PROTEIN

RCSB PDB-101

Introduction

Protein name is derived form a Greek word PROTOS which means “the first or the supreme’’.

Proteins are extremely complicated and nitrogenous molecule made up of variable number of amino acid residue joined to each other by a specific covalent bond called peptide bond.

20 amino acid which have been found to occur in all proteins, known as standard amino acid.

Why are proteins important to us?

- Proteins make up about 15% of the mass of the average person
- Enzymes act as a biological catalyst
- Storage and transport – Hemoglobin
- Defence -Antibodies
- Hormones – Insulin
- Ligaments and arteries (mainly formes by elastin Protein)
- Muscle – Proteins in the muscle respond to nerve impulses by changing the packing of their molecules (Actin and myosin)
- Hair, nails and skin: Protein keratin as main component

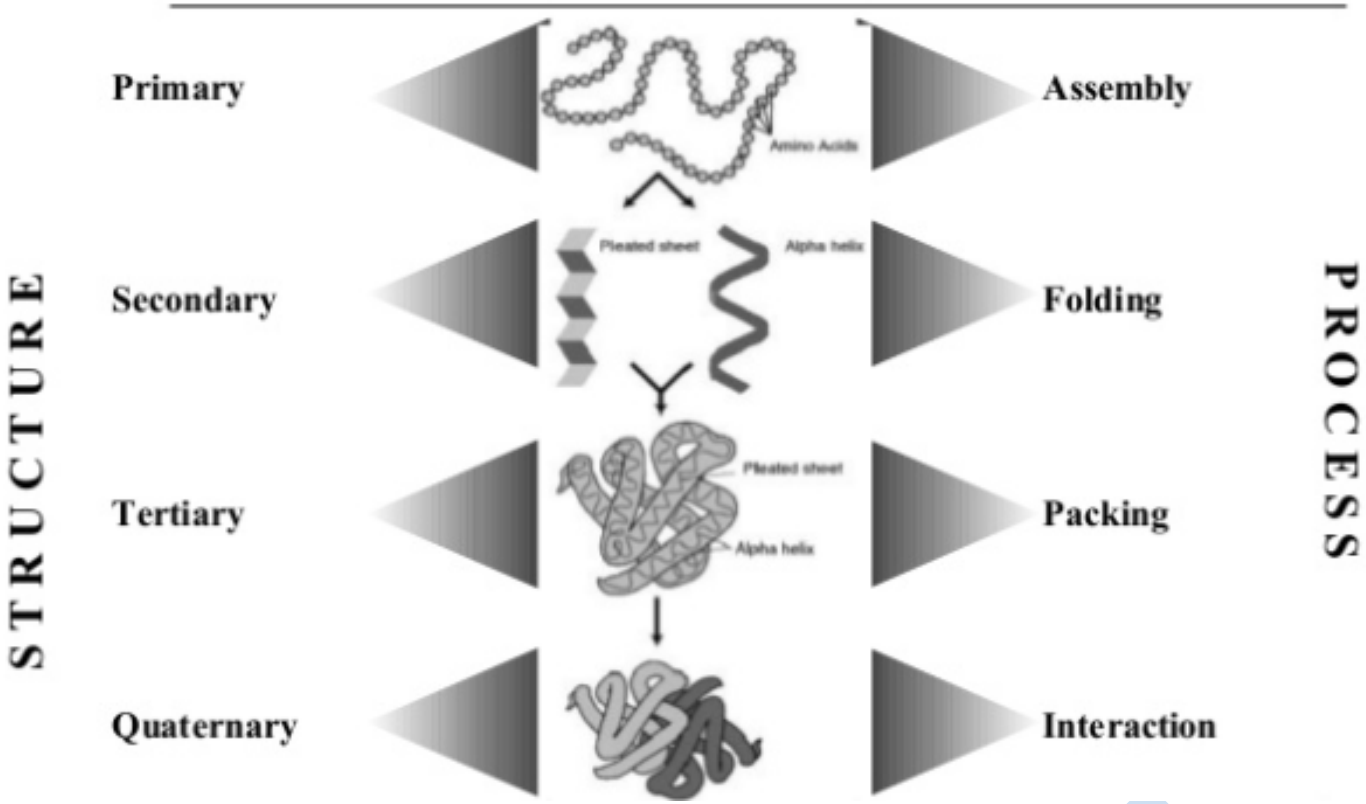
Levels in Protein structure

Majority of protein are compact and highly convoluted molecules.

Each polypeptide assumes at least three levels of structural organization termed as primary, secondary and tertiary structure.

Proteins which possess more than one polypeptide chain in their molecule also possess a fourth structure called quaternary structure.

Chemistry of Protein Structure



Primary structure

The sequence of amino acid residues along the peptide is called primary structure of the peptide.

It also include the determination of the number of amino acid residues in a peptide chain.

Shows whether the peptide chain is open, cyclic or branched.

Primary structure is linear, ordered and 1 dimensional.

Written from amino end to carboxyl end that is N to C.

primary structure of human insulin

CHAIN 1: GIVEQ CCTSI CSLYQ LENYC N

CHAIN 2: FVNQH LCGSH LVEAL YLVCG ERGFF YTPKT

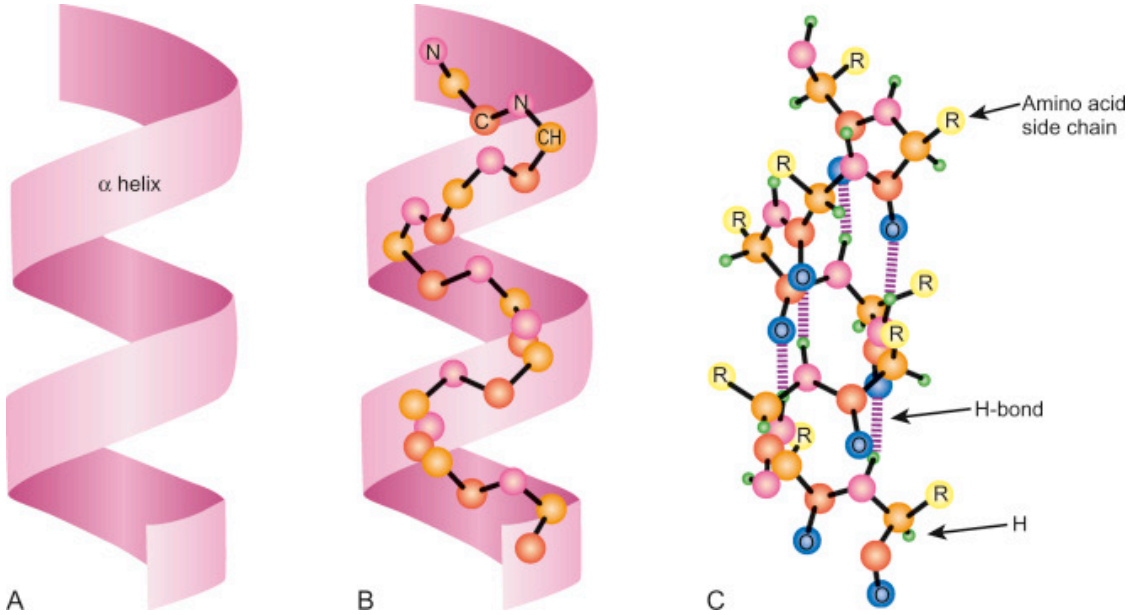
Secondary Structure

- Primary structure shows that peptide are quite straight and extended.
- X-rays diffraction on protein crystals shows that polypeptide chain tend to twist or coil upon themselves.
- The folding of the polypeptide chain into specific coiled structure held together by H bonds is called secondary structure of protein.
- Secondary structure may take one of the following form.

1. Alpha – Helix
2. Beta Pleated Sheet
3. Loop or Coil Conformation
4. Super secondary motifs

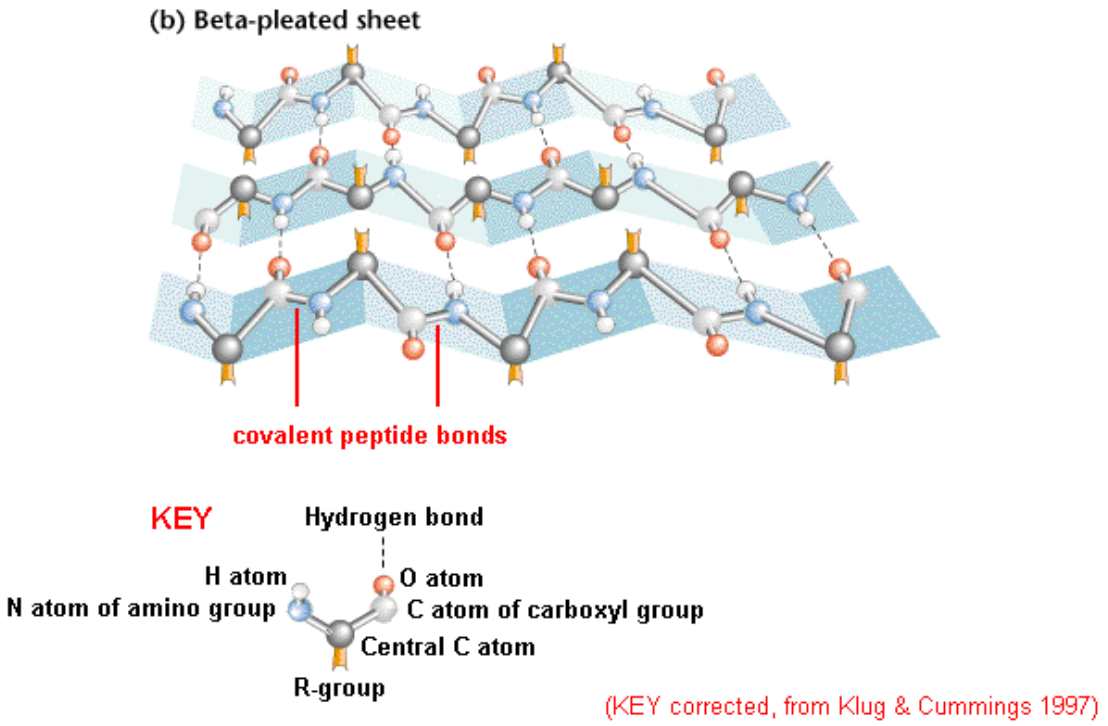
Alpha(α)- Helix

1. It is a clockwise rodlike spiral shape.
2. Formed by intrachain Hydrogen bonding between C=O group of each amino acid and NH_2 group that is present 4 residue ahead.
3. Proteins have great strength and elasticity.
4. Can easily be stretched due to tight coiling.



β- Pleated Sheath

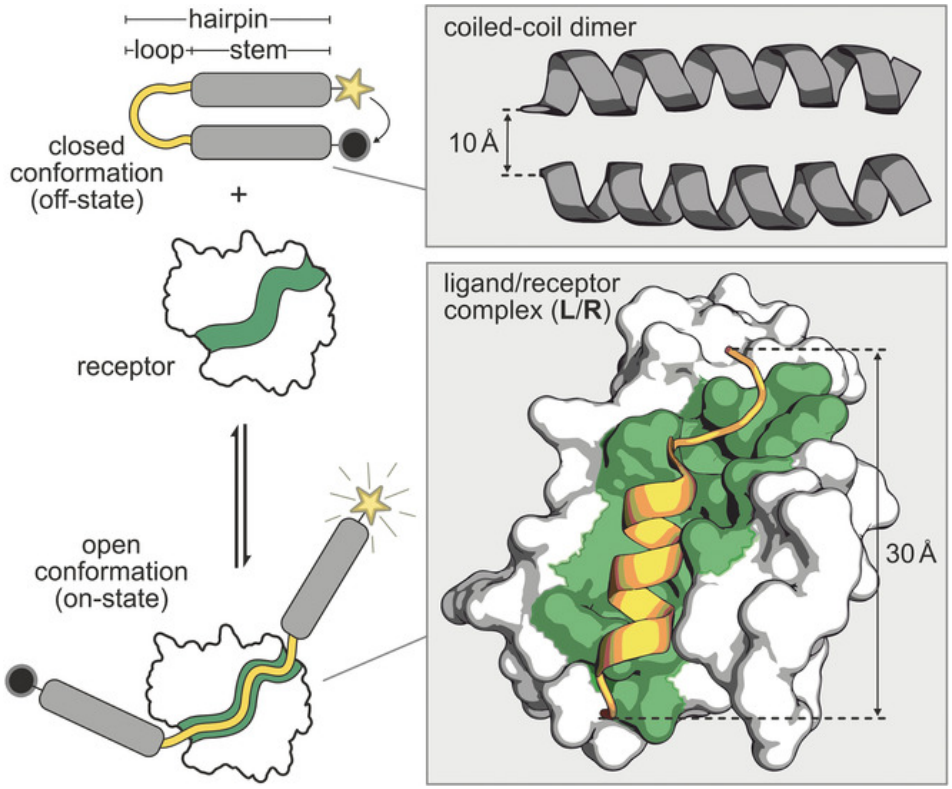
1. 5 to 10 amino acid in this structure line up side by side just like a sheath of cloth can be folded again and again
2. Hydrogen bond present between the peptide strands that is interstrand.
3. This form is fully expended and can't be further stretched and they are inelastic



(KEY corrected, from Klug & Cummings 1997)

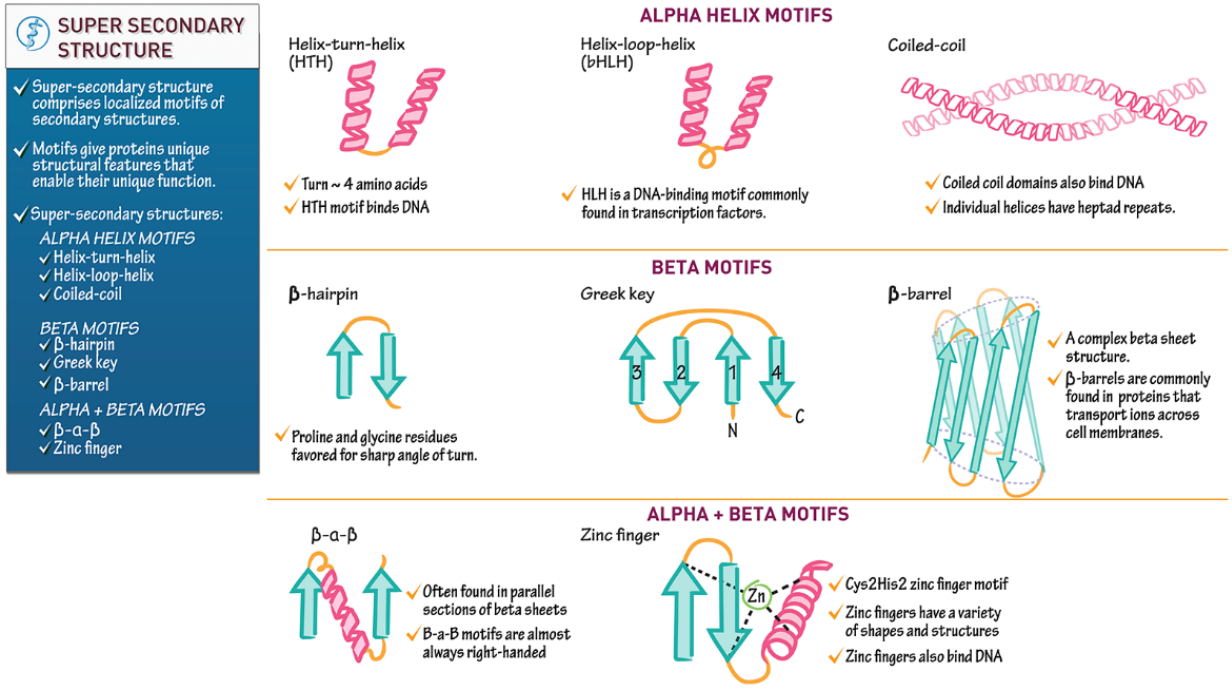
Loop or Coil Conformation

1. Present mainly in globular protein.
2. Connect two Alpha helix or Beta sheath.
3. Present in those area where bend is required.



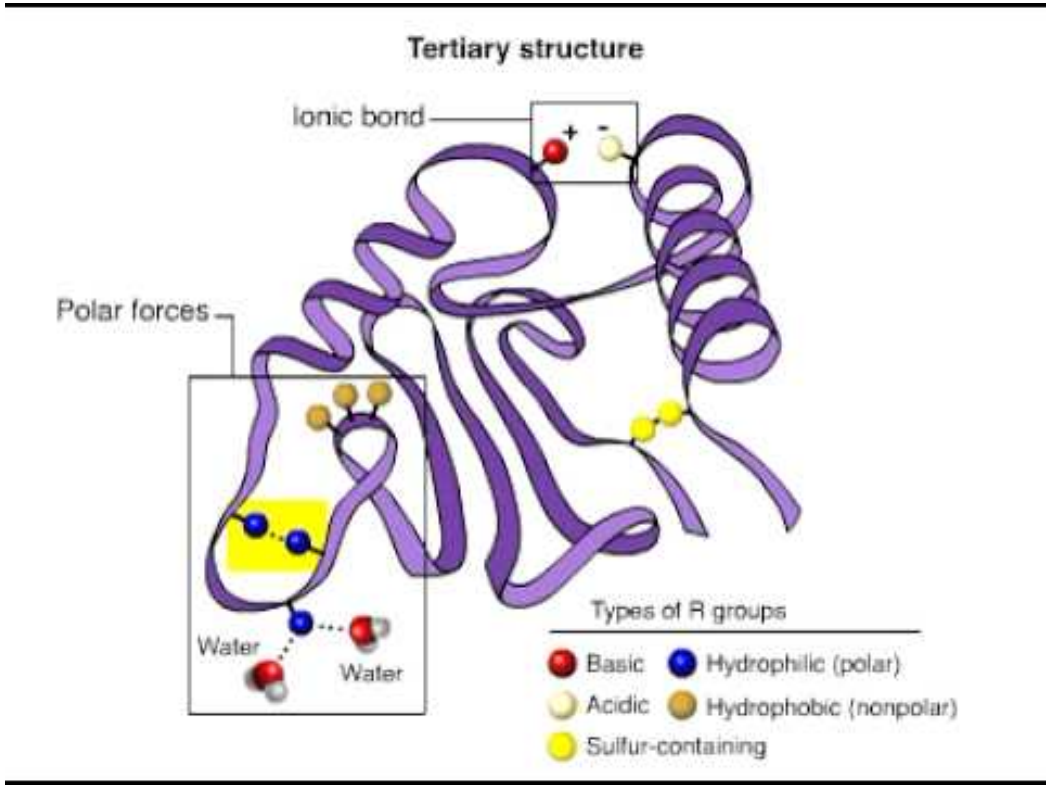
Super secondary Motifs

1. Present in Globular protein.
2. This structure form when two beta pleated sheath are connected to each other by an alpha helix.
3. For example β-α-β supersecondary motif



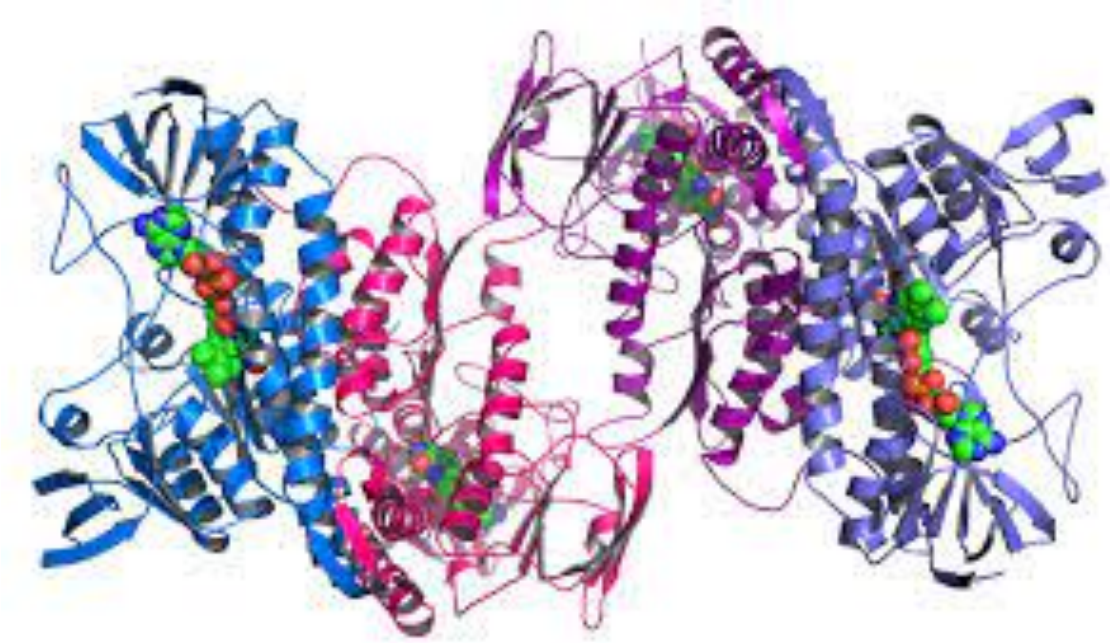
Tertiary structure

1. The tertiary structure mean the overall conformation of a polypeptide.
2. Myoglobin chain is when fully extended its length is 20 time than is width.
3. X-rays diffraction show that its structure is just like a foot ball i.e. globular.
4. The globular structure is due to folding and refolding

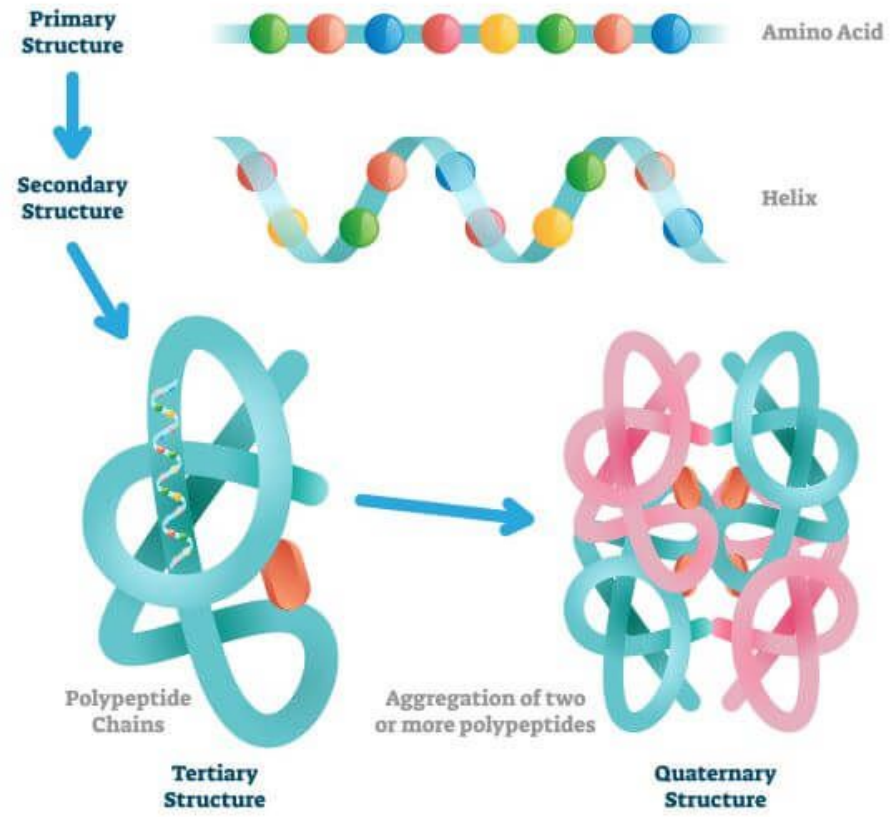


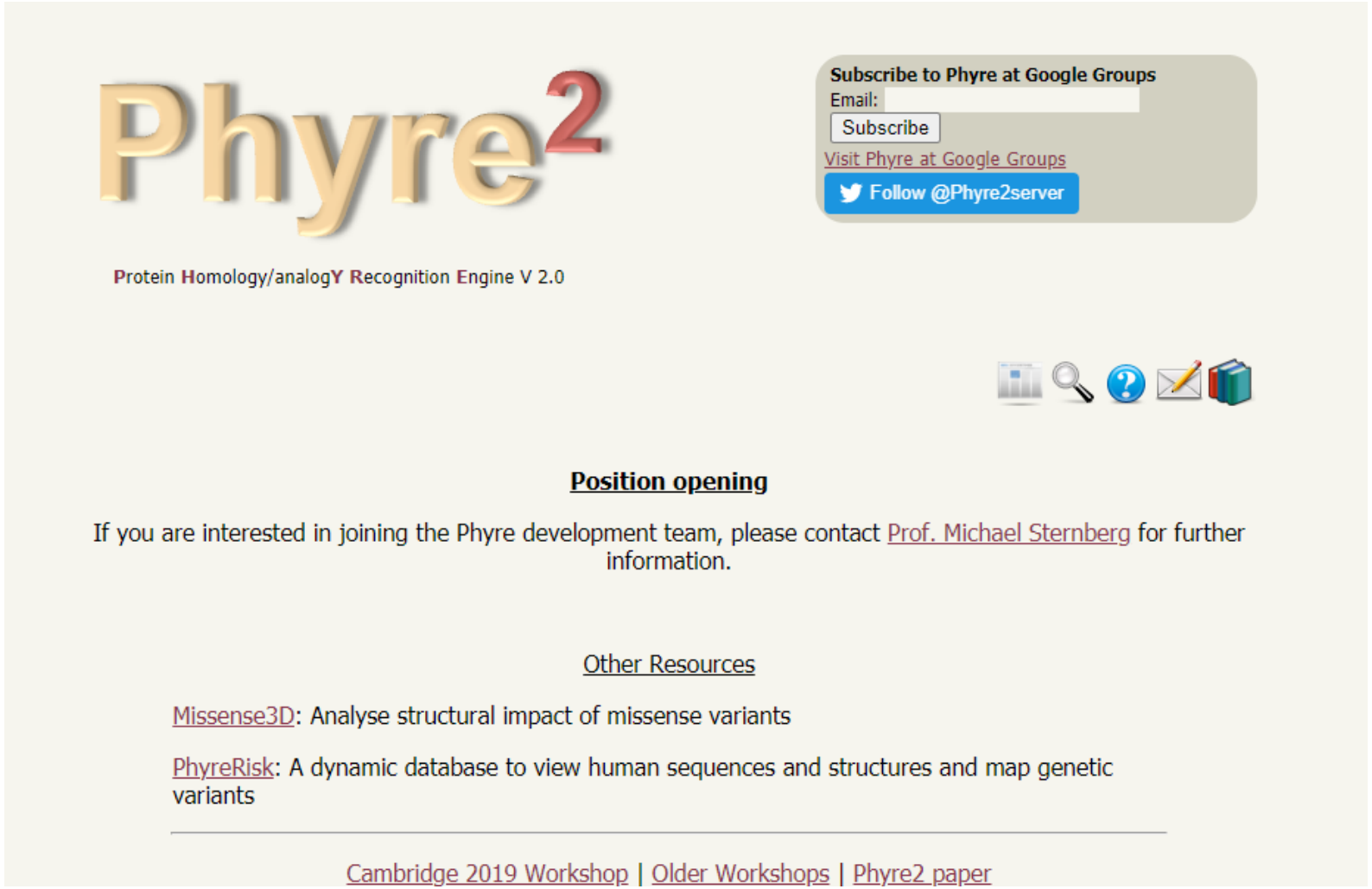
Quaternary Structure

1. Formed by those protein having more than one peptide chain subunit.
2. Each peptide have its own primary, secondary, and tertiary structure.
3. The number and arrangement of the over all structure of the peptide subunit is called quaternary structure.
4. For example structure of Hemoglobin.

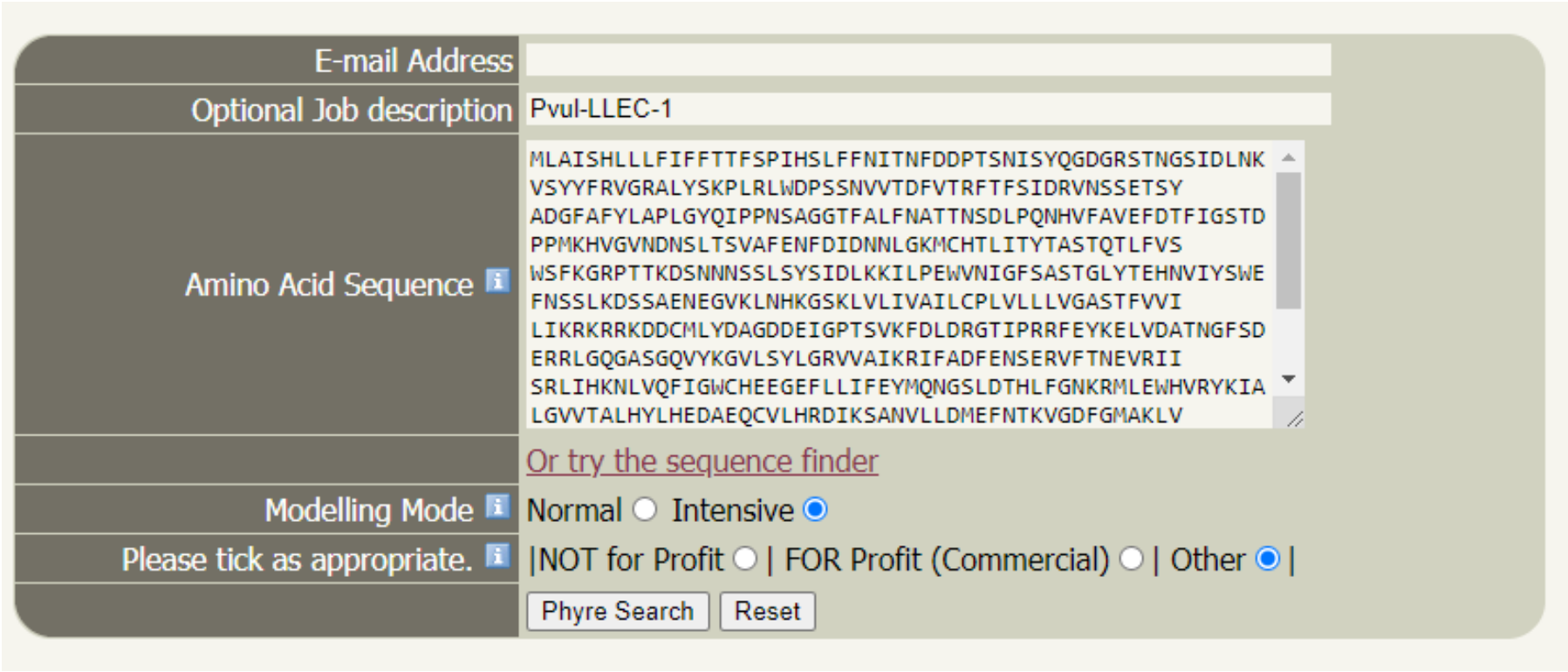


PROTEIN STRUCTURE





- http://www.sbg.bio.ic.ac.uk/phyre2/html/page.cgi?id=index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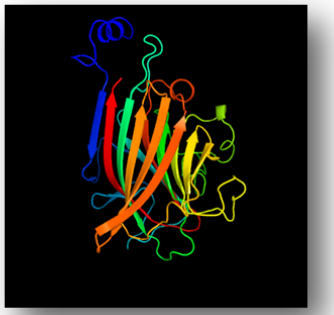
Normal
Intensive
Please tick as appropriate.
|NOT for Profit | FOR Profit (Commercial) | Other |
Phyre Search
Reset



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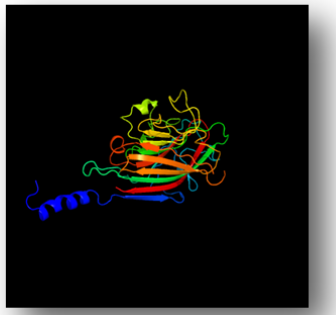
Pvul-BLEC-5



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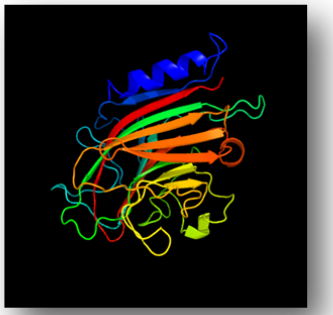

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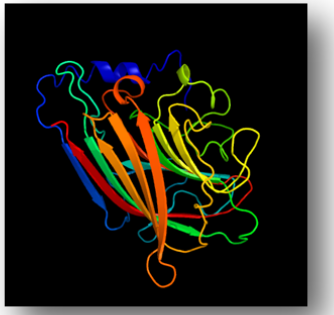

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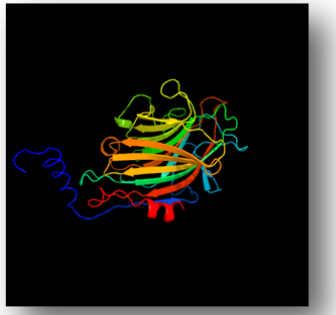

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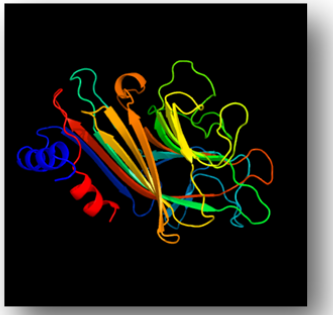

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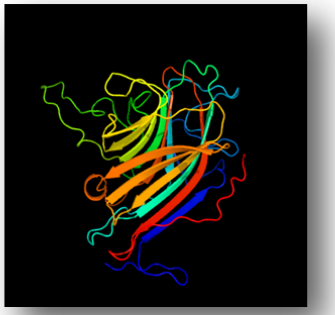

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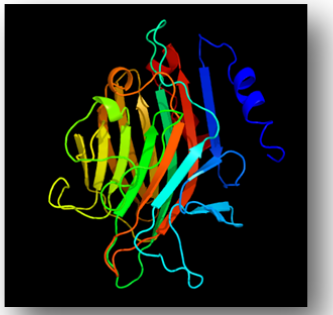

Pvul-BLEC-17

SECONDARY DATABASES

- **Secondary databases** make use of publicly available sequence data in primary **databases** to provide layers of information to DNA or protein sequence data.
- **Secondary databases** comprise data derived from analysing entries in primary **databases**.

- **ExPASy** (**Ex**pert **P**rotein **A**nalysis **Sy**stem)

https://web.expasy.org/protparam/

Expasy

ProtParam

ProtParam tool

ProtParam (References / Documentation) is a tool which allows the computation of various physical and chemical parameters for a given p
user entered protein sequence. The computed parameters include the molecular weight, theoretical pI, amino acid composition, atomic con
life, instability index, aliphatic index and grand average of hydropathicity (GR/

Please note that you may only fill out **one** of the following fields at a time.

Enter a Swiss-Prot/TrEMBL accession number (AC) (for example **P05130**) or

Or you can paste your own amino acid sequence (in one-letter code) in the b

RESET Compute parameters

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Please note that you may only fill out **one** of the following fields at a time.

Enter a Swiss-Prot/TrEMBL accession number (AC) (for example **P05130**) o

Or you can paste your own amino acid sequence (in one-letter code) in the

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RESET | Compute parameters

Expasy

ProtParam

User-provided sequence:

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       130        140        150        160        170        180
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       190        200        210        220        230        240
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```

Dalton

Measure of molecular weight or molecular mass. One molecular hydrogen molecular atom has molecular mass of 1 Da, so 1 Da = 1 g/mol. Proteins and other molecular macromolecule molecular weights are usually measured in molecular kDa or kD (kilodaltons) - 1000 Da. molecular average molecular amino molecular acid = 110 Da.

Protein Isoelectric Point calculates the theoretical **pI** (isoelectric point) for the protein sequence you enter.

Number of amino acids: 667

Molecular weight: 75271.53

Theoretical pI: 6.04

Amino acid composition: CSV format

Ala (A)	35	5.2%
Arg (R)	36	5.4%
Asn (N)	39	5.8%
Asp (D)	39	5.8%
Cys (C)	7	1.0%
Gln (Q)	16	2.4%
Glu (E)	36	5.4%
Gly (G)	45	6.7%
His (H)	19	2.8%
Ile (I)	33	4.9%
Leu (L)	69	10.3%
Lys (K)	29	4.3%
Met (M)	15	2.2%
Phe (F)	41	6.1%
Pro (P)	28	4.2%
Ser (S)	56	8.4%
Thr (T)	39	5.8%
Trp (W)	9	1.3%
Tyr (Y)	25	3.7%
Val (V)	51	7.6%
Pyl (O)	0	0.0%
Sec (U)	0	0.0%
(B)	0	0.0%
(Z)	0	0.0%
(X)	0	0.0%

- The **Instability index** is a measure of proteins, used to determine whether it will be stable in a test tube. If the **index** is less than 40, then it is probably stable in the test tube. If it is greater (for example, enaptin) then it is probably not stable.
- The aliphatic index of a protein is a measure of the relative volume occupied by aliphatic side chain of the following amino acids: alanine, valine, leucine and isoleucine. An increase in the aliphatic index increases the thermostability of globular proteins. The index is calculated by the following formula.
  Aliphatic index = X(Ala) + a*X(Val) + b*X(Leu) + b*(X)Ile$ X(Ala), X(Val), X(Ile) and X(Leu) are the amino acid compositional fractions. The constants a and b are the relative volume of valine (a=2.9) and leucine/isoleucine (b=3.9) side chains compared to the side chain of alanine
- **Grand average of hydropathicity** index (**GRAVY**) is used to represent the hydrophobicity value of a peptide, which calculates the sum of the **hydropathy** values of all the amino acids divided by the sequence length.

```
Instability index:

The instability index (II) is computed to be 32.38
This classifies the protein as stable.


Aliphatic index: 87.06

Grand average of hydropathicity (GRAVY): -0.176
```

ID	*Phaseolus vulgaris* Genomic Database Identifier	Physical position on *P. vulgaris* genome			Protein length (aa)	pI	Molecular weight (Da)	Instability index	Aliphatic index	GRAVY	Stable or unstable	NCBI Accession No.
		Chr.	Start position (bp)	End Position (bp)								
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Pvul-LLEC-4	Phvul.001G040600.1.p	1	4.339.156	4.340.979	607	6.01	67907.43	31.81	94.43	-0.064	stable	XP_007161074.1
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Pvul-LLEC-8	Phvul.001G040100.1.p	1	4.394.207	4.396.266	636	5.62	71103.50	34.65	90.66	-0.154	stable	XP_007161068.1
Pvul-LLEC-9	Phvul.001G040000.1.p	1	4.399.520	4.401.949	666	5.83	74151.24	25.70	88.11	-0.129	stable	XP_007161067.1
Pvul-LLEC-10	Phvul.001G234200.1.p	1	4.880.986	48.811.980	664	8.68	73859.86	33.83	92.30	-0.104	stable	XP_007163432.1
Pvul-LLEC-11	Phvul.002G214900.1.p	2	38.345.248	38.347.335	695	5.85	77309.63	32.79	87.80	-0.128	stable	XP_007159169.1
Pvul-LLEC-12	Phvul.002G215200.1.p	2	38.371.310	38.373.253	647	7.31	72858.74	30.71	85.09	-0.229	stable	XP_007159173.1
Pvul-LLEC-13	Phvul.002G215300.1.p	2	38.383.003	38.384.994	663	7.32	74176.59	31.47	90.89	-0.201	stable	XP_007159174.1
Pvul-LLEC-14	Phvul.002G215400.1.p	2	38.393.780	38.395.786	668	6.75	75537.69	36.90	91.44	-0.147	stable	XP_007159175.1
Pvul-LLEC-15	Phvul.003G204500.1.p	3	43.061.296	43.063.308	670	5.11	73707.66	42.72	86.10	-0.074	unstable	XP_007155476.1
Pvul-LLEC-16	Phvul.005G103200.1.p	5	32.195.113	32.197.596	691	5.99	77701.63	41.04	86.43	-0.115	unstable	XP_007149844.1
Pvul-LLEC-17	Phvul.005G103300.1.p	5	32.198.665	32.200.731	688	6.34	77072.28	34.86	91.89	-0.078	stable	XP_007149845.1
Pvul-LLEC-18	Phvul.006G087700.1.p	6	19.974.245	19.976.281	678	5.75	72719.33	36.68	85.27	-0.040	stable	XP_007146994.1
Pvul-LLEC-19	Phvul.006G185000.1.p	6	28.613.191	28.616.354	692	5.51	78507.66	36.34	89.22	-0.143	stable	XP_007148157.1
Pvul-LLEC-20	Phvul.006G200800.1.p	6	29.750.251	29.752.428	639	6.96	72045.08	36.62	88.17	-0.155	stable	XP_007148350.1
Pvul-LLEC-21	Phvul.007G078200.1.p	7	7.489.146	7.491.182	678	6.24	75420.09	41.56	84.10	-0.087	unstable	XP_007143518.1
Pvul-LLEC-22	Phvul.007G260300.1.p	7	38.169.156	38.172.057	670	6.25	74866.04	36.79	84.51	-0.263	stable	XP_007145693.1
Pvul-LLEC-23	Phvul.007G260400.2.p	7	38.176.633	38.178.637	450	7.61	50666.97	39.48	84.60	-0.294	stable	XP_007145694.1
Pvul-LLEC-24	Phvul.007G260500.1.p	7	38.182.876	38.185.141	657	6.43	72940.88	37.51	88.23	-0.212	stable	XP_007145695.1
Pvul-LLEC-25	Phvul.008G117700.1.p	8	14.407.039	14.409.057	672	7.01	74202.12	34.28	99.33	-0.066	stable	XP_007140498.1
Pvul-LLEC-26	Phvul.008G117800.1.p	8	14.436.075	14.438.400	668	7.32	73975.61	33.83	94.03	-0.115	stable	XP_007140499.1
Pvul-LLEC-27	Phvul.008G239600.1.p	8	58.823.983	58.826.861	699	5.59	74937.86	33.42	87.78	-0.018	stable	XP_007141948.1
Pvul-LLEC-28	Phvul.008G279300.1.p	8	62.071.477	62.073.771	662	6.64	72808.09	38.34	86.56	-0.003	stable	XP_007142422.1
Pvul-LLEC-29	Phvul.010G015800.1.p	10	2.345.298	2.347.358	686	5.74	75220.67	36.40	93.76	-0.068	stable	XP_007134058.1
Pvul-LLEC-30	Phvul.011G119200.1.p	11	18.774.057	18.775.652	531	5.98	59066.39	34.97	94.11	-0.007	stable	XP_007132721.1