JOHANNES KEPLER UNIVERSITÄT LINZ

Genome data analysis
Computer lab session 4

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Overview

- **Protein structure**
- **UniProtKB**
- **ExPASy**
- **PDB – the protein databank**
  - **JSmol**

Overview

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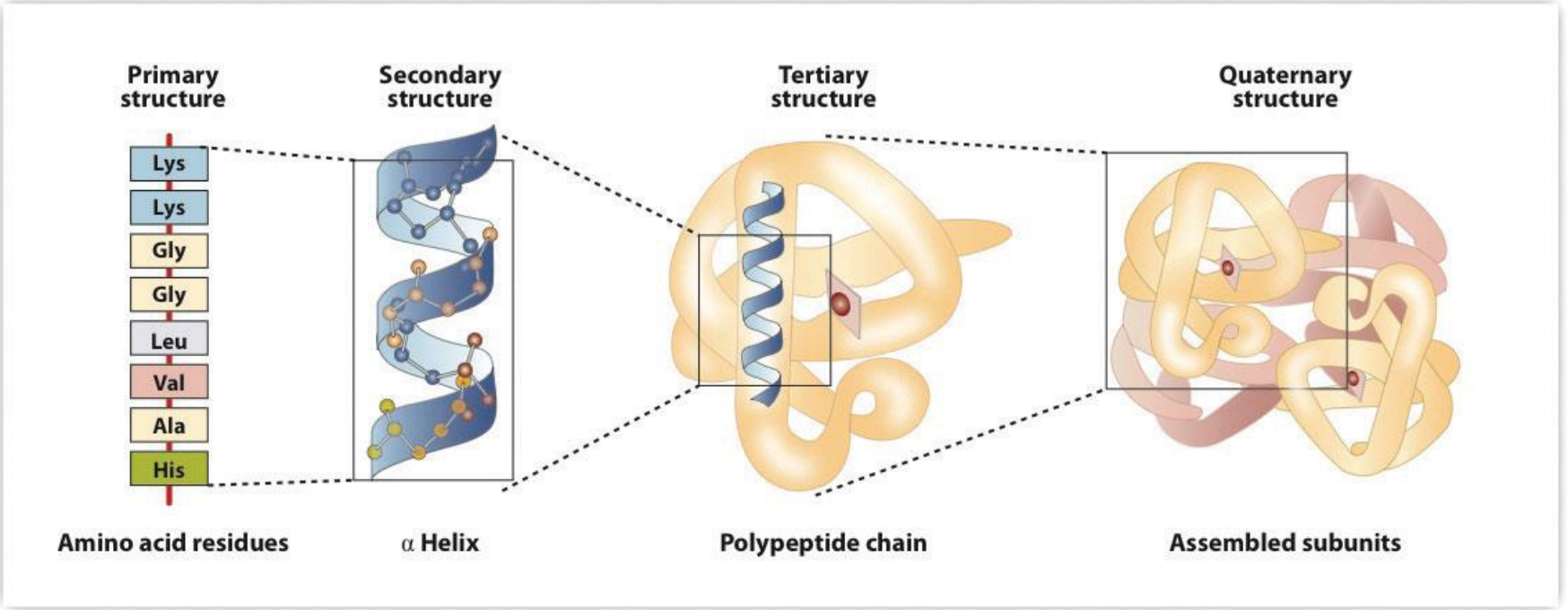
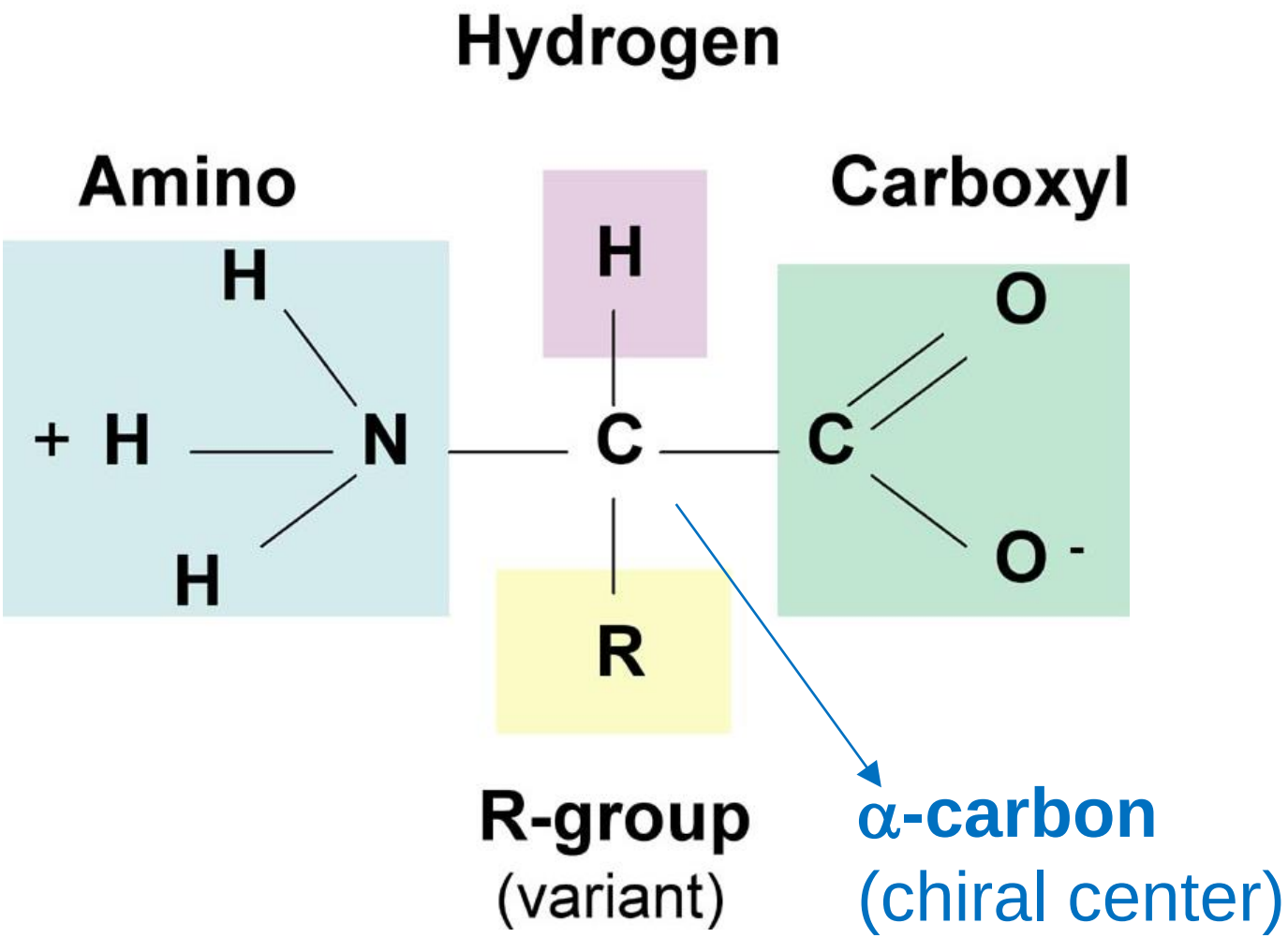
4 levels of protein structure

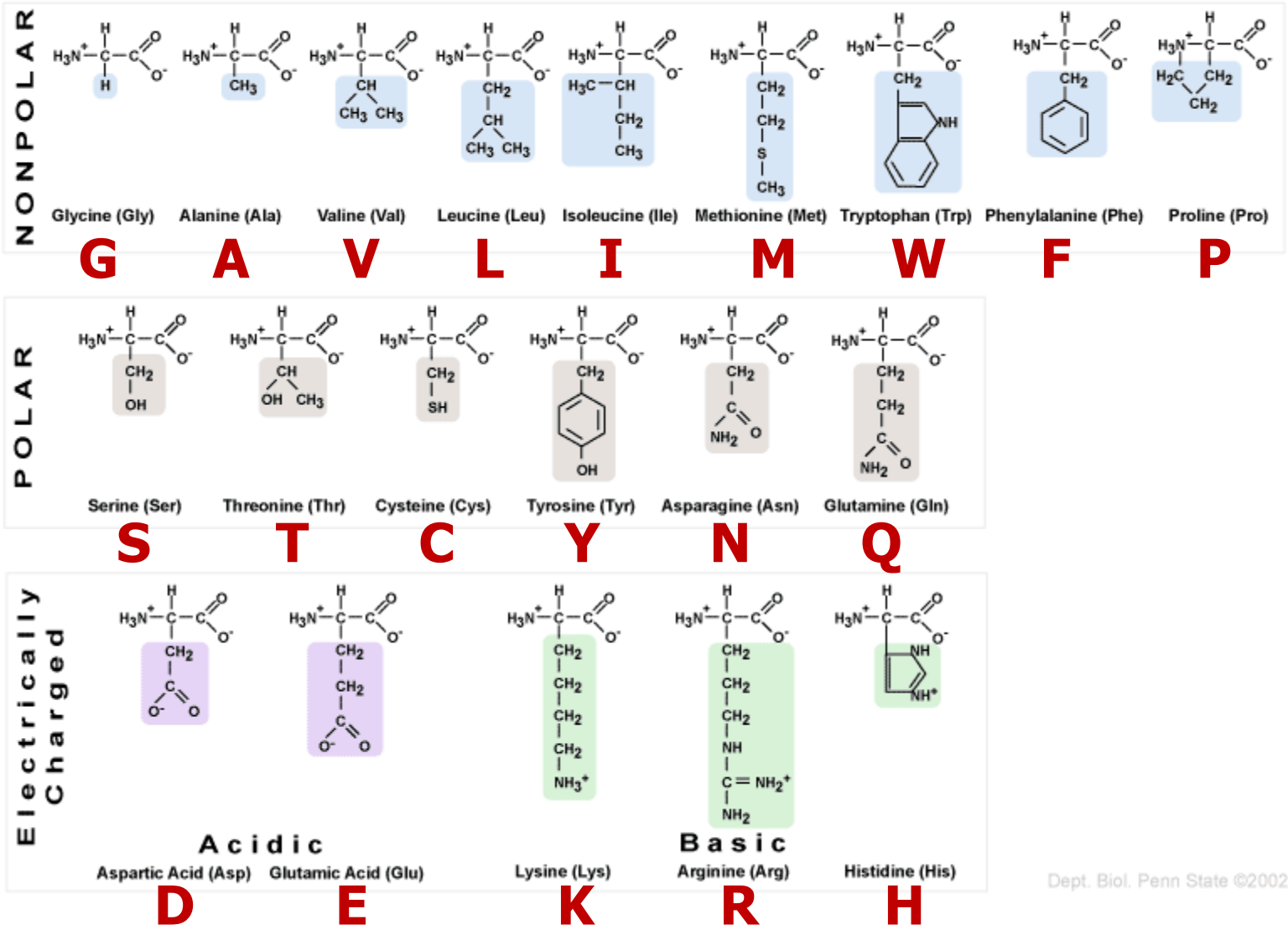


- **Primary structure:** amino acid sequence (peptide bond; polypeptide chain)
- **Secondary structure:** local folding of the polypeptide chain forming regular patterns → α-helices, β-sheets and β-turns (hydrogen bonds)
- **Tertiary structure:** global folding of the polypeptide chain = 3D structure / protein conformation (non-covalent bonds & disulfide bridges)
- **Quaternary structure:** assembly of multiple subunits (polypeptides) forming a big complex (non-covalent bonds & disulfide bridges)

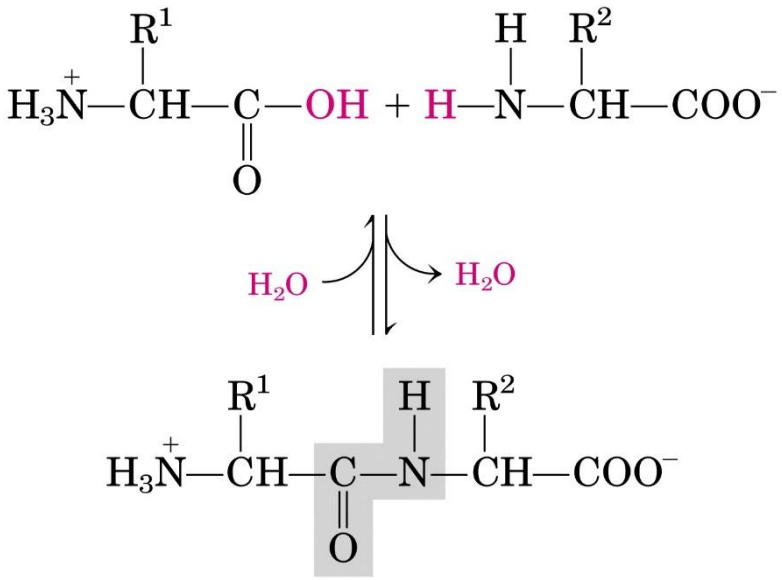
Amino acid structure



Classifications of amino acids



The chemistry of peptide bond formation



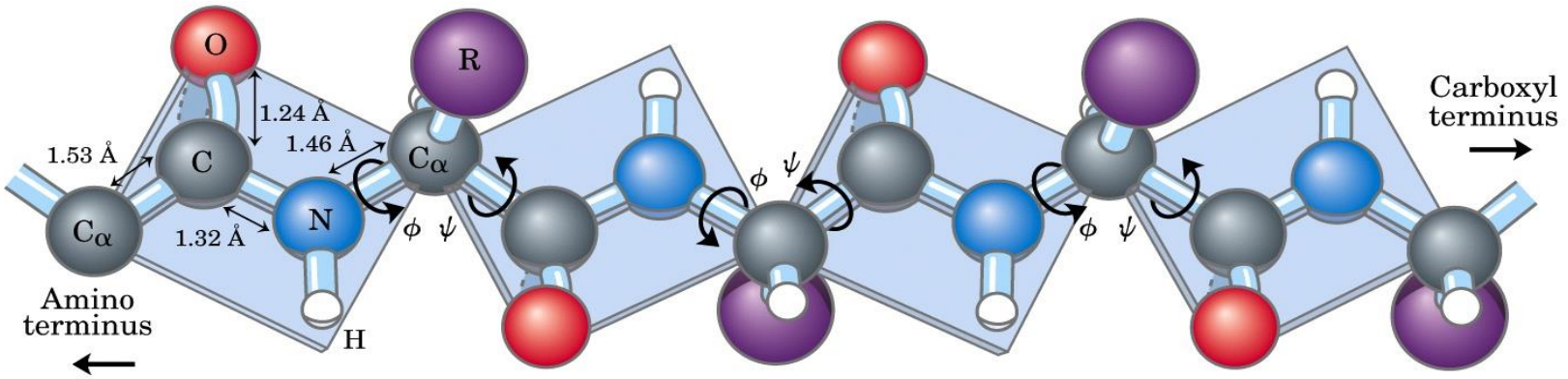
- With the removal of water two amino acids are connected via the carboxy- and amino-groups and a **peptide bond** has been formed

- The C-N bond has a partial double bond character because of delocalization of valence electrons on the nitrogen atom

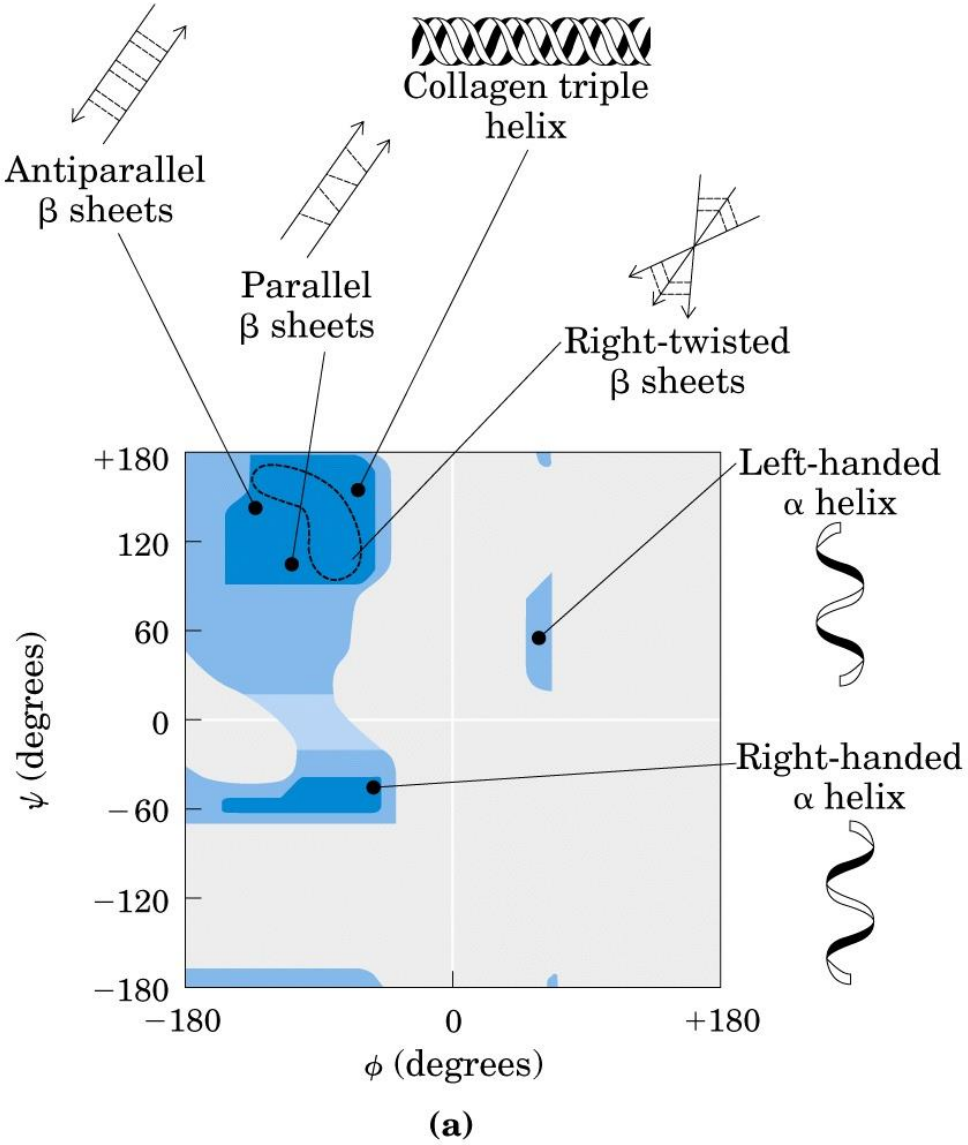
- The peptide bond is **rigid** and **planar**

Angle of rotation (Torsionswinkel)

- **Phi (φ)** – angle of rotation around N-Cα bond
- **Psi (ψ)** – angle of rotation around Cα-C bond
- Most combinations of φ and ψ angles for an amino acid are not allowed because of steric collisions between the side chains and the peptide backbone.
- The angle pairs are usually plotted against each other in a diagram called a **Ramachandran plot** showing sterically allowed regions



Ramachandran plot

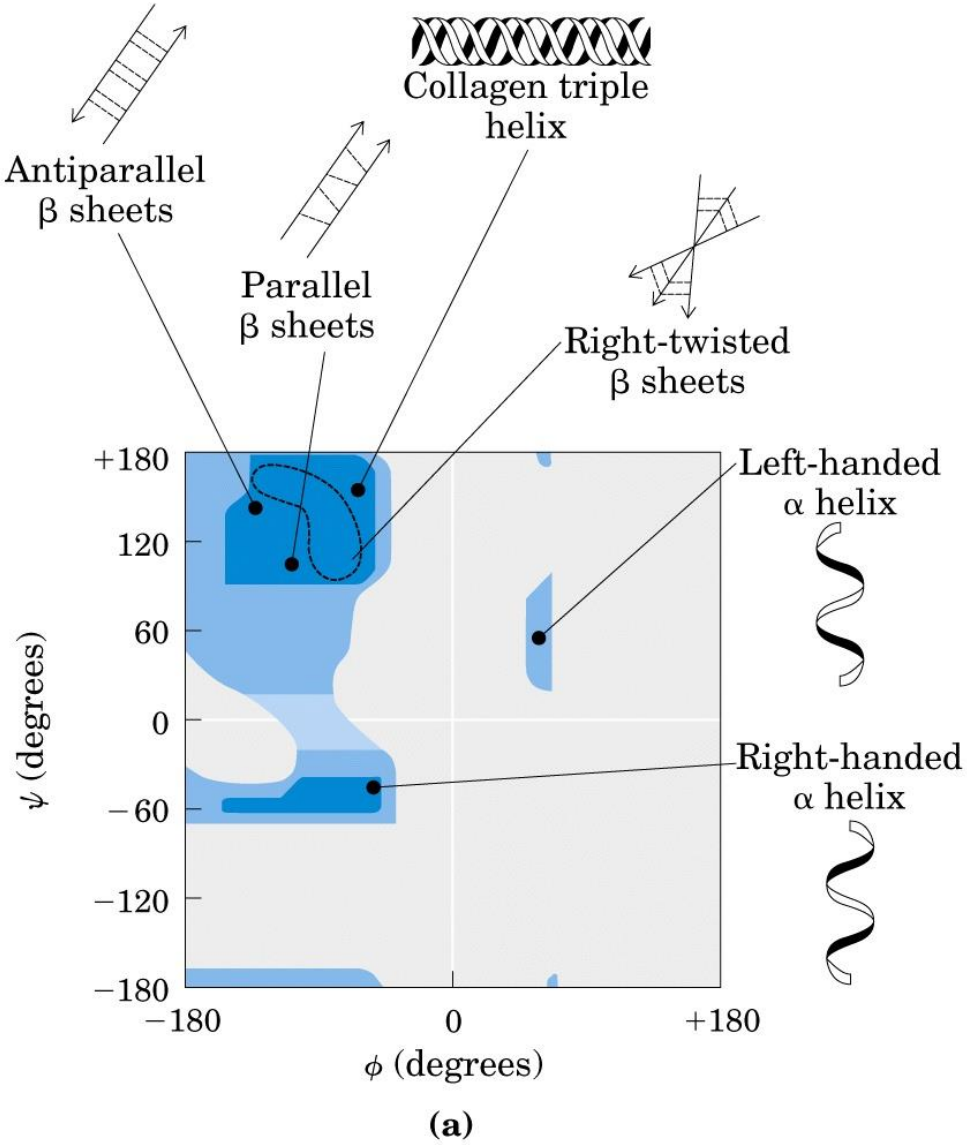


The conformation of the polypeptide chain of a protein is determined by two angles: phi (φ) and psi (ψ).

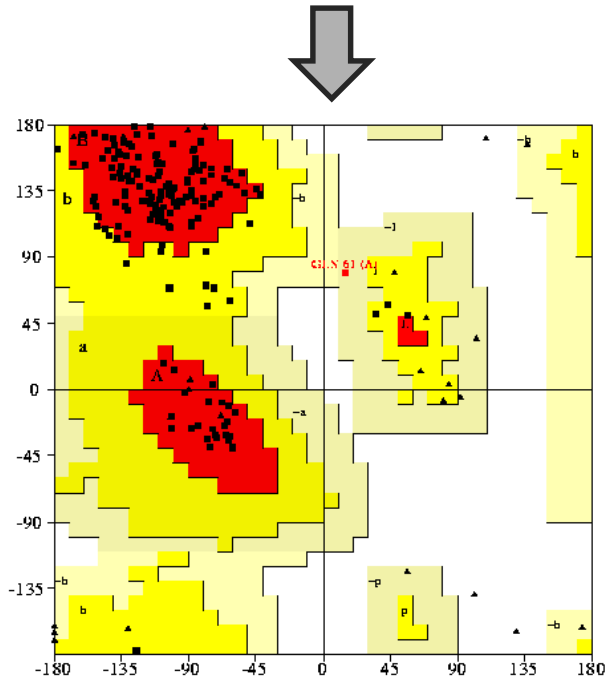
Only certain combinations of these angles are allowed because of **steric hindrance** between main-chain atoms and side-chain atoms, except for glycine.

The Ramachandran plot shows **allowed combinations** of the conformational angles phi (φ) and psi (ψ).

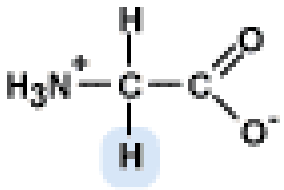
Ramachandran plot



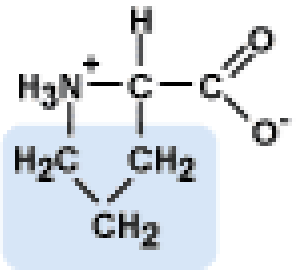
Distribution of the phi (φ) and psi (ψ) angles for 121,870 residues of 463 known protein structures.



Two special amino acids



- **Glycine**, with only a hydrogen atom as a side chain, can adopt a much wider range of conformations than the other residues. It allows unusual main-chain conformations in proteins. This is one of the main reasons why a high proportion of glycine residues are conserved among homologous protein sequences.



- **Proline** is said to be a helix breaker: proline destabilizes α-helices because of its irregular geometry; the side chain forms a ring with the amide group, which causes steric hindrance.

- **Proline** and **Glycine** are frequently found in beta turns. Proline because its cyclic structure is ideally suited for the beta turn, and glycine because with the smallest side chain of all the amino acids, it is the most sterically flexible.

Domains and Motifs

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- **Domain:**
  - A domain is a conserved part of a protein that forms a compact three-dimensional structure. A domain **can function independently** from the rest of the protein chain.
  - Many proteins consist of several domains.
  - One domain can occur in many different proteins. (Possible homology)

- **Motif:**
  - a short, conserved region of a protein: typically 5 to 20 contiguous amino acid residues
  - mostly **recognition sequences** for other proteins (proteases, ubiquitin ligases, kinases,…)
  - does not imply homology

common human protein domains

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Zinc finger, C2H2 type	1093 proteins
Immunoglobulin	1032
EGF-like	471
Homeobox	417
Pleckstrin-like	405
RNA-binding region RNP-1	400
SH3	394
Calcium-binding EF-hand	392
Fibronectin, type III	300
PDZ/DHR/GLGF	280
Small GTP-binding protein	261
BTB/POZ	236
Cadherin	226

Classes of proteins

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- **Function**
  - Enzymes: Catalyze biochemical reactions
  - Structural: Form biological structures
  - Transport: Carry biochemically important substances
  - Defense: Protect the body from foreign invaders
- **Structure**
  - Globular: Complex folds, irregularly shaped tertiary structures
  - Fibrous: Extended, simple folds $\rightarrow$ generally structural proteins
- **Cellular localization**
  - Membrane: In direct physical contact with a membrane; generally water insoluble.
  - Soluble: Water soluble; can be anywhere in the cell.

Co- and Post-translational modifications

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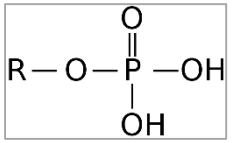
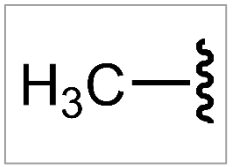
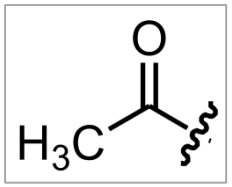
- **Phosphorylation:** on **serine**, **threonine** or **tyrosine** residues
  - important for the regulation of many cellular processes (cell cycle, growth, apoptosis…)
  - chromatin modification (histones)
  - kinases and phosphatases



- **Methylation:** on **lysine** and **arginine**
  - chromatin modification (histones)
  - methyltransferases and demethylases



- **Acetylation:** on **lysine**
  - chromatin modification (histones)
  - histone acetyltransferases (HATs) and histone deacetylases (HDACs).



- **N-terminal acetylation:** N-terminal methionine is replaced by an acetyl group
  - functional regulation
  - irreversible
  - methionine aminopeptidase (MAP) removes methionine and N-acetyltransferase (NAT) adds acetyl group

Co- and Post-translational modifications

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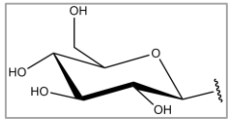
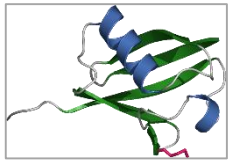
- **Glycosylation:** N-linked on **asparagine** or O-linked on **serine** or **threonine**
  - important for protein folding and stability
  - Glycosylases and deglycosylases



- **(Poly-)Ubiquitinylation:** on **lysine**
  - mark for degradation
  - Ubiquitin ligases and deubiquitinating enzymes (DUBs)



- **Proteolytic cleavage:** Proteases cut the peptide bond at a certain sequence.

- **Disulfid bonds** covalently link the sulfur atoms of two different cysteine residues (intermolecular or intramolecular).

3D structures

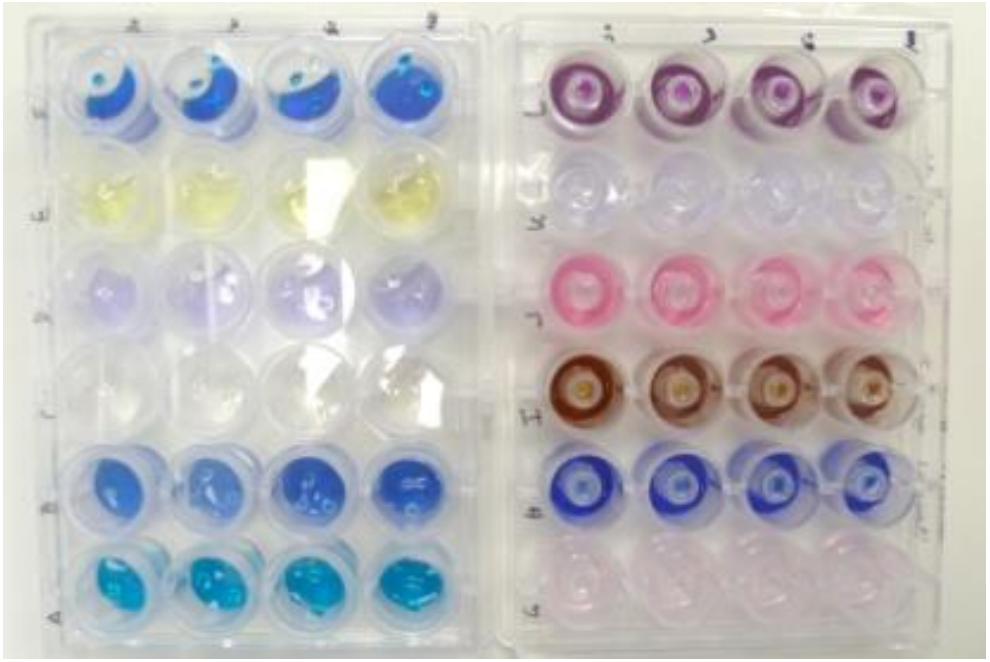
- **The tertiary structure is a good indicator of homology**
  - How is the 3D structure of a protein determined?

Main approaches:

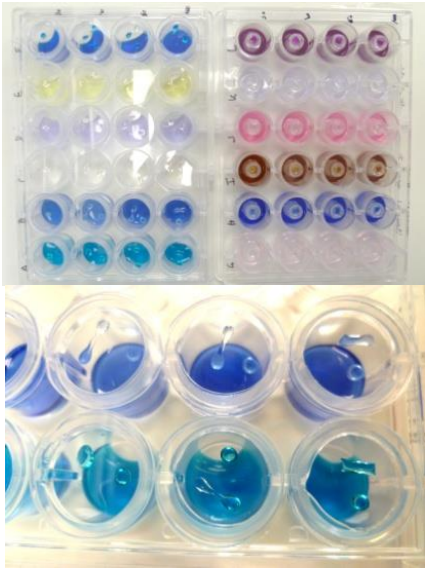
- Experimental determination
  - X-ray crystallography
  - Nuclear magnetic resonance (NMR) spectroscopy
  - Electron microscopy

X-ray crystallography

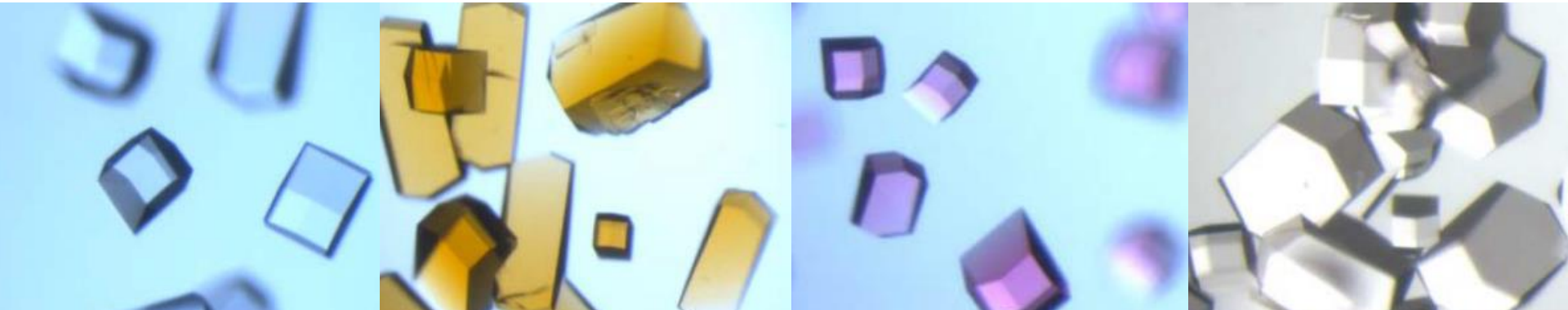
- X-ray crystallography is used to **solve the atomic and molecular structure of proteins**.
- Requirements: your protein of interest must be VERY pure and concentrated to get crystalized
- The growth of protein crystals can be tricky!



Crystallization by vapor diffusion



- The aim is to obtain a supersaturated solution → **vapour diffusion**: extract water from drops
- *Hanging or Sitting-drop method*: Drops sit on top, or hang on the wall of an airtight container. The droplet contains the purified protein, buffer, and precipitant at low concentrations. It can equilibrate with a larger reservoir in the container having high buffer and precipitant concentrations.
- as **water vaporizes from the drop** the precipitant concentration increases to an optimum level so that the protein crystalizes. Since the system is in equilibrium, these optimum conditions are maintained until the crystallization is complete.



X-ray crystallography

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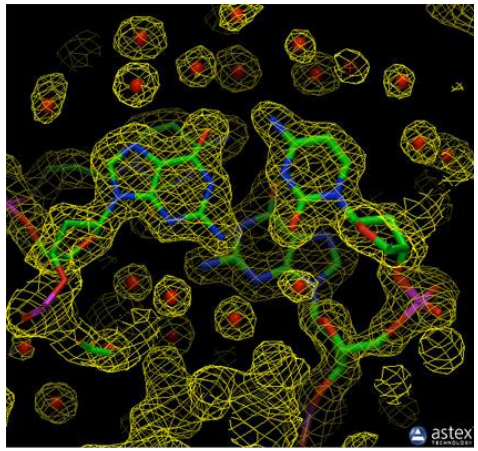
- Analysis of diffraction patterns (=Beugungsdiagramme):

  incident X-rays are diffracted by the crystalline atoms of the protein into many specific directions. By measuring the angles and intensities of these diffracted beams, a crystallographer can produce a three-dimensional picture of the density of electrons within the crystal. From this electron density, the mean positions of the atoms as well as the chemical bonds in the crystal can be determined.



- Best resolution → individual atoms and electron clouds
- Today 80% of protein structures are solved by crystallography

NMR and Electron Microscopy

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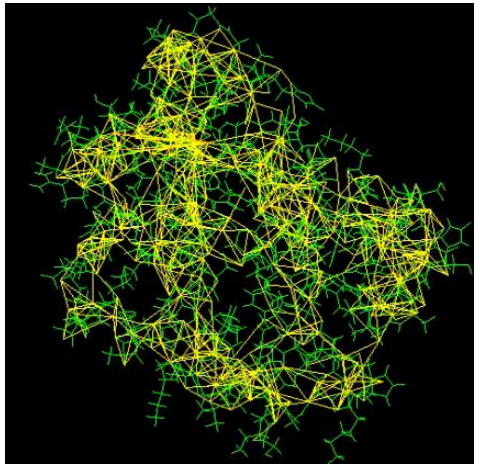
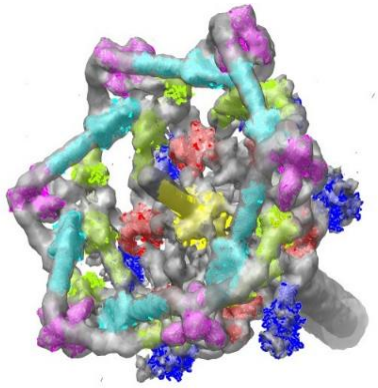
NMR:

- Magnetic field applied to proteins in solution
- Does not require crystallization
- Medium resolution → data on local conformation and distance between atoms (but no individual atoms)



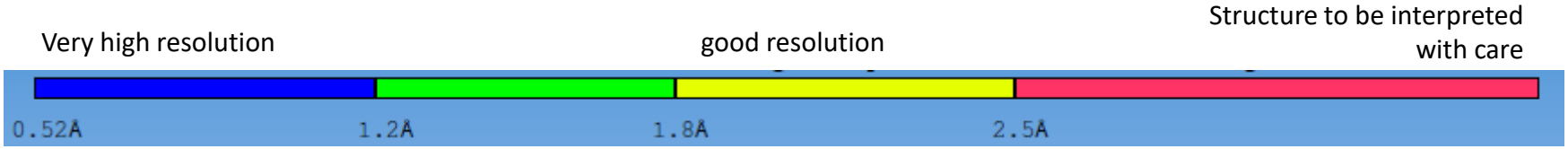
Electron Microscopy:

- Electron microscopy uses accelerated electrons as a source of illumination. Use of small crystals
- Low resolution → image of the overall shape of the protein



Resolution

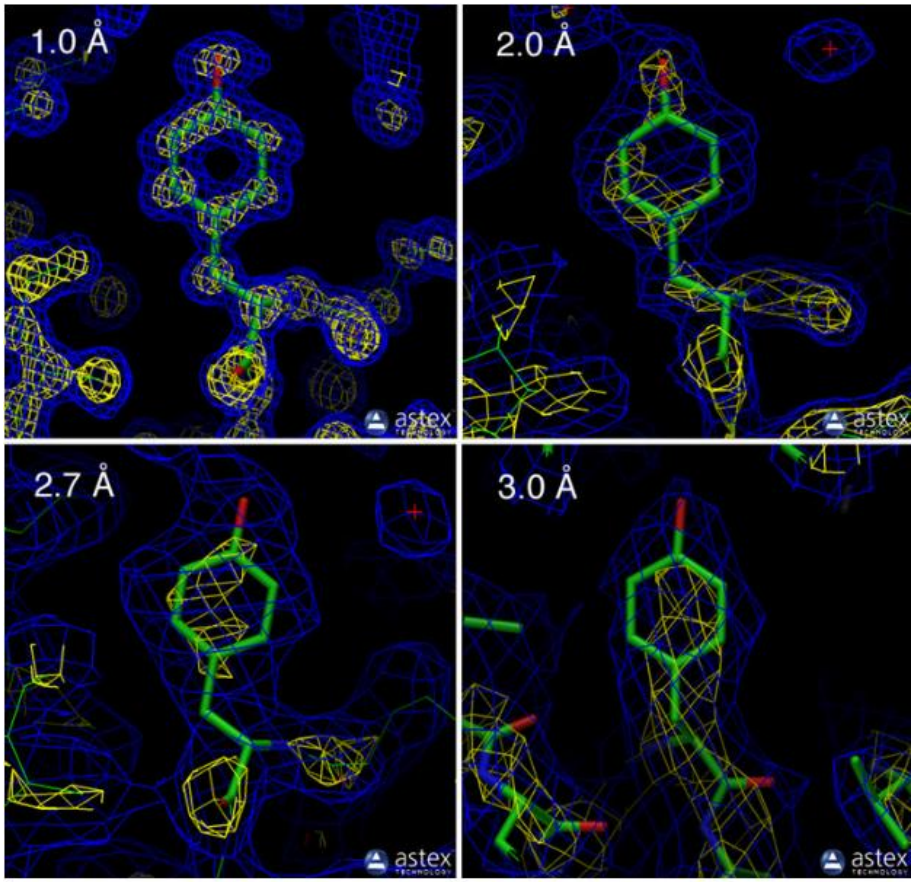
- Definition: Resolution is the minimum detectable distance between two distinguishable items



- High-resolution structures, with resolution values of ~1Å, are highly ordered and it is easy to see **every atom** in the electron density map.

1Å=0.1nm

- Lower resolution structures, with resolutions of 3 Å or higher, show only the **basic contours of the protein chain**, and the atomic structure must be inferred.



Resolution and R-value

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- The R-value is the measure of the **quality** of the atomic model obtained from the crystallographic data.
- When solving the structure of a protein, the researcher first builds an atomic model and then calculates a simulated diffraction pattern based on that model.
- The R-value measures how well the **simulated** diffraction pattern matches the **experimentally-observed** diffraction pattern.
- A totally random set of atoms will give an R-value of about **0.63**, whereas a perfect fit would have a value of **0**.
- Typical values are about **0.20**

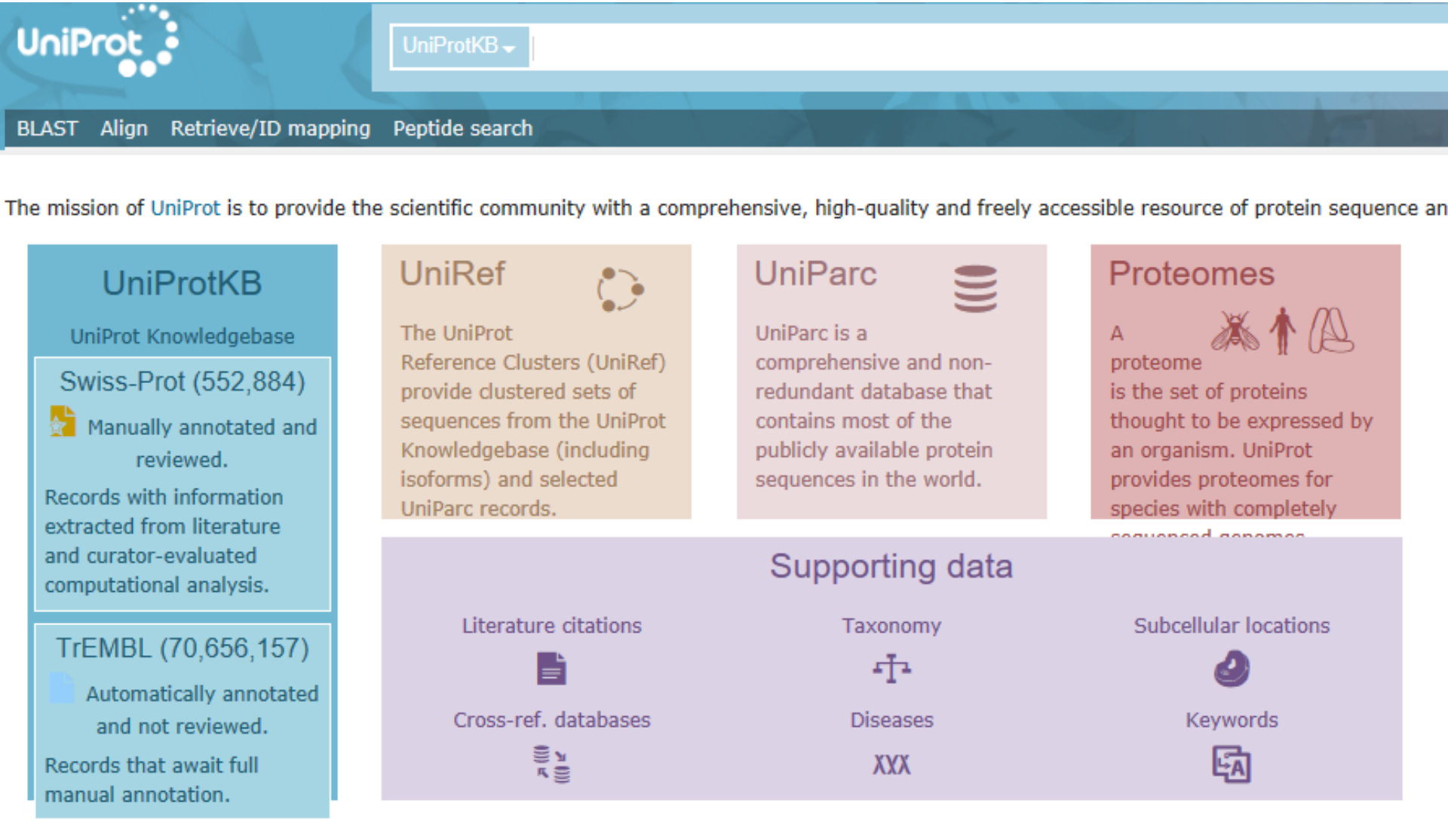
Overview

- Protein structure
- **UniProtKB**
- ExPASy
- PDB – the protein databank
  - JSmol

UniProtKB

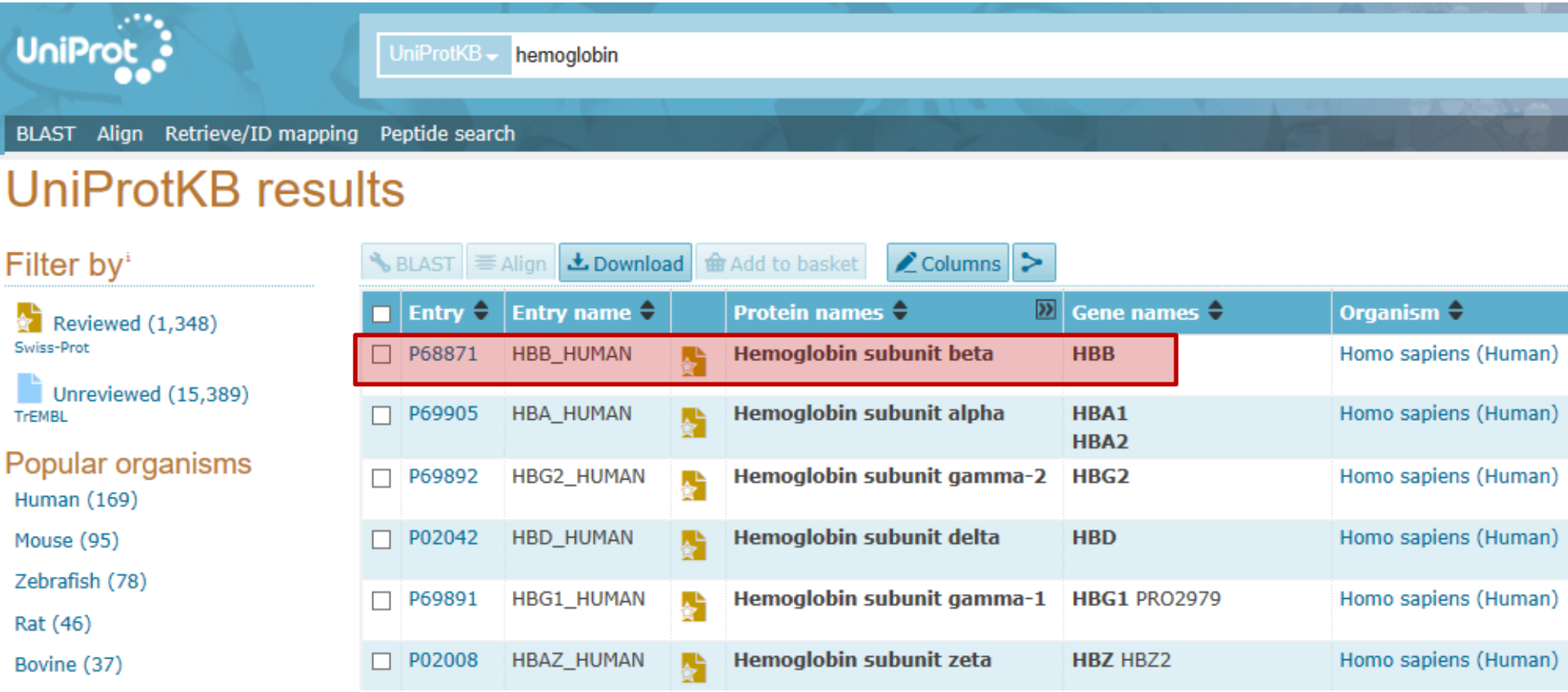
www.uniprot.org

to analyze amino acid sequences



UniProtKB

- Search for hemoglobin and select the first entry → **hemoglobin subunit beta (HBB)**



UniProtKB

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UniProtKB - P68871 (HBB_HUMAN)

Display

- Entry
- Publications
- Feature viewer
- Feature table

None

- Function
- Names & Taxonomy
- Subcellular location
- Pathology & Biotech
- PTM / Processing
- Expression
- Interaction
- Structure
- Family & Domains
- Sequence
- Cross-references
- Entry information
- Miscellaneous
- Similar proteins

Top

BLAST | Align | Format | Add to basket | History

Feedback | Help video

Protein **Hemoglobin subunit beta**

Gene **HBB**

Organism *Homo sapiens (Human)*

Status Reviewed - Annotation score: ●●●●● - Experimental evidence at protein level[i]

Function[i]

Involved in oxygen transport from the lung to the various peripheral tissues.
LVV-hemorphin-7 potentiates the activity of bradykinin, causing a decrease in blood pressure.
Spinorphin: functions as an endogenous inhibitor of enkephalin-degrading enzymes such as DPP3, and as a selective antagonist of the P2RX3 receptor which is invol
properties implicate it as a regulator of pain and inflammation.

Sites

Feature key	Position(s)	Length	Description	Graphical view	Featu
Binding site[i]	2 – 2	1	2,3-bisphosphoglycerate; via amino nitrogen		
Binding site[i]	3 – 3	1	2,3-bisphosphoglycerate		
Metal binding[i]	64 – 64	1	Iron (heme distal ligand)		
Binding site[i]	83 – 83	1	2,3-bisphosphoglycerate		
Metal binding[i]	93 – 93	1	Iron (heme proximal ligand)		
Binding site[i]	144 – 144	1	2,3-bisphosphoglycerate		

GO - Molecular function[i]

- heme binding Source: InterPro
- hemoglobin binding Source: UniProtKB
- iron ion binding Source: InterPro

UniProtKB

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GO - Molecular function

- heme binding — Source: InterPro
- hemoglobin binding — Source: UniProtKB
- iron ion binding — Source: InterPro
- oxygen binding — Source: UniProtKB
- oxygen transporter activity — Source: UniProtKB

GO - Biological process

- bicarbonate transport — Source: Reactome
- blood coagulation — Source: Reactome
- cellular oxidant detoxification — Source: GOC
- hydrogen peroxide catabolic process — Source: BHF-UCL
- nitric oxide transport — Source: UniProtKB
- oxygen transport — Source: UniProtKB
- platelet aggregation — Source: UniProtKB
- positive regulation of cell death — Source: BHF-UCL
- positive regulation of nitric oxide biosynthetic process — Source: UniProtKB
- protein heterooligomerization — Source: BHF-UCL
- receptor-mediated endocytosis — Source: Reactome
- regulation of blood pressure — Source: UniProtKB-KW
- regulation of blood vessel size — Source: UniProtKB-KW

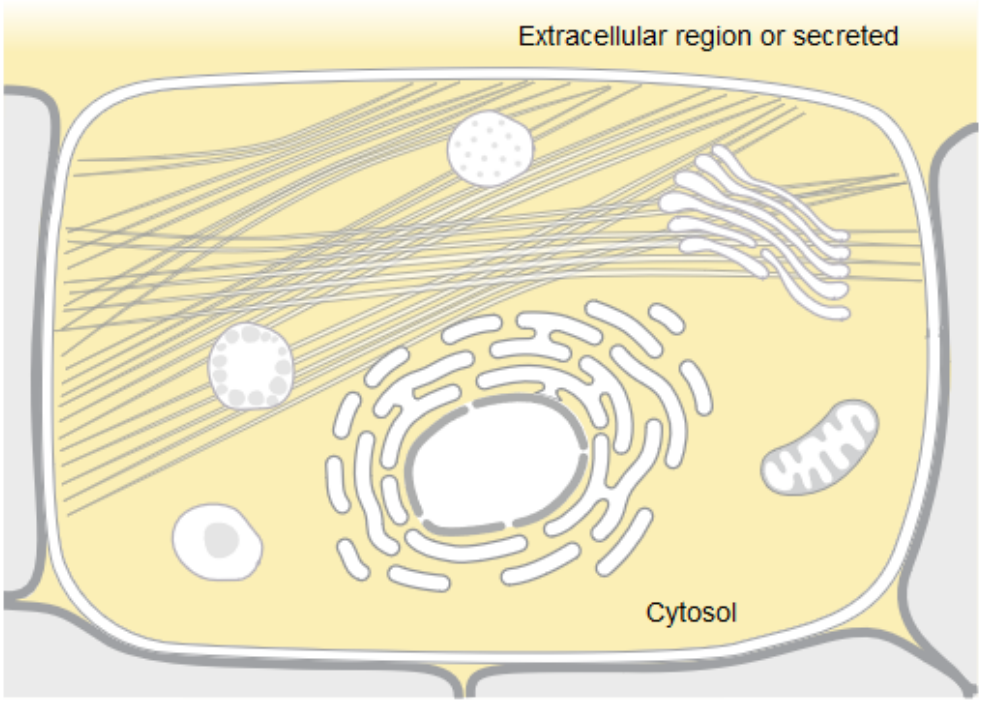
Subcellular location

GO - Cellular component

- blood microparticle — Source: UniProtKB
- cytosol — Source: Reactome
- endocytic vesicle lumen — Source: Reactome
- extracellular exosome — Source: UniProtKB
- extracellular region — Source: Reactome
- haptoglobin-hemoglobin complex — Source: BHF-UCL
- hemoglobin complex — Source: UniProtKB

Complete GO annotation...

Subcellular location



Graphics by Christian Stolte; Source: COMPARTMENTS

Manual annotation | Automatic computational assertion

GO - Cellular component

Cytosol

cytosol — Source: Reactome
hemoglobin complex — Source: BHF-UCL

Extracellular region or secreted

blood microparticle — Source: UniProtKB
extracellular exosome — Source: UniProtKB
extracellular region — Source: Reactome
extracellular space — Source: UniProtKB

Other locations

endocytic vesicle lumen — Source: Reactome
ficolin-1-rich granule lumen — Source: Reactome
haptoglobin-hemoglobin complex — Source: BHF-UCL
tertiary granule lumen — Source: Reactome

View the complete GO annotation on QuickGO ...

Pathology & Biotech

Involvement in disease

Heinz body anemias (HEIBAN) 4 Publications

The disease may be caused by mutations affecting the gene represented in this entry.
Disease description: Form of non-spherocytic hemolytic anemia of Dacie type 1. After splenectomy, which has little benefit, basophilic inclusions called Heinz bodies are demonstrable in the erythrocytes. Before splenectomy, diffuse or punctate basophilia may be evident. Most of these cases are probably instances of hemoglobinopathy. The hemoglobin demonstrates heat lability. Heinz bodies are observed also with the Ivemark syndrome (asplenia with cardiovascular anomalies) and with glutathione peroxidase deficiency.
See also OMIM:140700

Beta-thalassemia (B-THAL) 6 Publications

The disease is caused by mutations affecting the gene represented in this entry.
Disease description: A form of thalassemia. Thalassemias are common monogenic diseases occurring mostly in Mediterranean and Southeast Asian populations. The hallmark of beta-thalassemia is an imbalance in globin-chain production in the adult HbA molecule. Absence of beta chain causes beta(0)-thalassemia, while reduced amounts of detectable beta globin causes beta(+)-thalassemia. In the severe forms of beta-thalassemia, the excess alpha globin chains accumulate in the developing erythroid precursors in the marrow. Their deposition leads to a vast increase in erythroid apoptosis that in turn causes ineffective erythropoiesis and severe microcytic hypochromic anemia. Clinically, beta-thalassemia is divided into thalassemia major which is transfusion dependent, thalassemia intermedia (of intermediate severity), and thalassemia minor that is asymptomatic.
See also OMIM:613985

Feature key	Position(s)	Description	Actions	Graphical view	Length
Natural variant (VAR_002907)	27	E → K in B-THAL; Hb E; confers resistance to severe malaria. 4 Publications Corresponds to variant dbSNP:rs33950507	Ensembl, ClinVar.		1
Natural variant (VAR_010145)	115	L → P in B-THAL; Durham-N.C./Brescia. 3 Publications Corresponds to variant dbSNP:rs36015961	Ensembl, ClinVar.		1
Natural variant (VAR_003037)	116	A → D in B-THAL; Hradec Kralove; unstable. 1 Publication Corresponds to variant dbSNP:rs35485099	Ensembl, ClinVar.		1
Natural variant (VAR_003056)	127	V → G in B-THAL; Dhonburi/Neapolis; unstable. 1 Publication Corresponds to variant dbSNP:rs33925391	Ensembl, ClinVar.		1

Sickle cell anemia (SKCA) 5 Publications

The disease is caused by mutations affecting the gene represented in this entry.
Disease description: Characterized by abnormally shaped red cells resulting in chronic anemia and periodic episodes of pain, serious infections and damage to vital organs. Normal red blood cells are round and flexible and flow easily through blood vessels, but in sickle cell anemia, the abnormal hemoglobin (called Hb S) causes red blood cells to become stiff. They are C-shaped and resembles a sickle. These stiffer red blood cells can led to microvascular occlusion thus cutting off the blood supply to nearby tissues.
See also OMIM:603903

Feature key	Position(s)	Description	Actions	Graphical view	Length
Natural variant (VAR_002863)	7	E → V in SKCA; Hb S; at heterozygosity confers resistance to malaria. 3 Publications Corresponds to variant dbSNP:rs334	Ensembl, ClinVar.		1

Beta-thalassemia, dominant, inclusion body type (B-THALIB) 1 Publication

The disease is caused by mutations affecting the gene represented in this entry.
Disease description: An autosomal dominant form of beta thalassemia characterized by moderate anemia, lifelong jaundice, cholelithiasis and splenomegaly, marked morphologic changes in the red cells, erythroid hyperplasia of the bone marrow with increased numbers of multinucleate red cell precursors, and the presence of large inclusion bodies in the normoblasts, both in the marrow and in the peripheral blood after splenectomy.
See also OMIM:603902

PTM / Processing

PTM = Post-translational modifications

Molecule processing

Feature key	Position(s)	Length	Description	Graphical view	Feature identifier
Initiator methionine			Removed By similarity 1 Publication		
Chain	2 – 147	146	Hemoglobin subunit beta		PRO_0000052976
Peptide	33 – 42	10	LVV-hemorphin-7		PRO_0000296641
Peptide	33 – 39	7	Spinorphin		PRO_0000424226

Amino acid modifications

Feature key	Position(s)	Length	Description	Graphical view	Feature identifier
Modified residue	2 – 2	1	N-acetylvaline By similarity		
Modified residue	2 – 2	1	N-pyruvate 2-iminyl-valine; in Hb A1b		
Glycosylation	2 – 2	1	N-linked (Glc) (glycation); in Hb A1c		
Glycosylation	9 – 9	1	N-linked (Glc) (glycation)		
Modified residue	10 – 10	1	Phosphoserine Combined sources		
Modified residue	13 – 13	1	Phosphothreonine Combined sources		
Glycosylation	18 – 18	1	N-linked (Glc) (glycation)		
Modified residue	45 – 45	1	Phosphoserine Combined sources		
Modified residue	51 – 51	1	Phosphothreonine Combined sources		
Modified residue	60 – 60	1	N6-acetyllysine 1 Publication		
Glycosylation	67 – 67	1	N-linked (Glc) (glycation)		

Expression

Tissue specificity
Red blood cells. 1 Publication

Gene expression databases

Bgee	ENSG00000244734.
ExpressionAtlas	P68871. baseline and differential.
Genevisible	P68871. HS.

Organism-specific databases

HPA	CAB009526. HPA043234.

Interaction

Subunit structure
Heterotetramer of two alpha chains and two beta chains in adult hemoglobin A (HbA). Heterotetramer of two zeta chains and two beta chains in hemoglobin Portland-2, detected in fetuses and neonates with homozygous alpha-thalassemia. 3 Publications

Binary interactions

With	Entry	#Exp.	IntAct	Notes
HBA2	P69905	20	EBI-715554,EBI-714680	
HBZ	P02008	2	EBI-715554,EBI-719843	

Protein-protein interaction databases

BioGrid	109293. 54 interactions.
DIP	DIP-35526N.

UniProtKB

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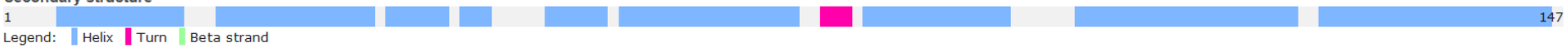
Structure

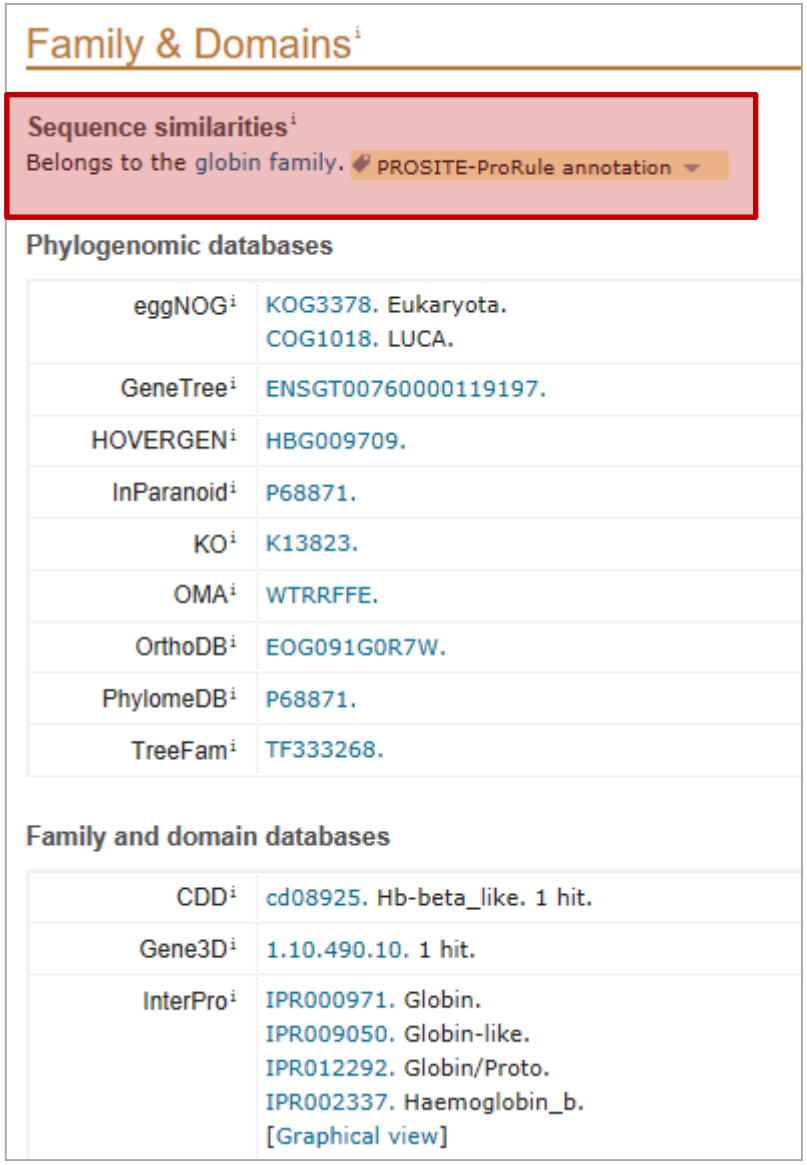
Secondary structure

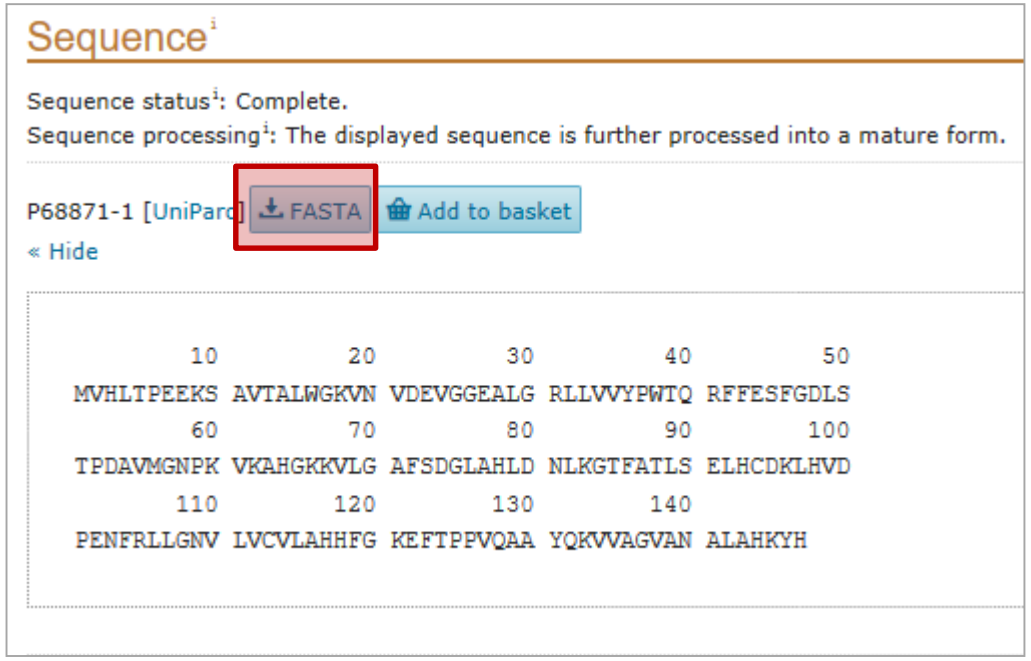


Show more details

Feature key	Position(s)	Length	Description	Graphical view	Feature identifier	Actions
Helix	6 – 17	12	Combined sources			
Helix	21 – 35	15	Combined sources			
Helix	37 – 42	6	Combined sources			
Helix	44 – 46	3	Combined sources			
Helix	52 – 57	6	Combined sources			
Helix	59 – 75	17	Combined sources			
Turn	78 – 80	3	Combined sources			
Helix	82 – 95	14	Combined sources			
Helix	102 – 119	18	Combined sources			
Helix	120 – 122	3	Combined sources			
Helix	125 – 143	19	Combined sources			
Helix	144 – 146	3	Combined sources			

UniProtKB





Click on FASTA and copy the amino acid sequence for further analysis with other tools.

Overview

- Protein structure
- UniProtKB
- **ExPASy**
- PDB – the protein databank
  - JSmol

ExPASy

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www.expasy.org

Query all databases | search | help

Visual Guidance

Categories

- proteomics
- genomics
- structure analysis
- systems biology
- evolutionary biology
- population genetics
- transcriptomics
- biophysics
- imaging
- IT infrastructure
- medicinal chemistry
- glycomics

Resources A..Z

ExPASy is the **SIB Bioinformatics Resource Portal** which provides access to scientific databases and software tools (i.e., *resources*) in different areas of life sciences including proteomics, genomics, phylogeny, systems biology, population genetics, transcriptomics etc. (see Categories in the left menu). On this portal you find resources from many different SIB groups as well as external institutions.

Featuring today

Myristoylator

Predict N-terminal myristoylation of proteins by neural networks.
[details]

How to use this portal?

ExPASy

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There are a lot of tools to analyze proteins.

Visual Guidance

Categories

- proteomics
  - protein sequences and identification
  - proteomics experiment
  - function analysis
  - sequence sites, features and motifs
  - protein modifications
  - protein structure
  - protein interactions
  - similarity search/alignment
- genomics
- structure analysis
- systems biology
- evolutionary biology
- population genetics
- transcriptomics
- biophysics
- imaging
- IT infrastructure
- medicinal chemistry
- glycomics

Resources A..Z

Links/Documentation

SIB resources
External resources - *(No support from the ExPASy Team)*

Databases

- UniProtKB • functional information on proteins • [more]
- UniProtKB/Swiss-Prot • protein sequence database • [more]
- STRING • protein-protein interactions • [more]
- SWISS-MODEL Repository • protein structure homology models • [more]
- PROSITE • protein domains and families • [more]
- ViralZone • portal to viral UniProtKB entries • [more]
- neXtProt • human proteins • [more]

- EMBnet services • bioinformatics tools, databases and courses • [more]
- ENZYME • enzyme nomenclature • [more]
- GlyTouCan • international glycan structure repository • [more]
- GPSDB • gene and protein synonyms • [more]
- HAMAP • UniProtKB family classification and annotation • [more]
- MatrixDB • protein-glycosaminoglycan interactions • [more]
- MetaNetX • Metabolic Network Repository & Analysis • [more]
- MIAPEGelDB • MIAPE document edition • [more]
- MyHits • protein domains database and tools • [more]
- PaxDb • protein abundance database • [more]
- Prolune • Popular science articles (in French) • [more]
- Protein Model Portal • structural information for a protein • [more]
- Protein Spotlight • Informally written reviews on proteins • [more]
- Rhea • expert curated resource of biochemical reactions • [more]
- SugarBind • pathogen sugar-binding • [more]
- SWISS-2DPAGE • proteins on 2-D and SDS PAGE maps • [more]
- SwissBioIsostere • bioIsosteres for small molecules • [more]
- SwissLipids • knowledge resource for lipid biology • [more]

Tools

- SWISS-MODEL Workspace • structure homology-modeling • [more]
- SwissDock • protein ligand docking server • [more]

- 2ZIP • Prediction of leucine zipper domains • [more]
- 3of5 • find user-defined patterns in protein sequences • [more]
- AACompIdent • protein identification by aa composition • [more]
- AACompSim • amino acid composition comparison • [more]
- Agadir • Prediction of the helical content of peptides • [more]
- ALF • simulation of genome evolution • [more]
- Alignment tools • Four tools for multiple alignments • [more]
- AllAll • protein sequences comparisons • [more]
- APSSP • Advanced Protein Secondary Structure Prediction • [more]
- Ascalaph • Molecular modeling software • [more]
- big-PI • predict GPI modification sites • [more]
- Biochemical Pathways • Biochemical Pathways • [more]
- BLAST • sequence similarity search • [more]
- BLAST (UniProt) • BLAST search on the UniProt web site • [more]
- BLAST - NCBI • Biological sequence similarity search • [more]
- BLAST - PBIL • BLAST search on protein sequence databases • [more]
- Blast2Fasta • Blast to Fasta conversion • [more]
- boxshade • MSA pretty printer • [more]
- CFSSP • Protein secondary structure prediction • [more]
- ChloroP • chloroplast transit peptides & cleavage sites • [more]
- Click2Drug • Directory of computational drug design tools • [more]
- ClustalO (UniProt) • Align two or more protein sequences • [more]
- ClustalW • Multiple sequence alignment • [more]

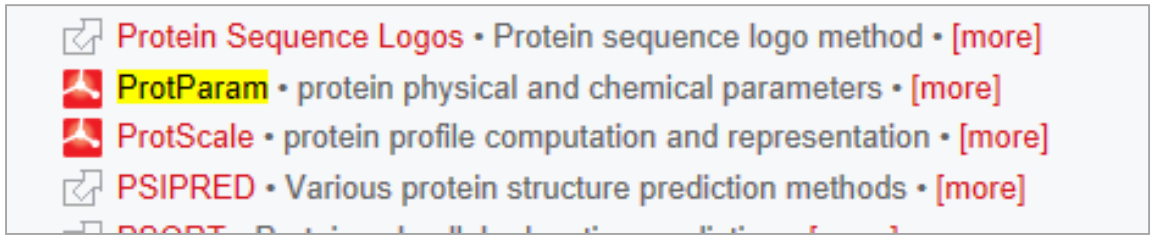
ExPASy

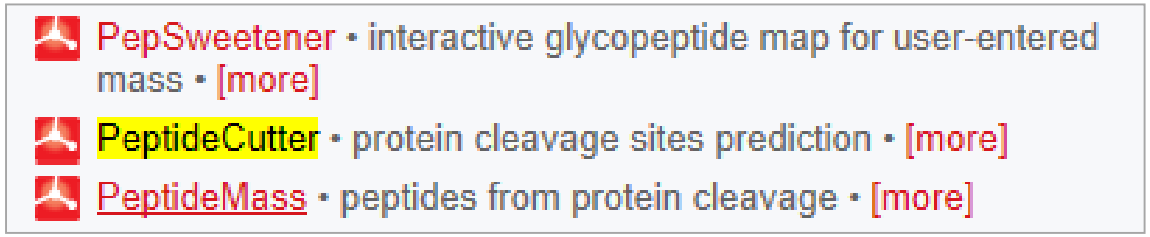
In the following we will get to know to three different tools:

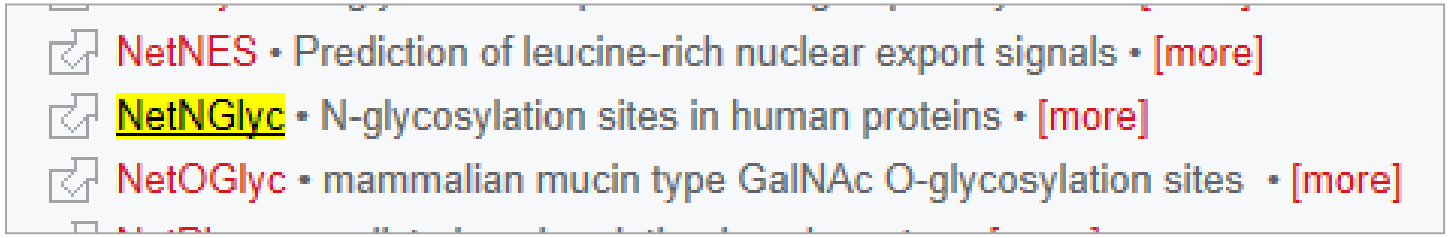
ProtParam

PeptideCutter

NetNGlyc







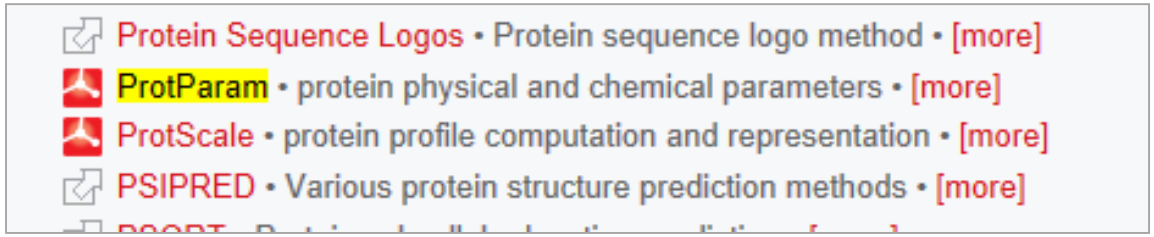
ExPASy

In the following we will get to know to three different tools:

ProtParam

PeptideCutter

NetNGlyc



ExPASy – ProtParam

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ProtParam tool

ProtParam (References / Documentation) is a tool which allows the computation of various physical and chemical parameters for a giv
weight, theoretical pI, amino acid composition, atomic composition, extinction coefficient, estimated half-life, instability index, aliphatic ir

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 a sequence identifier (ID) (for example **KPC1_DROME**):

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

```
MVHLTPEEKSAVTALWGKVNVDEVGGEALGRLLVVYPWTQRFFESFGDLSTPDAVMGNPK
VKAHGKKVLGAFSDGLAHLDNLKGTFATLSELHCDKLHVDPENFRLLGNVLVCVLAHHFG
KEFTPPVQAAYQKVVAGVANALAHKYH
```

Enter the sequence of your protein of interest

RESET | Compute parameters

ExPASy – ProtParam

ProtParam

User-provided sequence:

```
        10         20         30         40         50         60
MVHLTPEEKS AVTALWGKVN VDEVGGEALG RLLVVYPWTQ RFFESFGDLS TPDAVMGNPK

        70         80         90        100        110        120
VKAHGKKVLG AFSDGLAHLD NLKGTFATLS ELHCDKLHVD PENFRLLGNV LVCVLAHHFG

       130        140
KEFTPPVQAA YQKVVAGVAN ALAHKYH
```

References and documentation are available.

Number of amino acids: 147

Molecular weight: 15998.41

Theoretical pI: 6.74

Note: The unit for the molecular weight is Dalton (Da = g/mol)

ExPASy – ProtParam

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Amino acid composition

Amino acid composition: CSV format

Ala (A)	15	10.2%
Arg (R)	3	2.0%
Asn (N)	6	4.1%
Asp (D)	7	4.8%
Cys (C)	2	1.4%
Gln (Q)	3	2.0%
Glu (E)	8	5.4%
Gly (G)	13	8.8%
His (H)	9	6.1%
Ile (I)	0	0.0%
Leu (L)	18	12.2%
Lys (K)	11	7.5%
Met (M)	2	1.4%
Phe (F)	8	5.4%
Pro (P)	7	4.8%
Ser (S)	5	3.4%
Thr (T)	7	4.8%
Trp (W)	2	1.4%
Tyr (Y)	3	2.0%
Val (V)	18	12.2%
Pyl (O)	0	0.0%
Sec (U)	0	0.0%
(B)	0	0.0%
(Z)	0	0.0%
(X)	0	0.0%

Total number of negatively charged residues (Asp + Glu): 15
Total number of positively charged residues (Arg + Lys): 14

Atomic composition:

Carbon	C	729
Hydrogen	H	1128
Nitrogen	N	196
Oxygen	O	202
Sulfur	S	4

Formula: $C_{729}H_{1128}N_{196}O_{202}S_4$
Total number of atoms: 2259

Extinction coefficients

Extinction coefficients:

Extinction coefficients are in units of M^{-1} cm^{-1}, at 280 nm measured in water.

Ext. coefficient	15595
Abs 0.1% (=1 g/l)	0.975, assuming all pairs of Cys residues form cystines
Ext. coefficient	15470
Abs 0.1% (=1 g/l)	0.967, assuming all Cys residues are reduced

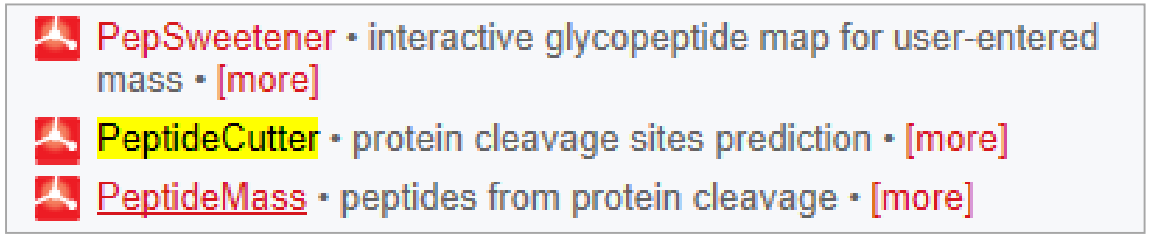
ExPASy

In the following we will get to know to three different tools:

ProtParam

PeptideCutter

NetNGlyc



ExPASy – Peptide Cutter

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Use the PeptideCutter to predict the cleavage of your protein by using specific proteases or chemicals.

PeptideCutter

PeptideCutter [references / documentation] predicts potential cleavage sites cleaved by proteases or chemicals in a given protein sequence. PeptideCutter returns the query sequence cleavage sites mapped on it and /or a table of cleavage site positions.

Enter a UniProtKB (Swiss-Prot or TrEMBL) protein identifier, ID (e.g. ALBU_HUMAN), or accession number, AC (e.g. P04406), **or** an amino acid sequence (e.g. 'SERVELAT'):

```
MVHLTPEEKSAVTALWGKVNVDEVGGEALGRLLVVYPWTQRFFESFGDLST
PDAVMGNPK
VKAHGKKVLGAFSDGLAHLDNLKGTFATLSELHCDKLHVDPENFRLLGNVL
VCVLAHHFG
KEFTPPVQAAYQKVVAGVANALAHKYH
```

Enter the sequence of your protein of interest

Perform the cleavage of the protein. Reset the fields.

Please, select

- all available enzymes and chemicals
- only the following selection of **enzymes and chemicals**

Arg-C proteinase	Asp-N endopeptidase	Asp-N endopeptidase + N-terminal Glu
BNPS-Skatole	Caspase1	Caspase2
Caspase3	Caspase4	Caspase5
Caspase6	Caspase7	Caspase8
Caspase9	Caspase10	
Chymotrypsin-high specificity (C-term to [FYW], not before P)	Chymotrypsin-low specificity (C-term to [FYWML], not before P)	
Clostripain (Clostridiopeptidase B)	CNBr	Enterokinase
Factor Xa	Formic acid	Glutamyl endopeptidase

ExPASy – Peptide Cutter

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PeptideCutter

The sequence to investigate:

```
         10         20         30         40         50         60
MVHLTPEEKS AVTALWGKVN VDEVGGEALG RLLVVYPWTQ RFFESFGDLS TPDAVMGNPK

         70         80         90        100        110        120
VKAHGKKVLG AFSDGLAHLD NLKGTFATLS ELHCDKLHVD PENFRLLGNV LVCVLAHHFG

        130        140
KEFTPPVQAA YQKVVAGVAN ALAHKYH
```

The sequence is 147 amino acids long.

Available enzymes

The enzyme(s) that you have chosen:

- Asp-N endopeptidase
- Enterokinase
- Factor Xa

You have chosen to display all possible cleaving enzymes.

These enzymes cleave the sequence:

Name of enzyme	No. of cleavages	Positions of cleavage sites
Asp-N endopeptidase	7	21 47 52 73 79 94 99

These chosen enzymes do not cut:

Enterokinase

Factor Xa

Scroll down to see map

Theresa Schwarz

ExPASy – Peptide Cutter

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The cleavage specificities of selected enzymes and chemicals:

Click on enzyme to see its cleavage specificities

Arg-C proteinase:

The Arg-C proteinase preferentially cleaves at Arg in position P1. The cleavage behaviour seems to be only moderately affected by residues in position P1' (Keil, 1992).

Asp-N Endopeptidase:

The Asp-N Endopeptidase cleaves specifically bonds with Asp in position P1' (Keil, 1992).

Asp-N Endopeptidase + N-terminal Glu:

The Asp-N Endopeptidase cleaves specifically bonds with Asp or Glu in position P1' (Keil, 1992).

BNPS-Skatole:

BNPS-skatole [2-(2-nitrophenylsulfenyl)-3-methylindole] is a mild oxidant and brominating reagent that leads to polypeptide cleavage on the C-terminal side of tryptophan residues).

Caspase 1:

Caspase-1 is acting on Interleukin-1 beta [Precursor] (P01584) to release it by specific cleavage at 116-Asp-|-Ala-117 (YVHDA) and 27-Asp-|-Gly-28 (EADG) bonds. It also hydrolyzes small-molecule substrate such as Ac-Tyr-Val-Ala-Asp-|-NHMec. Generally the substrate/enzyme interaction is located between the positions P4 and P1'. Various different patterns were proposed such as YEVD|X (Talanian et al., 1997) or WEHD|X (Thornberry et al., 1997), where X is any amino acid but Pro, Glu, Asp, Gln, Lys, Arg (Stennicke et al., 2000, Talanian et al., 1997). The pattern implemented for PeptideCutter considers an extended rule based on the study by Earnshaw et al., 1999, to optimise the caspase-1 endoproteolytic specificity, and can be found in the table at the end of this document, describing the possible variations on the different interacting sites from P4 to P'1.

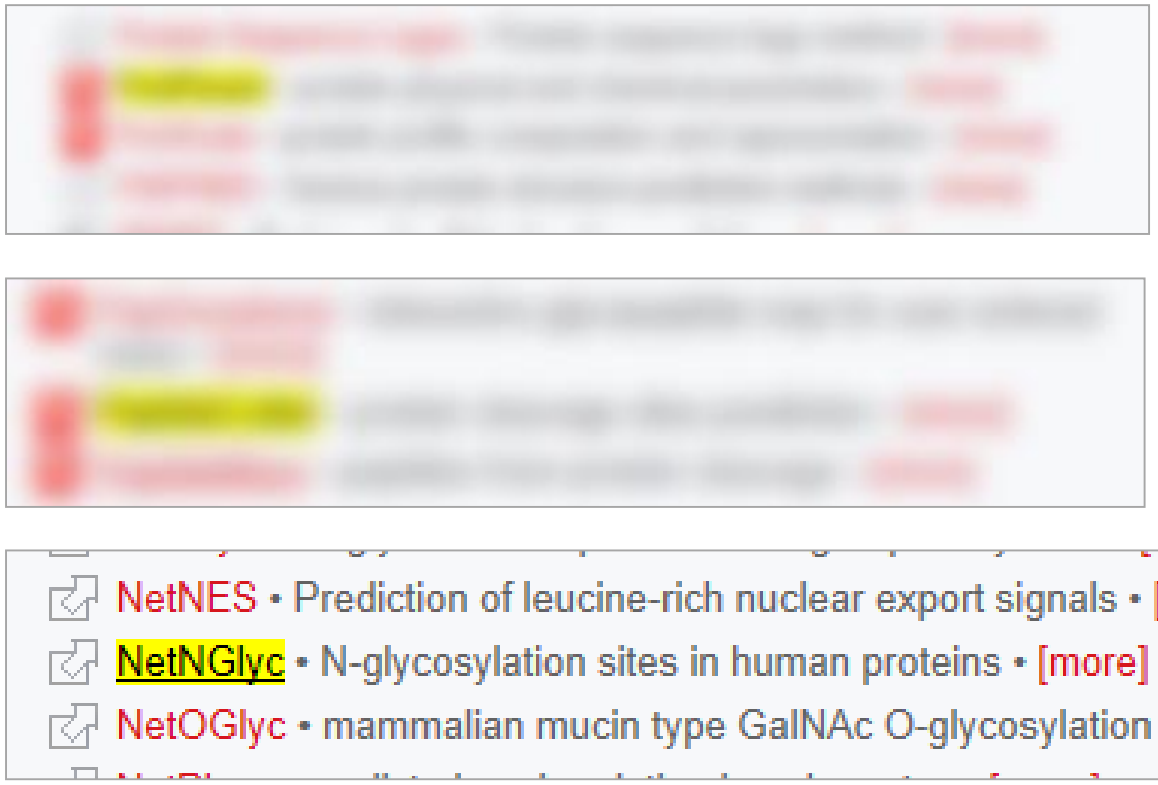
ExPASy

In the following we will get to know to three different tools:

ProtParam

PeptideCutter

NetNGlyc



ExPASy – NetNGlyc

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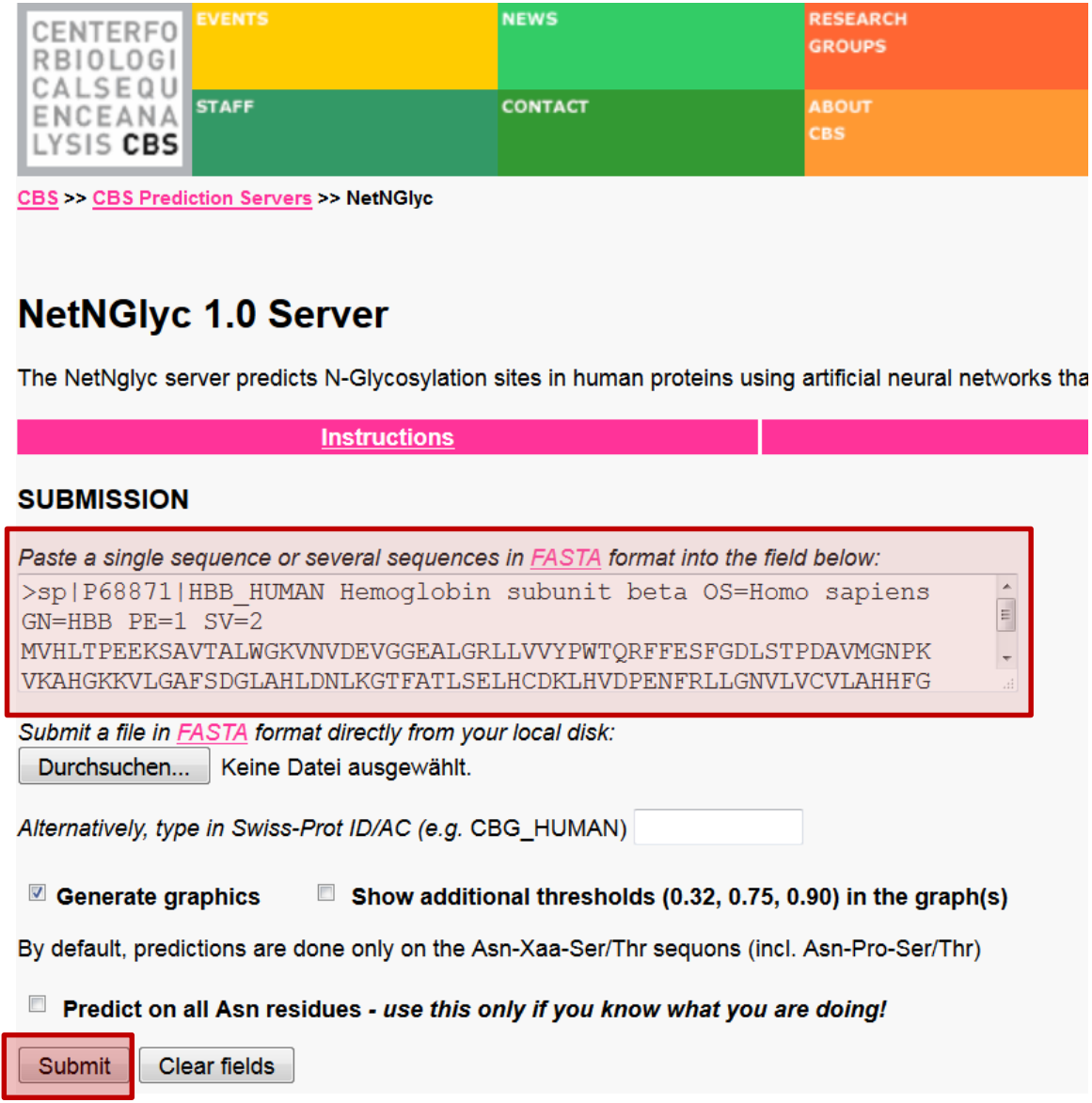
Use the NetNGlyc tool to predict N-glycosylation sites in proteins



Enter the sequence of your protein of interest in the FASTA format

ExPASy – NetNGlyc

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Output for 'Sequence'

```
########################################################################################################
```

Warning: This sequence may not contain a signal peptide!!

Proteins without signal peptides are unlikely to be exposed to the N-glycosylation machinery and thus may not be glycosylated (in vivo) even though they contain potential motifs.

SignalP-NN euk predictions are as follows:

# name	Cmax	pos	?	Ymax	pos	?	Smax	pos	?	Smean	?	D	?
Sequence	0.285	27	N	0.062	27	N	0.310	3	N	0.088	N	0.075	N

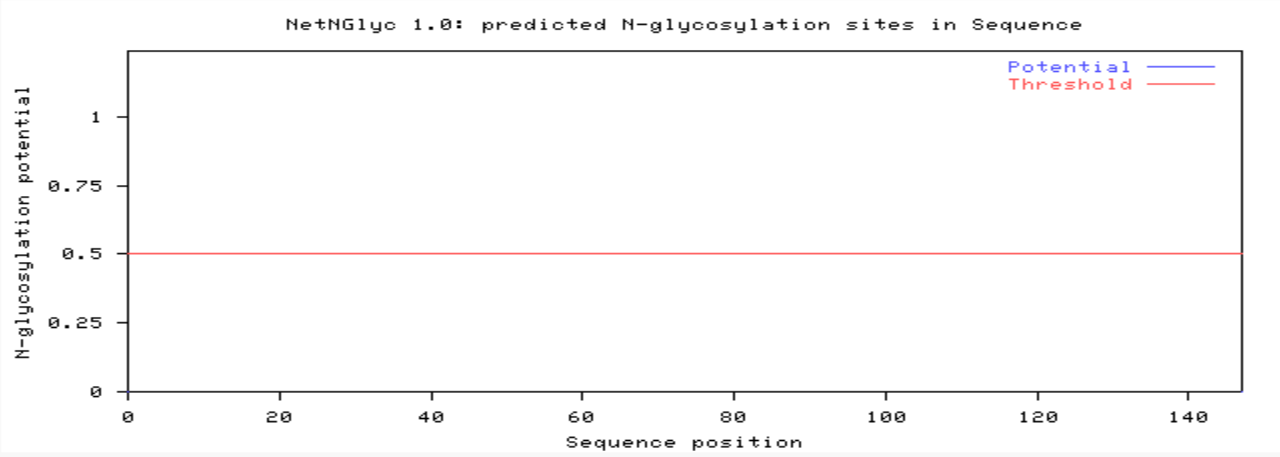
SignalP output is explained at http://www.cbs.dtu.dk/services/SignalP/output.html

```
########################################################################################################

Name:   Sequence          Length:  147
MVHLTPEEKSAVTALWGKVNVDEVGGEALGRLLVVYPWTQRFFESFGDLSTPDAVMGNPKVKAHGKKVLGAFSDGLAHLD       80
NLKGTFATLSELHCDKLHVDPENFRLLGNVLVCVLAHHFGKEFTPPVQAAYQKVVAGVANALAHKYH
.....................................................................................      80
.....................................................................                     160

(Threshold=0.5)
```

No sites predicted in this sequence.



ExPASy – NetNGlyc

CENTERFORBIOLOGICALSEQUENCEANALYSIS CBS

NetNGlyc 1.0 Server - prediction results

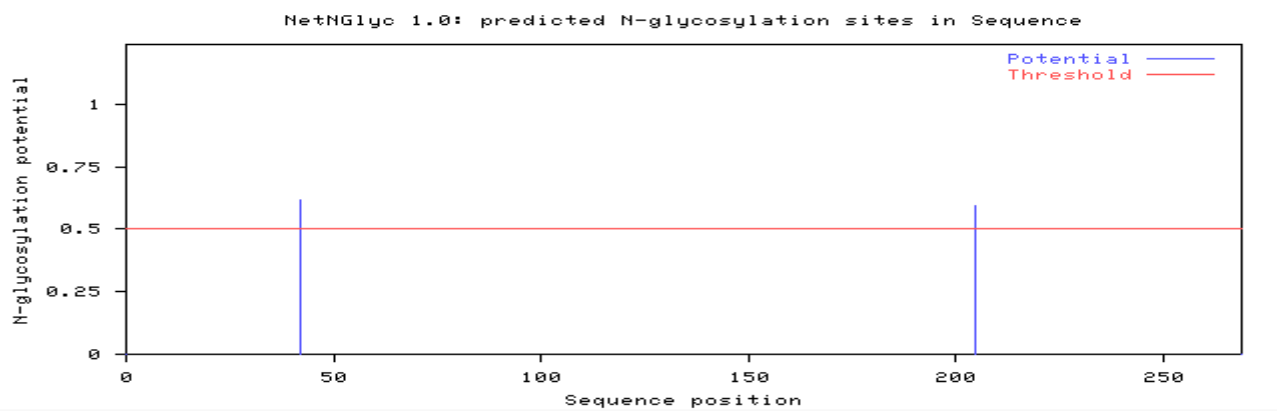
Technical University of Denmark

Asn-Xaa-Ser/Thr sequons in the sequence output below are highlighted in blue.
Asparagines predicted to be N-glycosylated are highlighted in red.

Output for 'Sequence'

```
Name:   Sequence          Length:  269
MASEFKKKLFWRAVVAEFLATTLFVFISIGSALGFKYPVGNNQTAVQDNVKVSLAFGLSIATLAQSVGHISGAHLNPAVT      80
LGLLLSCQISIFRALMYIIAQCVGAIVATAILSGITSSLTGNSLGRNDLADGVNSGQGLGIEIIGTLQLVLCVLATTDRR     160
RRDLGGSAPLAIGLSVALGHLLAIDYTGCGINPARSFGSAVITHNFSNHWIFWVGPFIGGALAVLIYDFILAPRSSDLTD     240
RVKVWTSGQVEEYDLDADDINSRVEMKPK
.........................................N.......................................      80
........................................................................................     160
.........................................N.......................................     240
.............................                                                           320

(Threshold=0.5)
--------------------------------------------------------------------------------
SeqName       Position  Potential    Jury agreement  N-Glyc result
--------------------------------------------------------------------------------
Sequence        42 NQTA    0.6188      (7/9)    +
Sequence       205 NFSN    0.5971      (8/9)    +
--------------------------------------------------------------------------------
```



Overview

- Protein structure
- UniProtKB
- ExPASy
- **PDB – the protein databank**
  - **JSmol**

PDB – The protein data bank

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www.rcsb.org

Search for hemoglobin.

RCSB PDB | Deposit | Search | Visualize | Analyze | Download | Learn | More | MyPDB Login

RCSB PDB PROTEIN DATA BANK

An Information Portal to 124588 Biological Macromolecular Structures

hemoglobin

Go

Advanced Search | Browse by Annotations

PDB-101 | wwPDB | EMDataBank | NDB Nucleic Acid Database | StructuralBiology Knowledgebase | Worldwide Protein Data Bank Foundation

- Welcome
- Deposit
- Search
- Visualize
- Analyze
- Download
- Learn

A Structural View of Biology

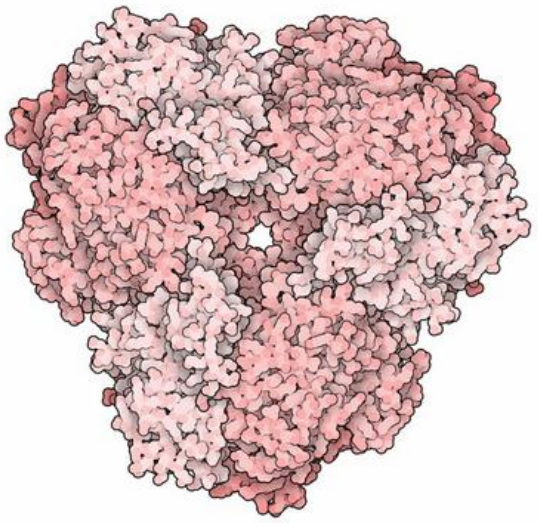
This resource is powered by the Protein Data Bank archive-information about the 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease.

As a member of the wwPDB, the RCSB PDB curates and annotates PDB data.

The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.

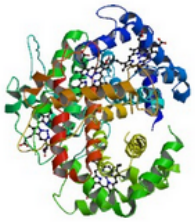
Discovering Biology Through Crystallography

November **Molecule of the Month**



Aminopeptidase 1 and Autophagy

PDB – The protein data bank



3D View

1FN3 Download File | View File

CRYSTAL STRUCTURE OF NICKEL RECONSTITUTED HEMOGLOBIN-A CASE FOR PERMANENT, T-STATE HEMOGLOBIN

Venkateshrao, S., Deepthi, S., Pattabhi, V., Manoharan, P.T.

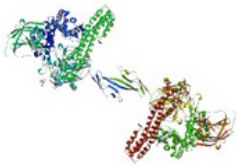
PubMed ID is not available.

Released: 10/7/2003
Method: X-ray Diffraction
Resolution: 2.48 Å
Residue Count: 574

Macromolecule:
HEMOGLOBIN ALPHA CHAIN (protein)
HEMOGLOBIN BETA CHAIN (protein)
Unique Ligands: HNI
Search term match score: 269.06

Matched fields in 1FN3.cif:

- **_citation.title**: Crystal Structure of Nickel Reconstituted **Hemoglobin** - A Case for Permanent, T-State **Hemoglobin**
- **_entity.pdbx_description**: **HEMOGLOBIN** ALPHA CHAIN, **HEMOGLOBIN** BETA CHAIN, PROTOPORPHYRIN IX CONTAINING NI(II)
- **_struct.title**: CRYSTAL STRUCTURE OF NICKEL RECONSTITUTED **HEMOGLOBIN** -A CASE FOR PERMANENT, T-STATE **HEMOGLOBIN**



3D View

4WJG Download File | View File

Structure of T. brucei haptoglobin-hemoglobin receptor binding to human haptoglobin-hemoglobin

Stdkilde, K., Torvund-Jensen, M., Moestrup, S.K., Andersen, C.B.F.

(2014) Nat Commun **5** 5487-5487

Released: 11/26/2014
Method: X-ray Diffraction
Resolution: 3.1 Å
Residue Count: 6546

Macromolecule:
Hemoglobin subunit alpha (protein)
Hemoglobin subunit beta (protein)
Haptoglobin (protein)
Iron-regulated surface determinant ... (protein)
Haptoglobin-hemoglobin receptor (protein)
Unique Ligands: HEM, NAG, OXY
Search term match score: 269.06

Matched fields in 4WJG.cif:

- **_entity.pdbx_description**: **Hemoglobin** subunit alpha, **Hemoglobin** subunit beta, Haptoglobin, Iron-regulated surface determinant protein H, Haptoglobin-**hemoglobin** receptor, PROTOPORPHYRIN IX CONTAINING FE, OXYGEN MOLECULE, N-ACETYL-D-GLUCOSAMINE
- **_entity_name_com.name**: Alpha-globin, **Hemoglobin** alpha chain, Beta-globin, **Hemoglobin** beta chain, Zonulin, Haptoglobin receptor A,Staphylococcus aureus surface protein I
- **_struct.title**: Structure of T. brucei haptoglobin-**hemoglobin** receptor binding to human haptoglobin-**hemoglobin**

You can find a lot of entries all about published hemoglobin structures

- substructures
- mutants
- …

We want to get the entire structure of the human hemoglobin protein.
The PDB-ID is: **4HHB**

→ **Search for 4HHB.**

PDB – The protein data bank

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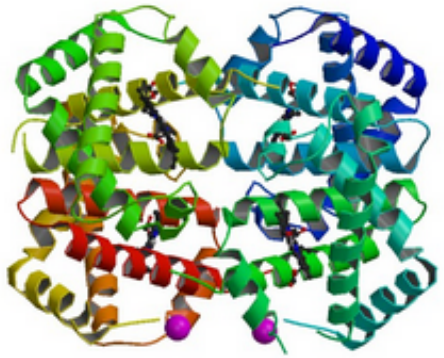
Biological Assembly 1



3D View: Structure | Ligand Interaction

Standalone Viewers
Ligand Explorer

Global Symmetry: Cyclic - C2 (3D View)
Global Stoichiometry: Hetero 4-mer - A2B2

Pseudo Symmetry: Dihedral - D2 (3D View)
Pseudo Stoichiometry: Homo 4-mer -A4

Biological assembly 1 assigned by ... generated by PISA (software)

Stoichiometry

general information

Macromolecule Content

- Total Structure Weight: 64736.99
- Atom Count: 4558
- Residue Count: 574
- Unique protein chains: 2

Display Files | Download Files

4HHB **PDB-ID**

THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT 1.74 ANGSTROMS RESOLUTION

DOI: 10.2210/pdb4HHB/pdb Entry 4HHB **supersedes** 1HHB

Classification: OXYGEN TRANSPORT
Organism(s): Homo sapiens

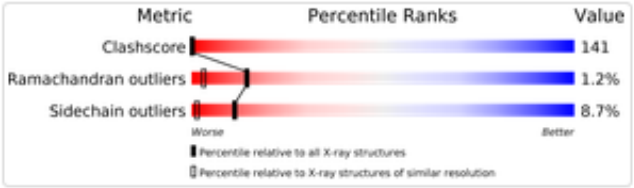
Deposited: 1984-03-07 **Released:** 1984-07-17
Deposition Author(s): Fermi, G., Perutz, M.F.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 1.74 Å
R-Value Work: 0.135

Experimental technique

wwPDB Validation | 3D Report | Full Report



This is version 1.2 of the entry. See complete history.

Literature | Download Primary Citation

The crystal structure of human deoxyhaemoglobin at 1.74 A resolution

Fermi, G., Perutz, M.F., Shaanan, B., Fourme, R.
(1984) J.Mol.Biol. **175**: 159-174

PubMed: 6726807 Search on PubMed
Primary Citation of Related Structures:
3HHB, 2HHB

Information about the literature

PubMed Abstract:
The structure of human deoxyhaemoglobin was refined at 1.74 A resolution using data collected on film at room temperature from a synchrotron X-ray source. The crystallographic R-factor is 16.0%. The estimated error in atomic positions is 0.1 A overal ...

PDB – The protein data bank

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Modifications:

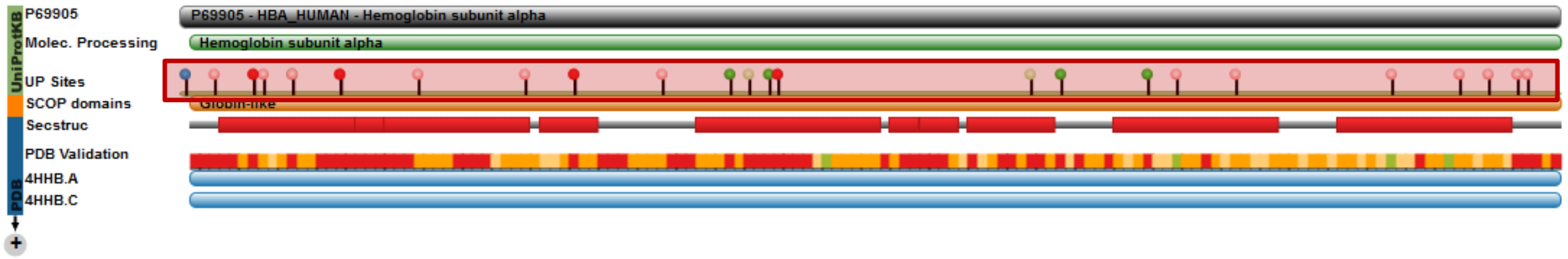
Move your curser over the dots to see what kind of modification it is.

Entity ID: 1

Molecule	Chains	Sequence Length	Organism	Details
HEMOGLOBIN (DEOXY) (ALPHA CHAIN)	A, C	141	Homo sapiens	**Gene Names**: HBA1, HBA2

Find proteins for P69905 *(Homo sapiens)* Go to Gene View: HBA1 HBA2 Go to UniProtKB: P69905

Protein Feature View Full Protein Feature View for P69905



Entity ID: 2

Molecule	Chains	Sequence Length	Organism	Details
HEMOGLOBIN (DEOXY) (BETA CHAIN)	B, D	146	Homo sapiens	**Gene Names**: HBB

Find proteins for P68871 *(Homo sapiens)* Go to Gene View: HBB Go to UniProtKB: P68871

Protein Feature View Full Protein Feature View for P68871

PDB – The protein data bank

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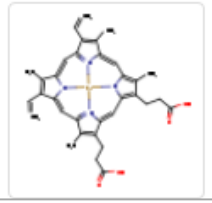
Information about ligands that are present in the structure

Small Molecules

Ligands 2 Unique

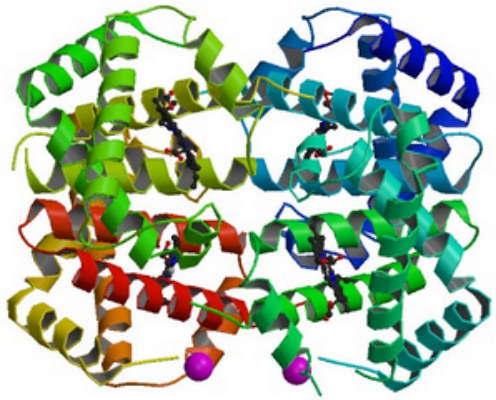
ID	Chains	Name / Formula / InChI Key	2D Diagram & Interactions	3D Interactions
PO4 Query on PO4 Download SDF File Download CCD File	B, D	**PHOSPHATE ION** O_4 P NBIIXXVUZAFLBC-UHFFFAOYSA-K		Ligand Interaction
HEM Query on HEM Download SDF File Download CCD File	A, B, C, D	**PROTOPORPHYRIN IX CONTAINING FE** *HEME* C_{34} H_{32} Fe N_4 O_4 KABFMIBPWCXCRK-RGGAHWMASA-L		Ligand Interaction

PDB – The protein data bank

For more detailed information you can choose the tabs at the top of the page.

Structure Summary | 3D View | Annotations | Sequence | Sequence Similarity | Structure Similarity | Experiment

Biological Assembly 1



3D View: Structure | Ligand Interaction

Standalone Viewers
Protein Workshop | Ligand Explorer

Display Files | Download Files

4HHB

THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT 1.74 ANGSTROMS RESOLUTION

DOI: 10.2210/pdb4HHB/pdb Entry 4HHB **supersedes** 1HHB

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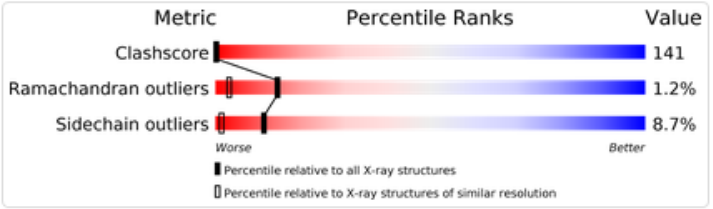
Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 1.74 Å
R-Value Work: 0.135

wwPDB Validation 3D Report | Full Report

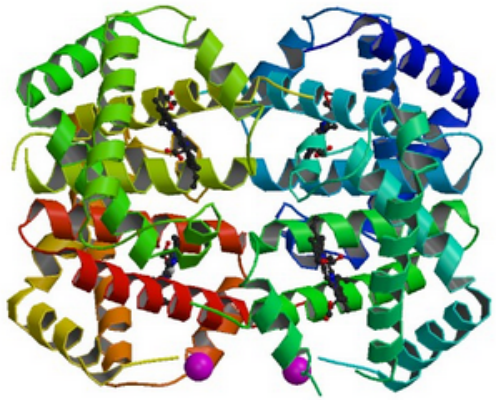


This is version 1.2 of the entry. See complete history.

View the 3D structure of the protein

Structure Summary | 3D View | Annotations | Sequence | Sequence Similarity | Structure Similarity | Experiment

Biological Assembly 1



3D View: Structure | Ligand Interaction

Standalone Viewers
Protein Workshop | Ligand Explorer

Display Files | Download Files

4HHB

THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT 1.74 ANGSTROMS RESOLUTION

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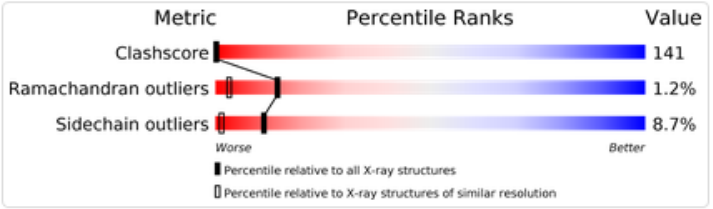
wwPDB Validation 3D Report | Full Report



This is version 1.2 of the entry. See complete history.

PDB – JSmol

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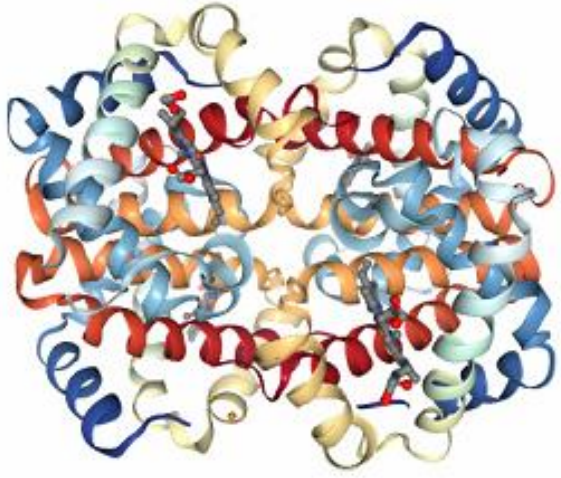
Structure Summary | 3D View | Annotations | Sequence | Sequence Similarity | Structure Similarity | Experiment

4HHB

THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT 1.74 ANGSTROMS RESOLUTION

Display Files | Download Files

Note: Use your mouse to drag, rotate, and zoom in and out of the structure. Mouse-over to identify atoms and bonds. Mouse controls documentation.



Structure View | Electron Density Maps | Ligand View

Structure View Documentation

Assembly: Asymmetric Un
Model: Model 1
Symmetry: None
Style: Cartoon
Color: Rainbow
Ligand: Ball & Stick
Quality: Automatic
Water ☐ Ions ☑
Hydrogens ☑ Clashes ☐
Default Structure View

Spin | Center | Fullscreen | Screenshot | Perspective Camera | White background | Focus

NGL is a WebGL based 3D viewer powered by MMTF.

Select a different viewer: NGL (WebGL) / NGL (WebGL) / JSmol (JavaScript)

Citation

PDB – JSmol

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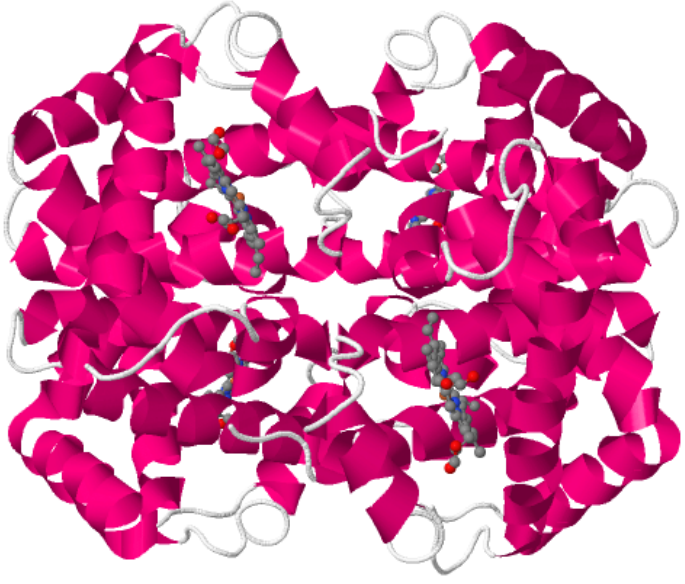
4HHB

THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT 1.74 ANGSTROMS RESOLUTION

Display Files | Download Files

NOTE: Use your mouse to drag, rotate, and zoom in and out of the structure. Help



JSmol

Biological assembly 1 assigned by authors and generated by PISA

Select a Viewer

JSmol (JavaScript)

Structure Details

Structure	Biological Assembly 1
Symmetry Type	Global Symmetry
Symmetry	C2
Stoichiometry	A2B2

Select Orientation

◀ *Front C2 axis* ▶

Select Display Mode

Secondary Structure | Subunit | Symmetry

Display Options

Style	Cartoon
Color	Secondary Structure
Surface	None

- ☐ H-Bonds
- ☐ Rotation
- ☐ Polyhedron
- ☐ SS-Bonds
- ☐ Black Background
- ☐ Axes

PDB – JSmol

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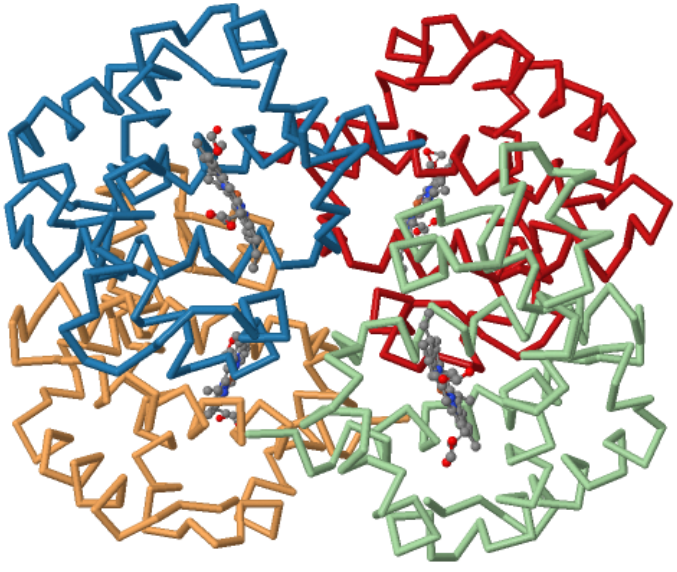
THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT 1.74 ANGSTROMS RESOLUTION

Display Files | Download Files

NOTE: Use your mouse to drag, rotate, and zoom in and out of the structure. Help



Biological assembly 1 assigned by authors and generated by PISA

Select a Viewer

JSmol (JavaScript)

Structure Details

Structure	Biological Assembly 1
Symmetry Type	Global Symmetry
Symmetry	C2
Stoichiometry	A2B2

Select Orientation

Front C2 axis

Select Display Mode

Secondary Structure | Subunit | Symmetry

Display Options

Style	Backbone
Color	Subunit
Surface	None

- H-Bonds
- Rotation
- Polyhedron
- SS Bonds
- Black Background
- Axes

PDB – JSmol

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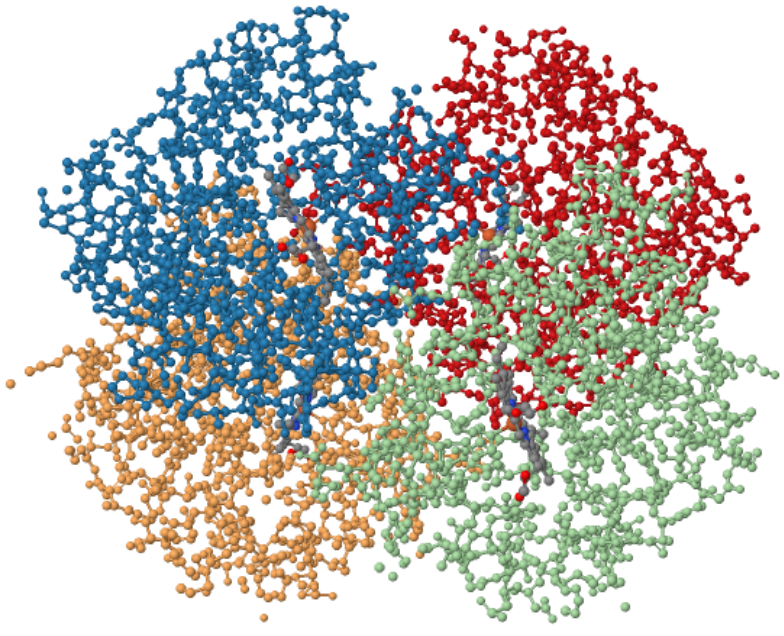
4HHB

THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT 1.74 ANGSTROMS RESOLUTION

Display Files | Download Files

NOTE: Use your mouse to drag, rotate, and zoom in and out of the structure. Help



JSmol

Use mouse to drag, rotate, and zoom

Biological assembly 1 assigned by authors and generated by PISA

Select a Viewer

JSmol (JavaScript)

Structure Details

Structure	Biological Assembly 1
Symmetry Type	Global Symmetry
Symmetry	C2
Stoichiometry	A2B2

Select Orientation

Front C2 axis

Select Display Mode

Secondary Structure | Subunit | Symmetry

Display Options

Style	Ball and Stick
Color	Subunit
Surface	None

- H-Bonds
- SS Bonds
- Rotation
- Black Background
- Polyhedron
- Axes

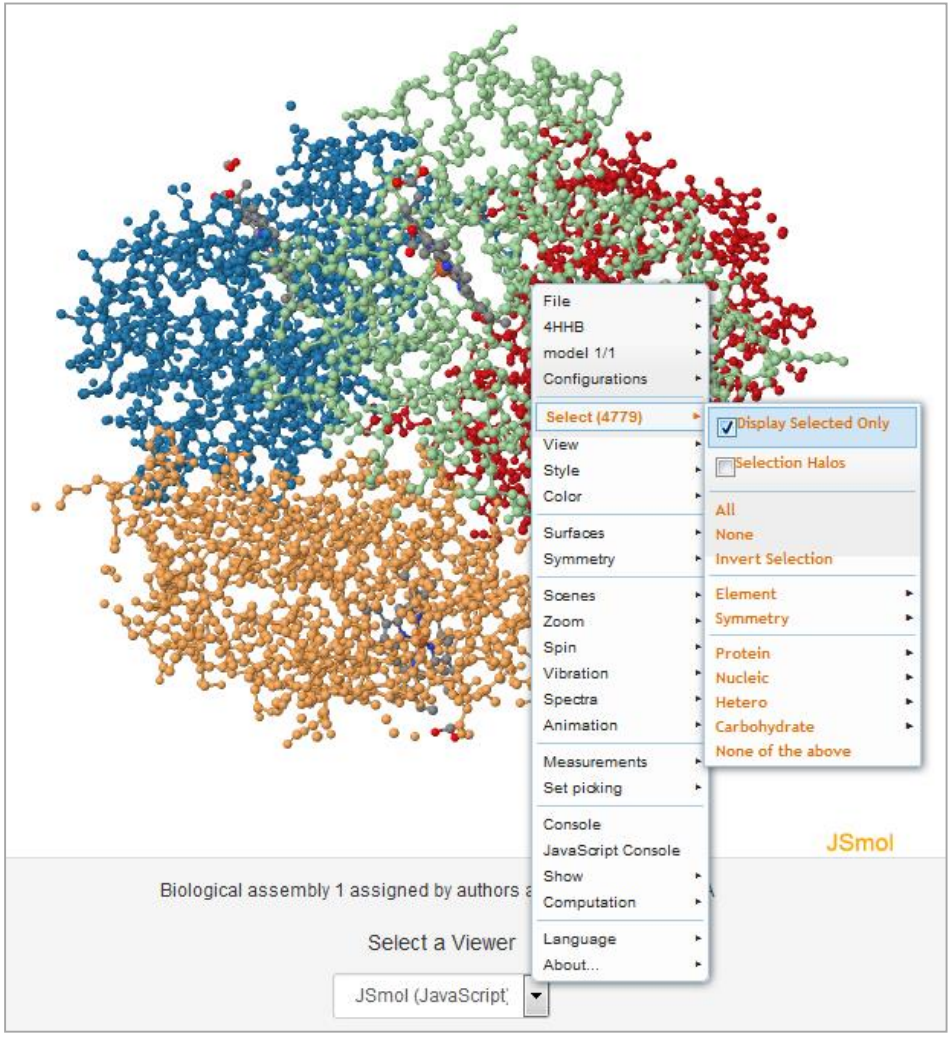
PDB – JSmol

Right click

Select

Display Selected Only

→ To make sure to just show selected settings



PDB – JSmol

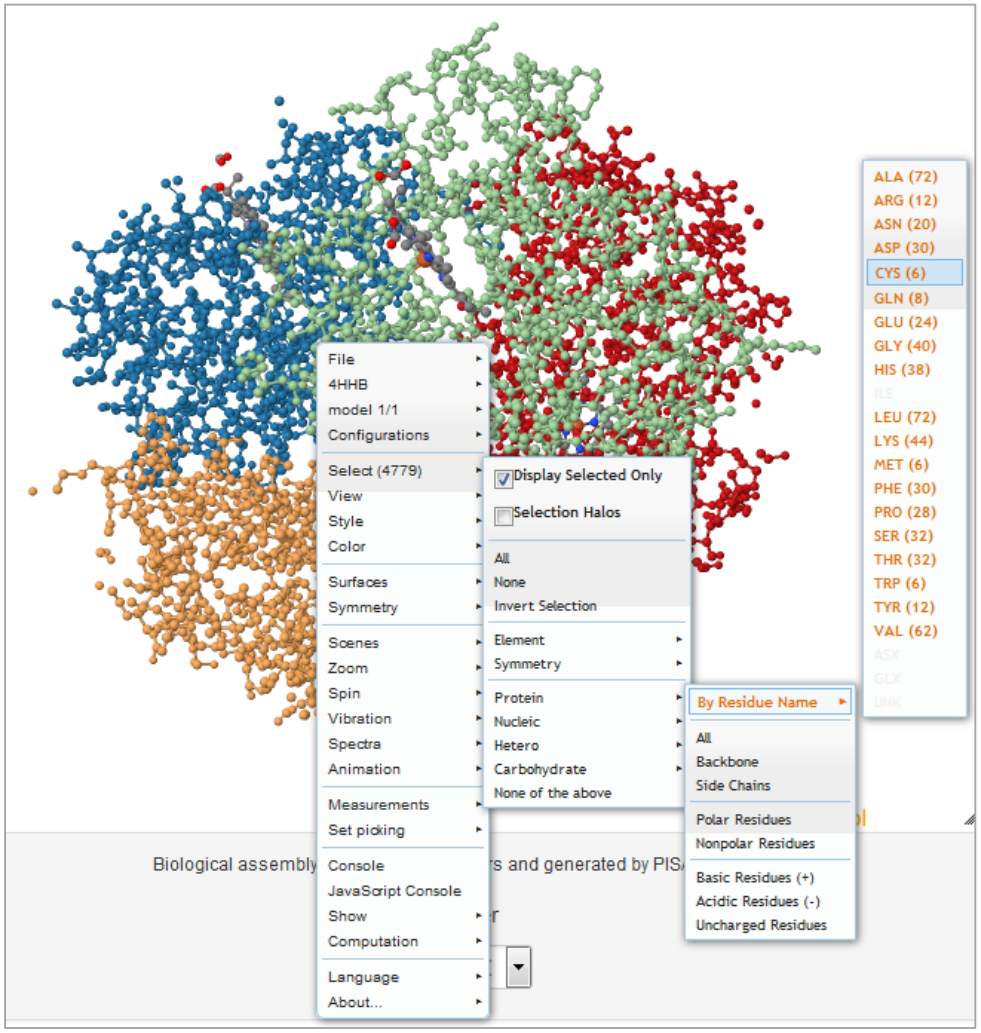
Right click

Select

Protein

By Residue Name

Cys



PDB – JSmol

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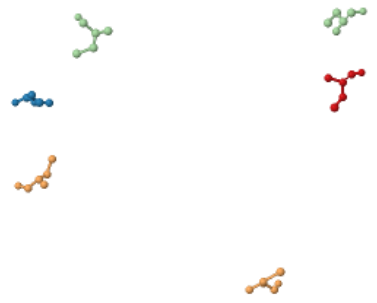
4HHB

THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT 1.74 ANGSTROMS RESOLUTION

Display Files | Download Files

NOTE: Use your mouse to drag, rotate, and zoom in and out of the structure. Help

You can see now all cysteines color coded by the subunits



Biological assembly 1 assigned by authors and generated by PISA

Select a Viewer

JSmol (JavaScript)

Structure Details

Structure	Biological Assembly 1
Symmetry Type	Global Symmetry
Symmetry	C2
Stoichiometry	A2B2

Select Orientation

◀ *Front C2 axis* ▶

Select Display Mode

Secondary Structure | Subunit | Symmetry

Display Options

Style	Ball and Stick
Color	Subunit
Surface	None

☐ H-Bonds ☐ SS Bonds
☐ Rotation ☐ Black Background
☐ Polyhedron ☐ Axes

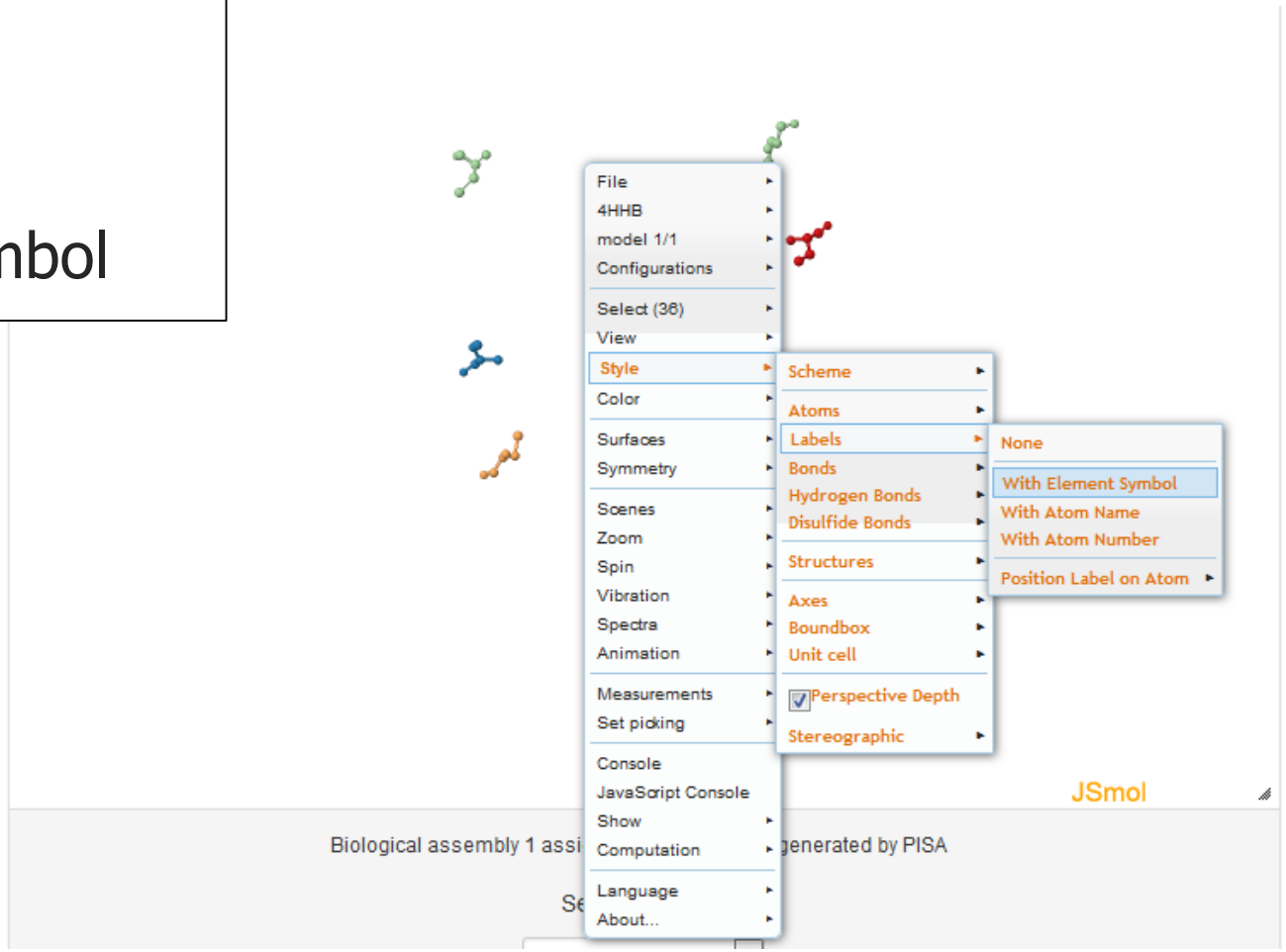
PDB – JSmol

Right click

Style

Labels

With Element Symbol



PDB – JSmol

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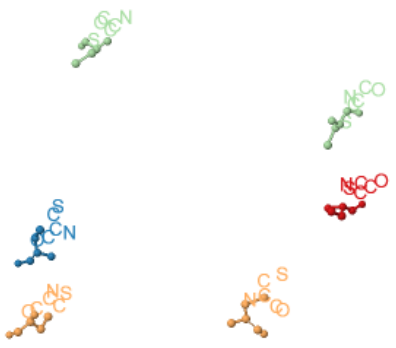
4HHB

THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT 1.74 ANGSTROMS RESOLUTION

Display Files | Download Files

The elements of Cys are labeled now

NOTE: Use your mouse to drag, rotate, and zoom in and out of the structure. Help



JSmol

Biological assembly 1 assigned by authors and generated by PISA

Select a Viewer

JSmol (JavaScript)

Structure Details

Structure	Biological Assembly 1
Symmetry Type	Global Symmetry
Symmetry	C2
Stoichiometry	A2B2

Select Orientation

◀ *Front C2 axis* ▶

Select Display Mode

Secondary Structure | Subunit | Symmetry

Display Options

Style	Ball and Stick
Color	Subunit
Surface	None

☐ H-Bonds ☐ SS Bonds
☐ Rotation ☐ Black Background
☐ Polyhedron ☐ Axes

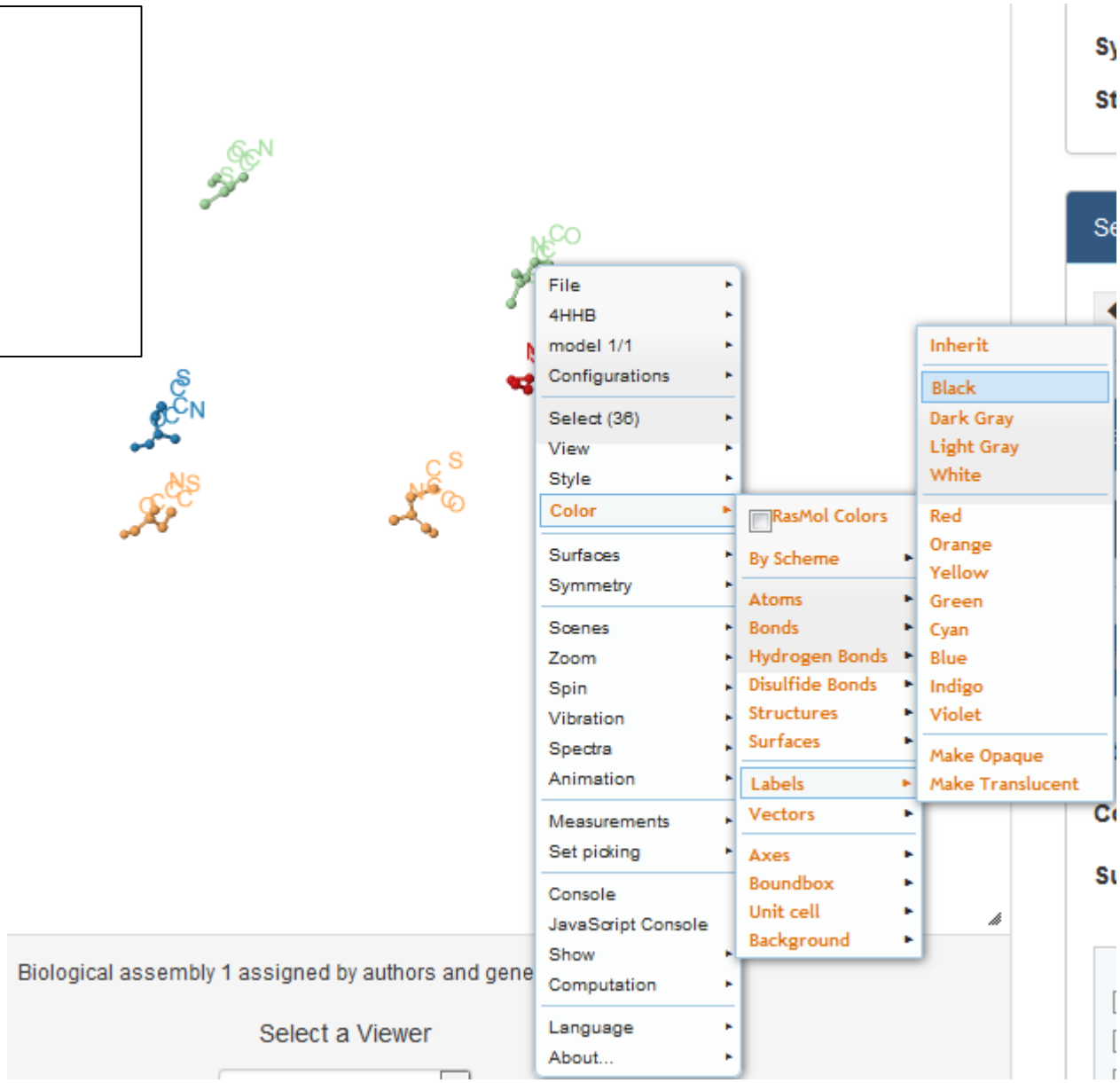
PDB – JSmol

Right click

Color

Labels

Black



PDB – JSmol

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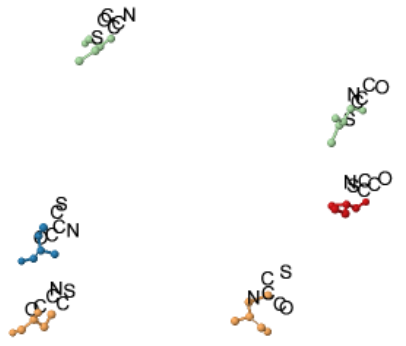
4HHB

THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT 1.74 ANGSTROMS RESOLUTION

Display Files | Download Files

You changed the color of the element labels to black.

NOTE: Use your mouse to drag, rotate, and zoom in and out of the structure. Help



JSmol

Biological assembly 1 assigned by authors and generated by PISA

Select a Viewer

JSmol / JavaScript

Structure Details

Structure	Biological Assembly 1
Symmetry Type	Global Symmetry
Symmetry	C2
Stoichiometry	A2B2

Select Orientation

Front C2 axis

Select Display Mode

Secondary Structure | Subunit | Symmetry

Display Options

Style	Ball and Stick
Color	Subunit
Surface	None

- H-Bonds
- SS Bonds
- Rotation
- Black Background
- Polyhedron
- Axes

PDB – JSmol

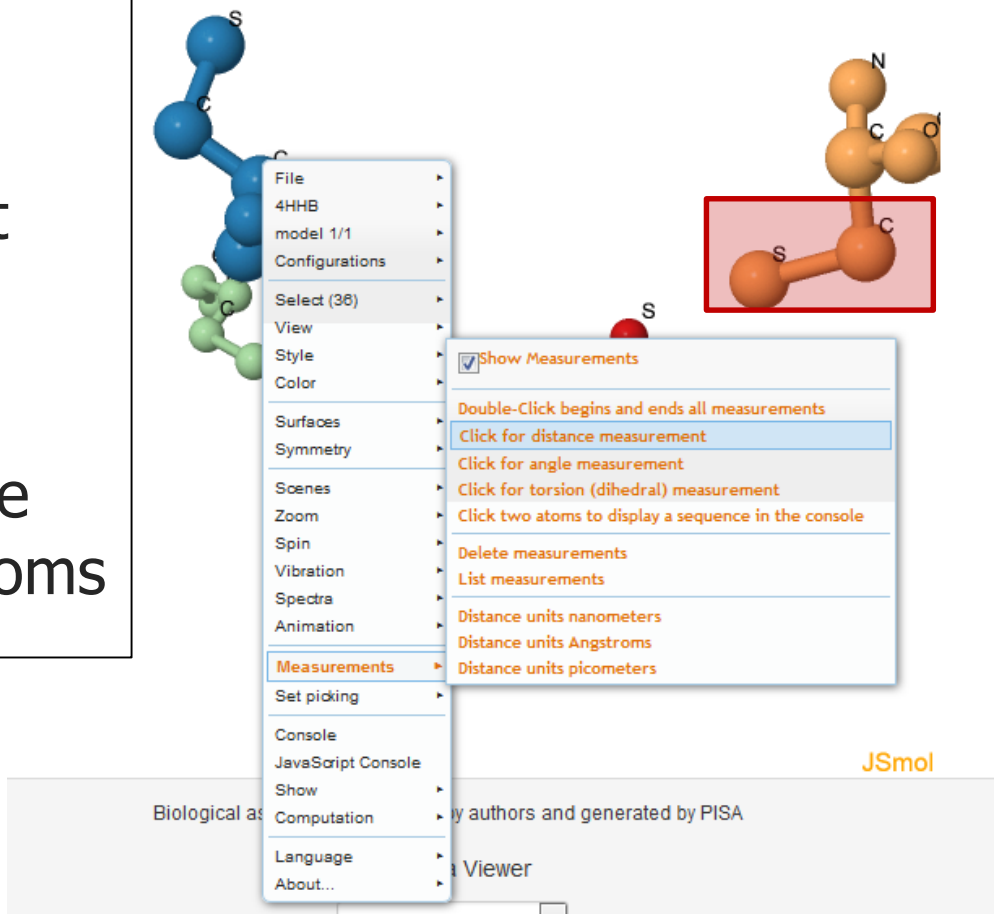
Zoom in

Right click

Measurements

Click for distance measurement

Click on S and C to measure the distance between those two atoms



PDB – JSmol

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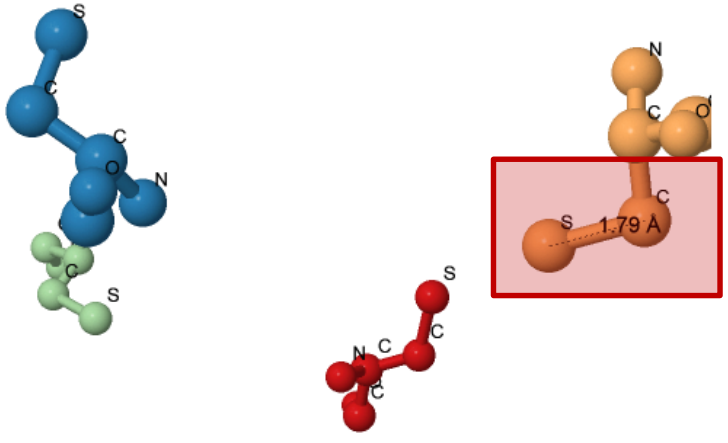
4HHB

THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT 1.74 ANGSTROMS RESOLUTION

Display Files | Download Files

NOTE: Use your mouse to drag, rotate, and zoom in and out of the structure. Help

You measured the distance between C and S of Cysteine which is about 1.79 angstroms



JSmol

Biological assembly 1 assigned by authors and generated by PISA

Select a Viewer

JSmol (JavaScript)

Structure Details

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Stoichiometry	A2B2

Select Orientation

◀ *Front C2 axis* ▶

Select Display Mode

Secondary Structure | Subunit | Symmetry

Display Options

Style	Ball and Stick
Color	Subunit
Surface	None

☐ H-Bonds ☐ SS Bonds
☐ Rotation ☐ Black Background
☐ Polyhedron ☐ Axes

- **QUESTIONS?**

- Please, download **Exercises #4** from MOODLE and upload until next Monday 8:00 a.m.

GOOD LUCK!