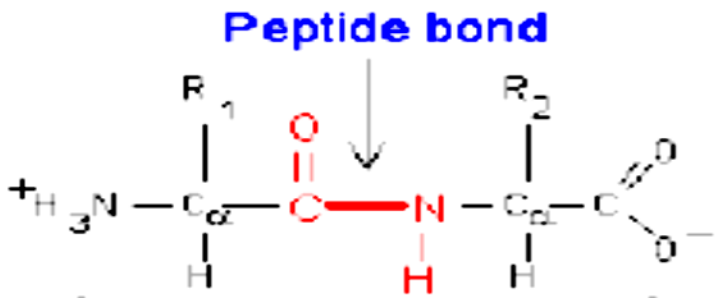




Characteristics of Peptide Bond

4. **Rotation around peptide bond (C-N) is not possible (because of partial double bond character). Only the Cα-N and Cα-C bonds rotation are possible.**
   The rotational (dihedral) angle between Cα-N is called as Φ,
   while Dihedral angle between Cα-C is called as Ψ.
   The dihedral Angle between Cα-R is called χ and N-C is called ω.





C_α-C=1.53 Å; N-C_α =1.46 Å; C=O =1.24 Å; C-N (Rigid) = 1.32 Å;

Alanine tripeptide: distance from residue *i* to (*i*+1) =C_α– C_α =3.8 Å

A fully extended polypeptide chain has Φ = Ψ= 180°