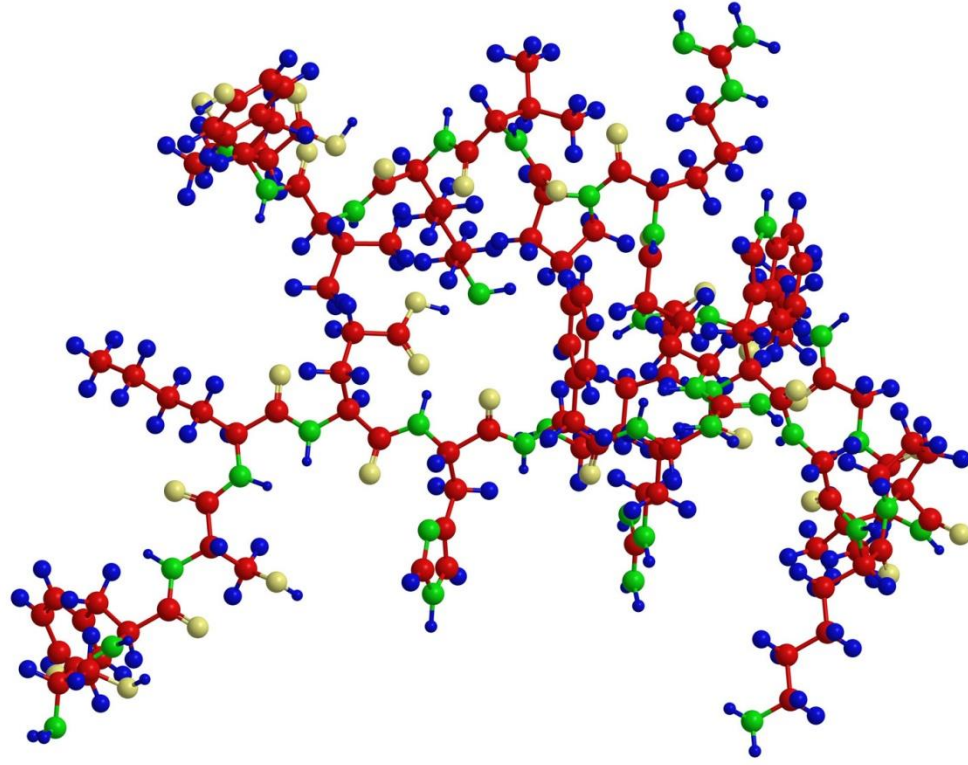
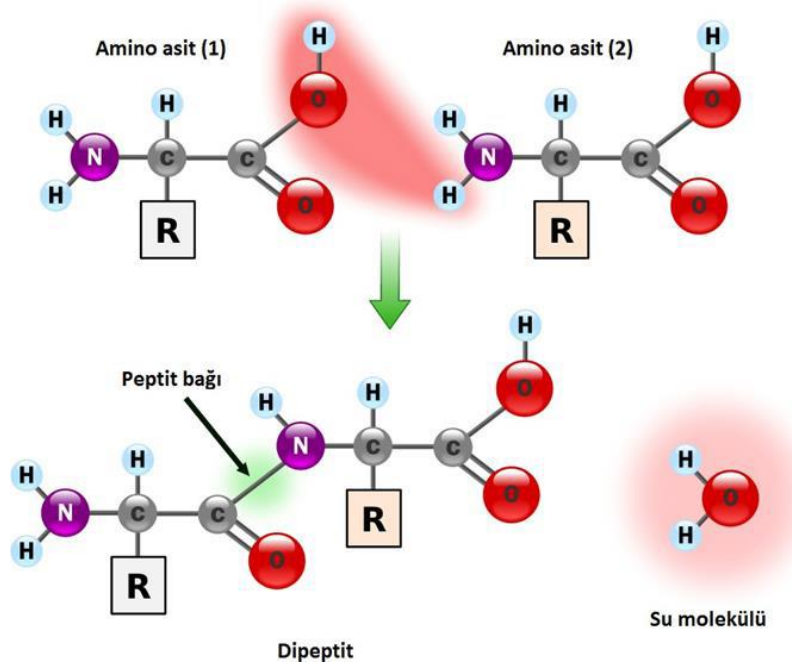


# Proteinlerin Yapısı ve Özellikleri-2



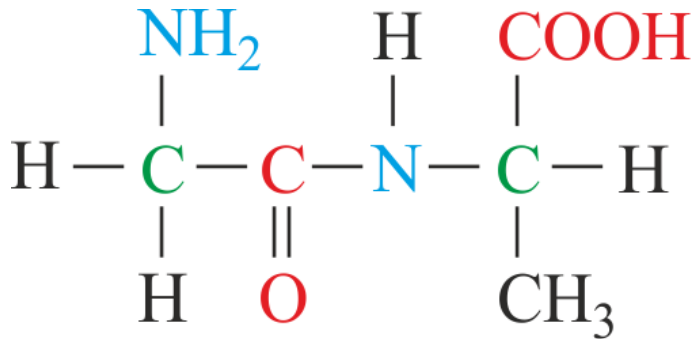
# Proteinler

- Peptitler/proteinler, amino asit polimerleridir.
- Bir peptidin en uçta bulunan serbest  $\alpha$ - amino kısmı amino ucu (N-terminal ucu), diğer uçta bulunan karboksil grubu ise karboksil ucu (C-terminal ucu) olarak adlandırılır.
- İki amino asit molekülü, değişken bir amit bağı olan peptit bağı ile kovalent olarak bağlanarak dipeptit oluşturur.
- Kondensasyon tepkimelerine bir örnek teşkil eden bu bağ oluşurken, bir amino asidin karboksil grubundaki OH grubu ile diğerinin amino grubundaki bir H atomu su oluşturarak uzaklaştırılır (dehidrasyon).

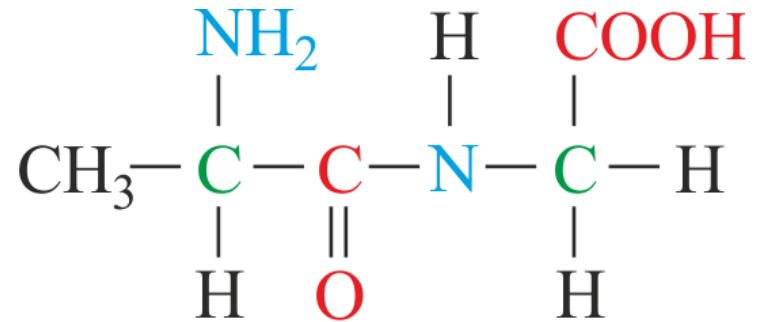


# Peptid bağları

- ❖ Peptid bağları normal yollarla veya ısıtılmak veya üre gibi yüksek konsantrasyonlarda proteinleri denature eden ajanlarla yıkılmazlar.
- ❖ Bu bağları nonenzimatik olarak yıkmak için yüksek ısıda uzun süre kuvvetli asit yada bazlarla maruz bırakmak gerekir.
- ❖ Genel bir kural olarak peptid zincirinin serbest amino ucu (N-terminal) sol tarafa, serbest karboksil ucu (C-terminal) sağ tarafa yazılır.



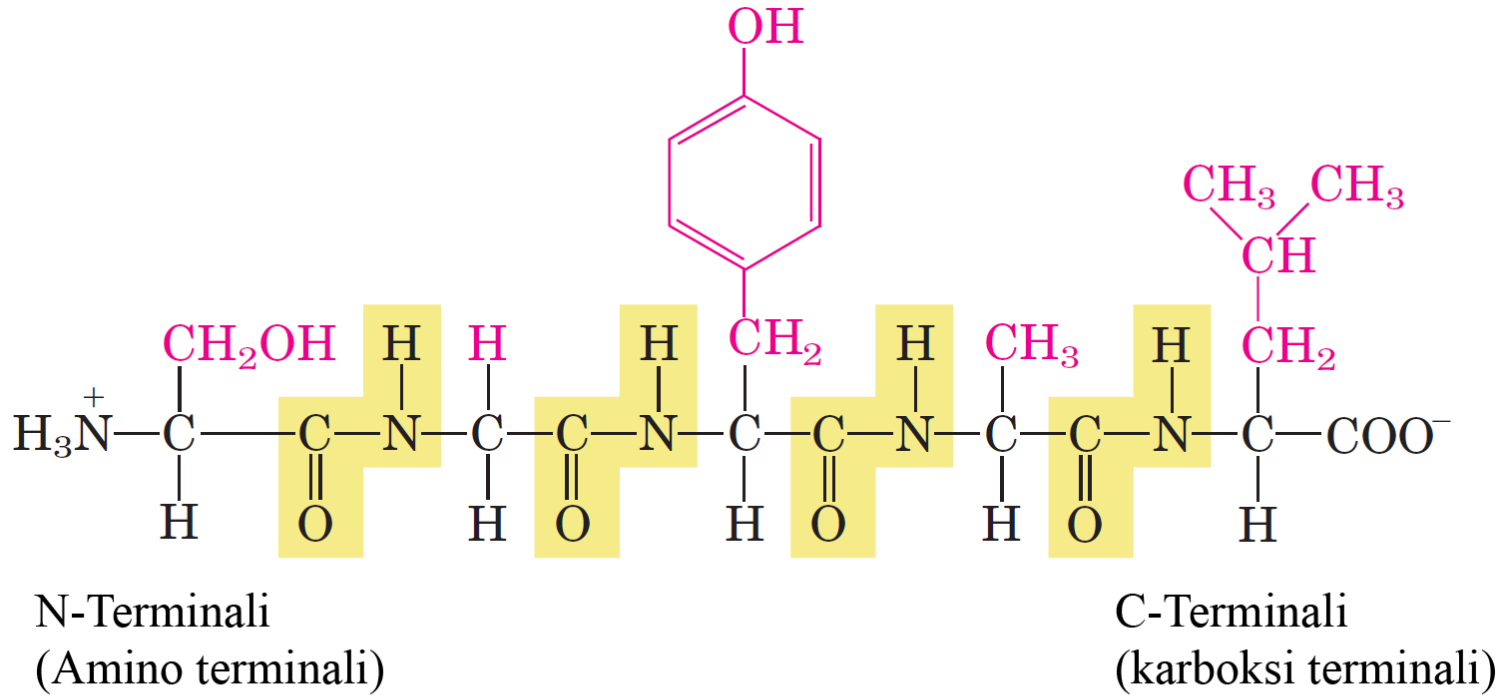
GlyAla



AlaGly

# Peptid bağları

❖ Polipeptiddeki her aa bir birim olarak adlandırılır. Bir polipeptid adlandırılırken C-terminal aa hariç, aa isimlerinin son ekleri (-in, -an, -ik, -at ..) -il ile değiştirilir.



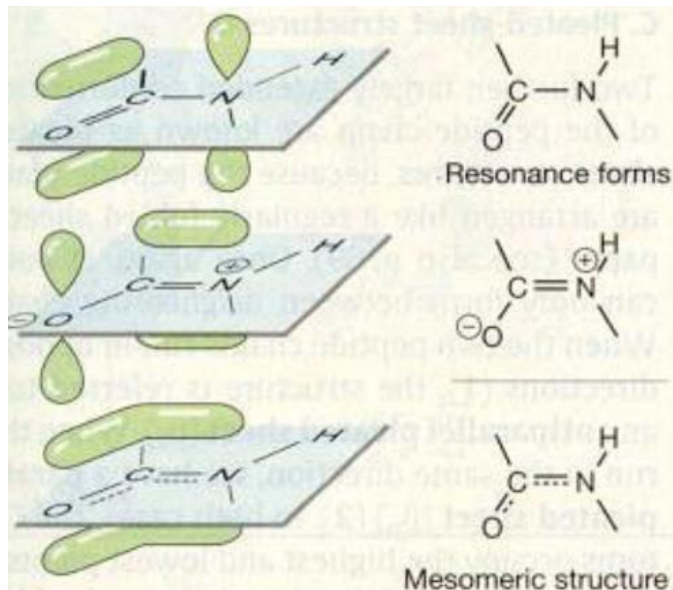
Serilglisiltirozilalanillösin penta peptidi

Ser-Gly-Tyr-Ala-Leu

# Peptid bağlarının özellikleri

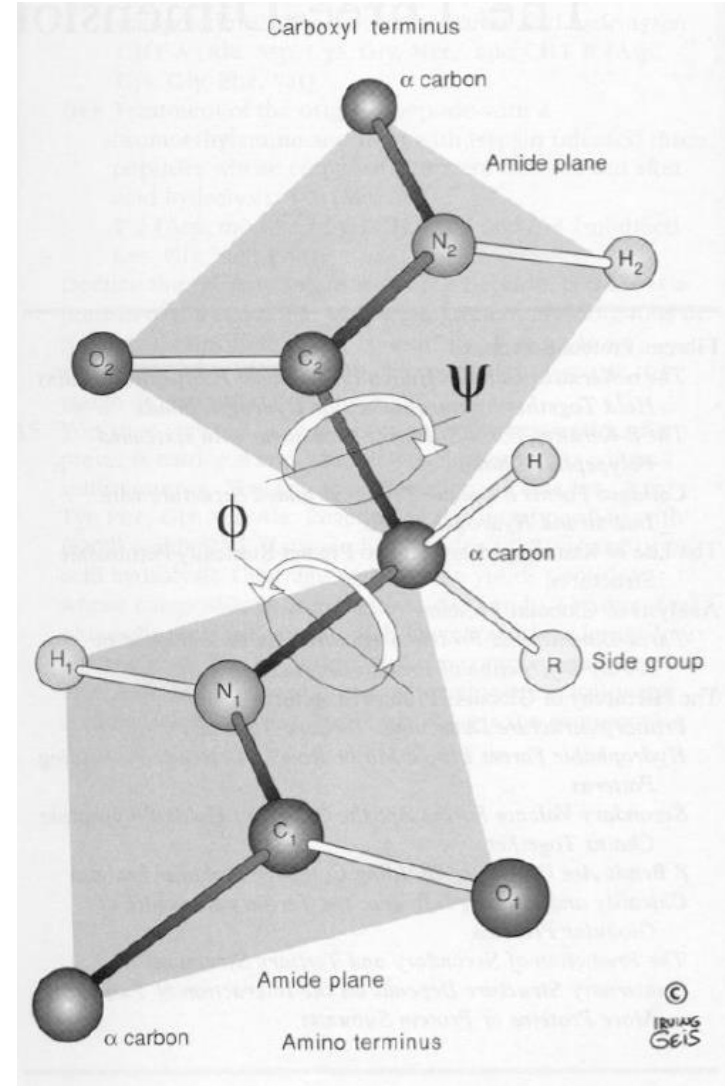
## a) Bağ etrafında rotasyon kısıtlılığı

Bir C–N tek bağının uzunluğu  $1,49\text{Å}$  ( $149\text{pm}$ ) ve bir C=N çift bağının uzunluğu  $1,27\text{Å}$  ( $127\text{pm}$ ) olduğu halde peptit bağının uzunluğu  $1,32\text{Å}$  ( $132\text{pm}$ ) kadardır. Peptit bağının uzunluğunun C=N çift bağının uzunluğundan büyük C–N tek bağının uzunluğundan küçük olması nedeniyle peptit bağının kısmen çift bağ olduğu kabul edilir. Bunun nedeni, peptit bağlarında rezonans veya mezomeri denen durum olmasıdır:



# Peptid bağlarının özellikleri

➤ Çift bağların eksen etrafında dönmeleri sınırlı olduğundan, peptid bağı oluşumuna katılan grupların atomları (3C, O, N ve H tomları) bir düzlemde bulunurlar; peptid bağı, rijit ve düzlemseldir.



# Peptid bağlarının özellikleri

b) Trans konfigürasyonu  
Peptid bağı, R gruplarının cis pozisyondaki streik etkileşiminden dolayı, genel olarak bir trans bağıdır.

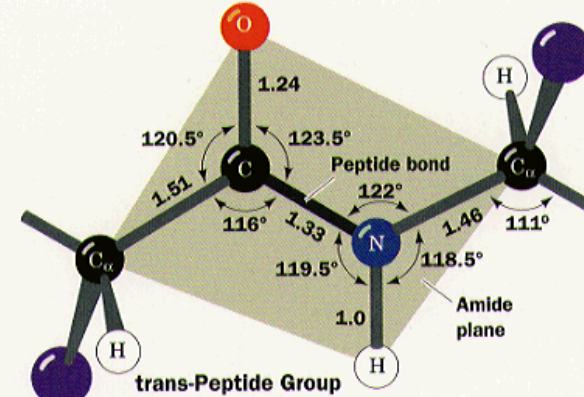


Figure 7-1. The trans-peptide group.

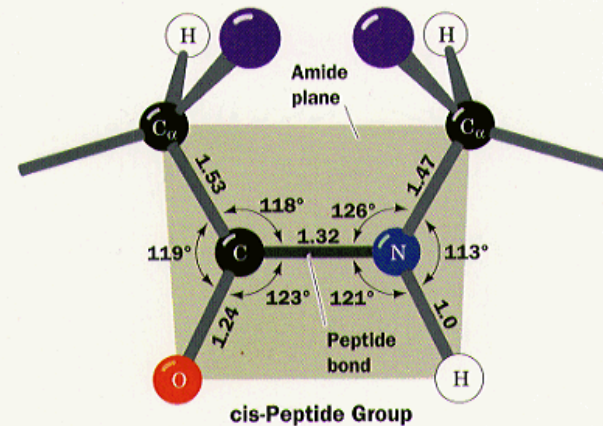


Figure 7-2. The cis-peptide group.

# Peptid bağlarının özellikleri

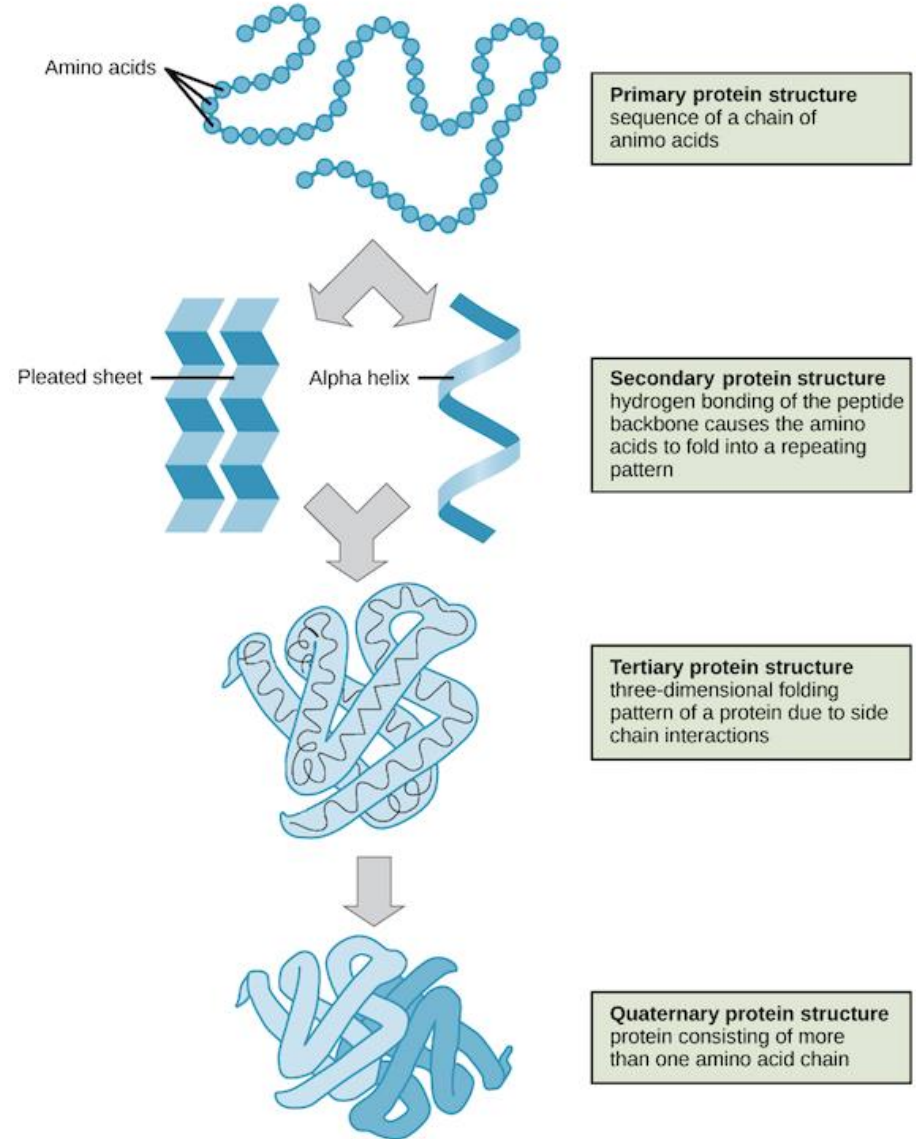
- c) Yüksüz fakat polar yapıdadır:
- Bütün amid bağları gibi, peptid bağının C=O ve –NH grupları 2 ila 12 pH dışında ne proton alırlar ne de proton verirler.
- Bu yüzden, polipeptidlerdeki yüklü gruplar sadece N-terminal  $\alpha$ -amino grubu, C-terminal  $\alpha$ -karboksil grubu ve yapıda yer alan amino asitlerin yan zincirlerindeki iyonize gruplardan oluşur.
- Peptid bağlarındaki –C=O ve –NH grupları polardır ve hidrojen bağı oluşumunda rol alırlar.



# Protein yapısı

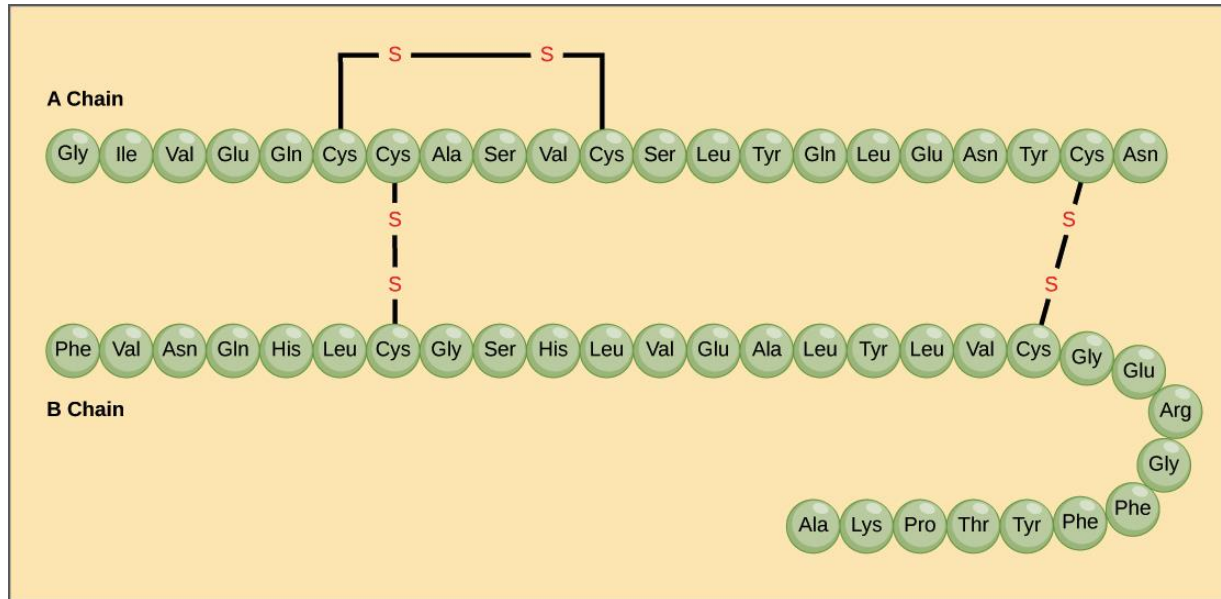
Proteinlerin dört yapısal düzeyi tanımlanmıştır:

- Birincil yapı,
- İkincil yapı,
- Üçüncül yapı (Tersiyer),
- Dördüncül yapı (Kuarterner).



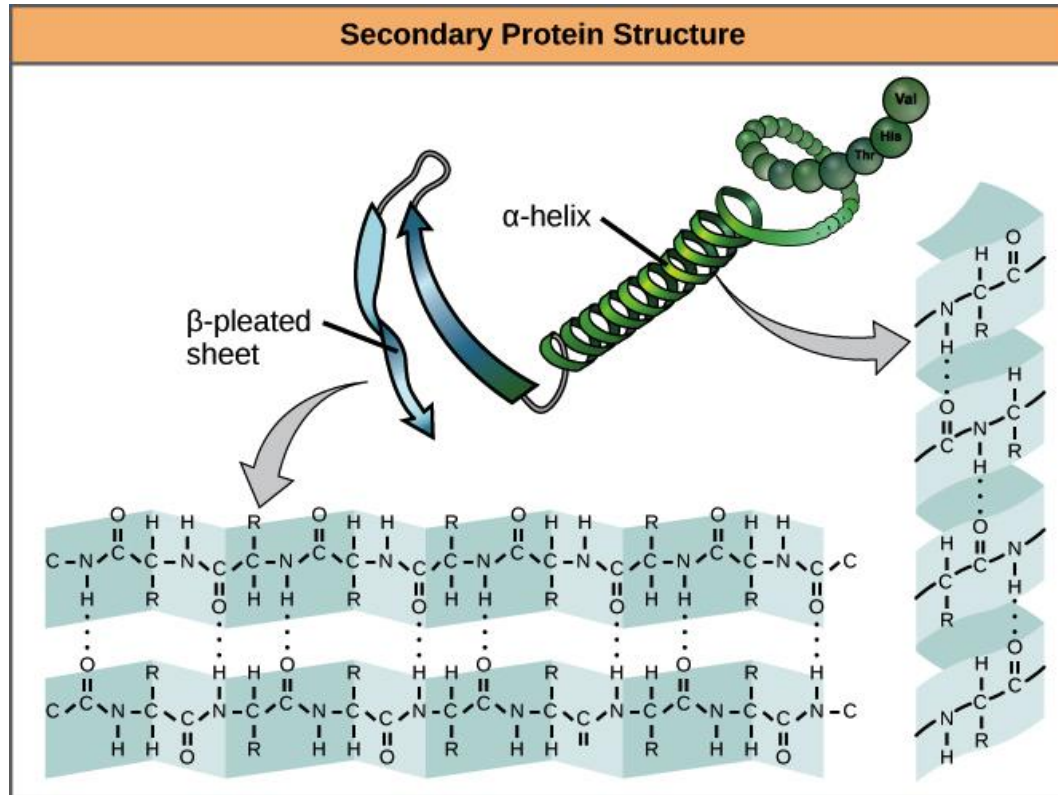
# Proteinlerin birincil yapısı

- Amino asitlerin peptit bağlarıyla birbirlerine bağlanıp oluşturdukları düz polimer (polipeptit) zinciri, proteinin birincil yapısını ifade eder.
- Polipeptit zincirinin biyolojik olarak aktif proteinlere dönüşebilmesi için özgül 3 boyutlu yapısını kazanması gerekmektedir.
- Bir proteinin birincil yapısı, onun 3 boyutlu yapısını belirler.
- Birincil yapıdaki amino asit değişiklikleri proteinin üç boyutlu konformasyonunu ve fonksiyonunu etkileyebilir.



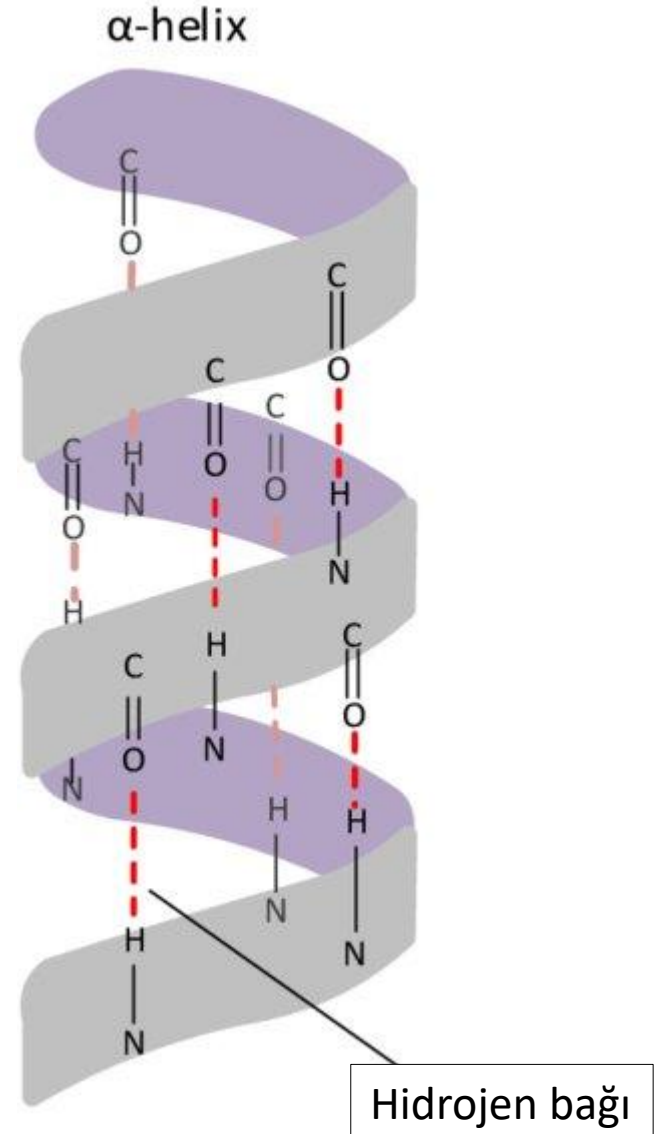
# Proteinlerin sekonder yapısı

- Proteinin ikincil yapısı, genel konformasyonunu etkileyen ve tekrarlanan kıvrım veya katlanmalarla tanımlanır.
- Bu katlanmalar, polipeptit omurgası boyunca düzenli aralıklarla kurulan hidrojen bağlarıyla oluşur.
- Proteinlerde sıklıkla karşılaşılan sekonder yapılar:
  - $\alpha$ -heliks
  - $\beta$ -tabakadır.



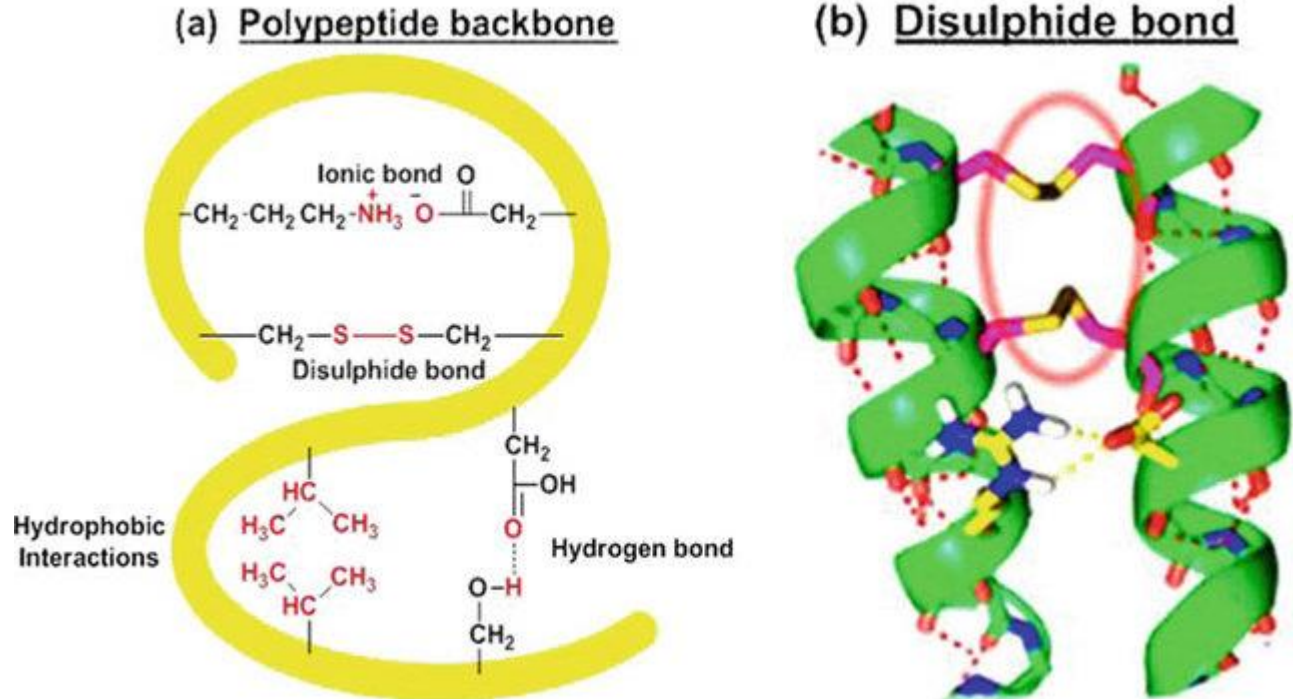
# Proteinlerin sekonder yapısı

- Doğada çeşitli polipeptid heliksleri bulunmaktadır. Ancak en sık karşılaşılan  $\alpha$ -helikstir.
- Bu yapıdaki aa lerin yan zincirlerinin birbiriyle sterik etkileşimi engellenecek şekilde merkez eksenenden dışarı doğru uzanan, kıvrılarak sıkıca birleşmiş bir spiral yapıdadır.



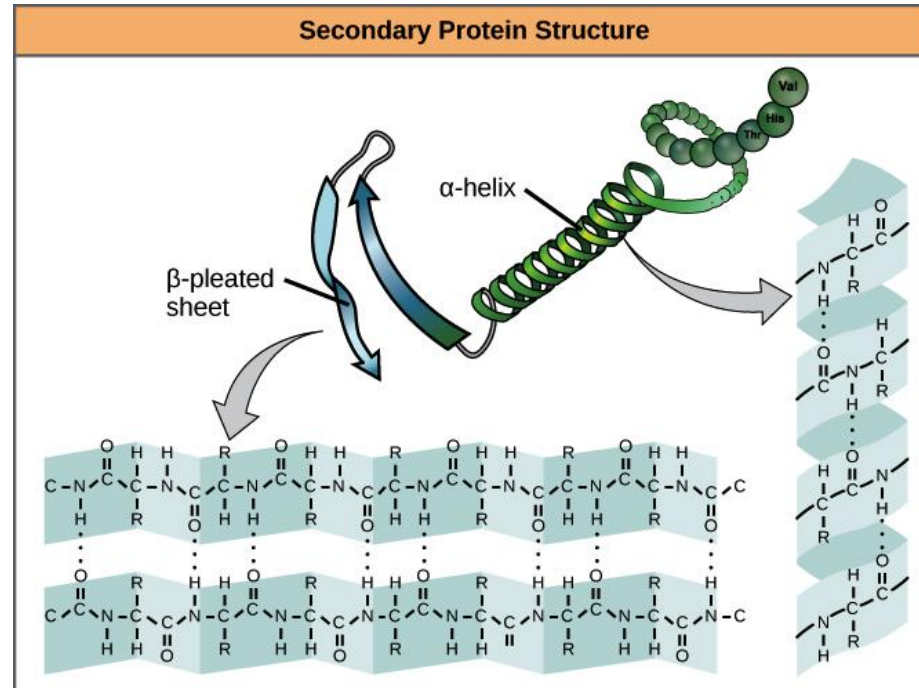
# Proteinlerin sekonder yapısı

- Farklı yapıdaki proteinler  $\alpha$ -heliks taşımaktadır:
- Keratinler yapılarının tamamına yakını  $\alpha$ -helikal olan birbirine sıkıca bağlı bir fibröz proteindir.
- Saç ve deri gibi dokuların ana bileşenidir.
- Sertlikleri yapılarındaki polipeptid zincirleri arasındaki disülfid bağlarının sayısına bağlıdır.
- Yapısı ortalama %80  $\alpha$ -helikslerden oluşan hemoglobin, keratinin aksine esnek bir globüler proteindir.



# Proteinlerin sekonder yapısı

- Bir  $\alpha$ -heliks, her 4 amino asitte bir, peptid bağı karbonil oksijenleri ile amid hidrojenleri arasında kurulan kovalent olmayan H bağları ile şeklini koruyan kıvrımlı bir yapıdır.
- Bu kıvrımlı yapısından dolayı dayanıklı bir formdur.
- Bu hidrojen bağları tek tek zayıf bağlardır ancak birlikte heliks yapısını stabilize etme görevini üstlenirler.
- Heliksin bir dönüşünde  $\sim 3,6$  aminoasit vardır ve bir dönüş uzunluğu  $5.4 \text{ \AA}$  dur.
- R grupları sarmaldan dışa doğru yönelmiştir.
- $\alpha$ -heliks yapısı globüler proteinlerde görülür.



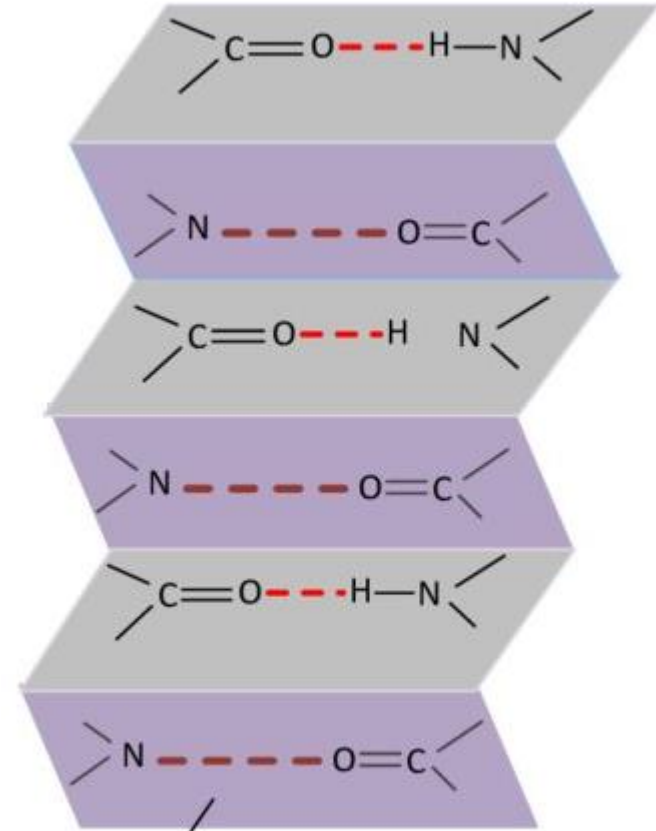


# Proteinlerin sekonder yapısı

$\beta$ -Sheet

## $\beta$ -tabaka:

- Bütün peptid bağı parçalarının hidrojen bağına katıldığı başka bir sekonder yapıdır.
- $\beta$ -tabakaları yüzeyleri kırmalı görünümündedir ve bu yüzden sıklıkla  $\beta$ -kırmalı tabaka denmektedir.
- Geniş oklar şeklinde görüntülenir.
- Hidrojen bağları polipeptid omurgaya dik konumdadır.

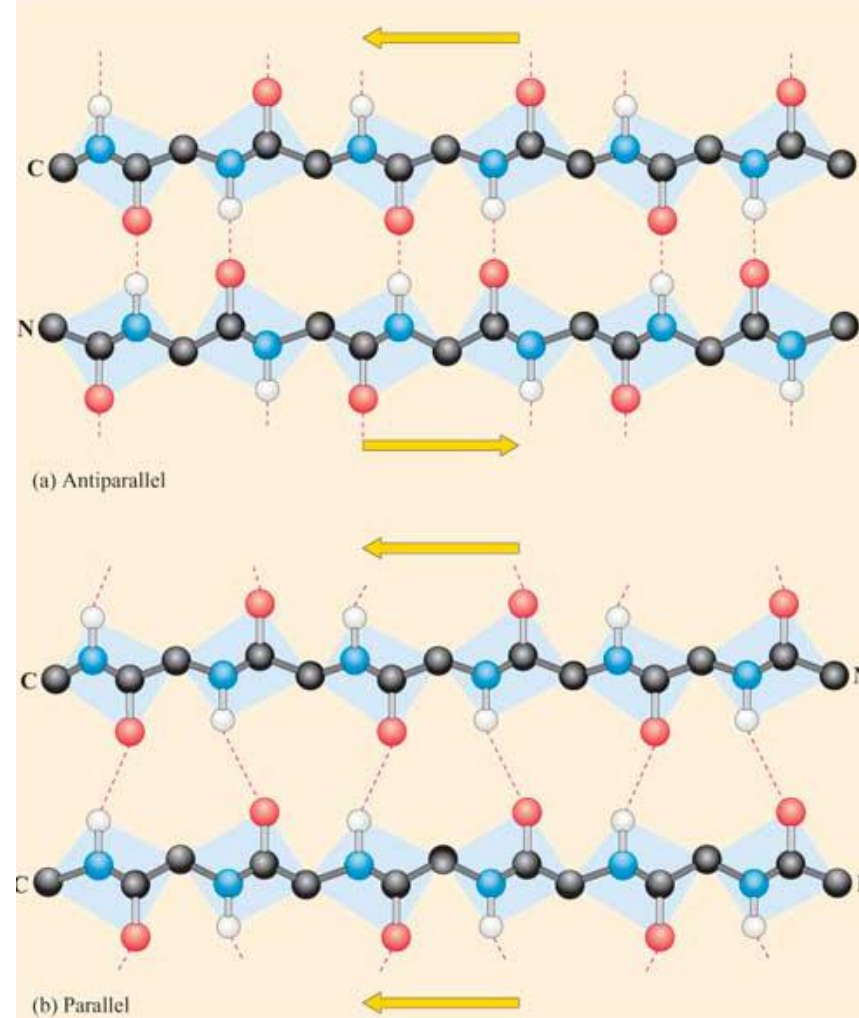


Hidrojen bağı

# Proteinlerin sekonder yapısı

## $\beta$ -tabaka:

- $\alpha$ -heliksin aksine  $\beta$ -tabakalarda hemen hemen tamamen açılmış iki veya daha çok peptid zinciri ( $\beta$ -zinciri) veya polipeptid parçası yer alır.
- Bir  $\beta$ -tabaka birbirine paralel ( $\beta$ -zincirin bütün N-uçları birarada) veya antiparalel ( $\beta$ -zincirinin N-terminal ve C-terminal uçları farklı yönlenmiş) olarak düzenlenmiş iki veya daha çok polipeptid zinciri veya polipeptid parçasından oluşabilir.





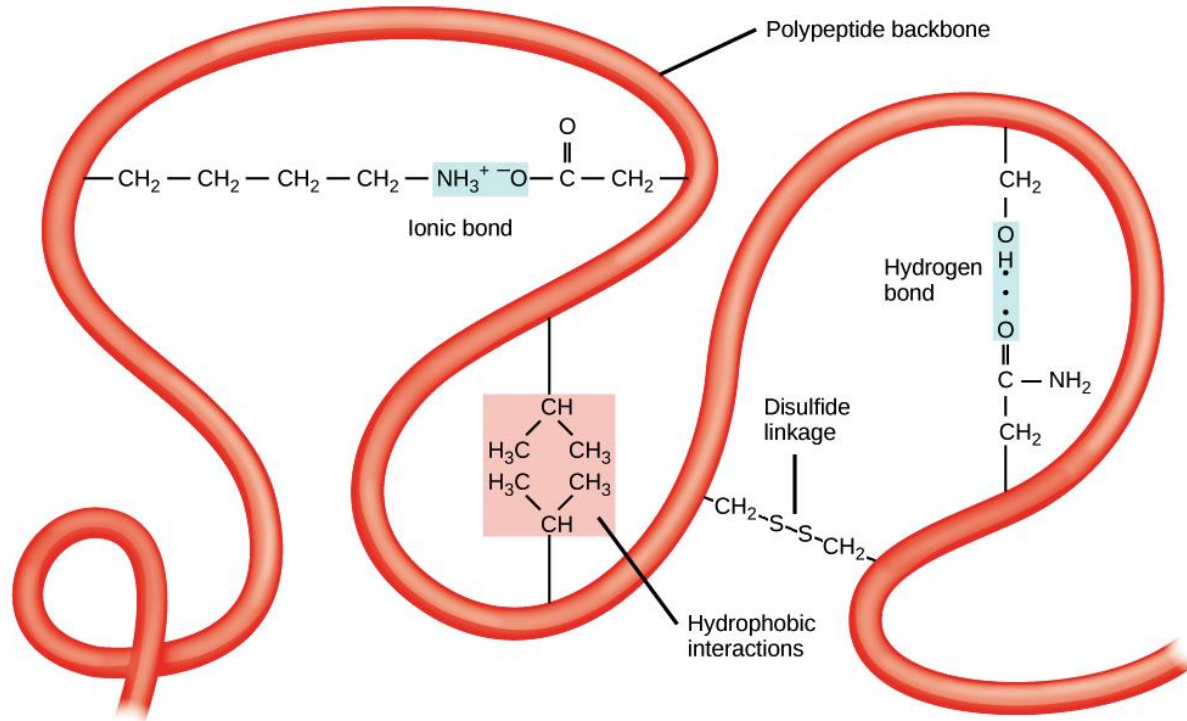
# Proteinlerin tersiyer yapısı

İkincil yapı elemanlarının daha üst düzeyde katlanmalarıyla oluşan üçüncül yapı, özellikle R grupları arasındaki etkileşimlerden kaynaklanır.

Üçüncül yapı ile üç boyutlu oluşuma katılan başlıca etkileşimler:

## ➤ Disülfid bağları:

İki sistein kalıntısının sülfidril (-SH) gruplarının sistin kalıntısı oluşturacak şekilde kovalent olarak bağlanmasıdır. Protein yapısının üç boyutlu yapısının stabilitesini sağlarlar.



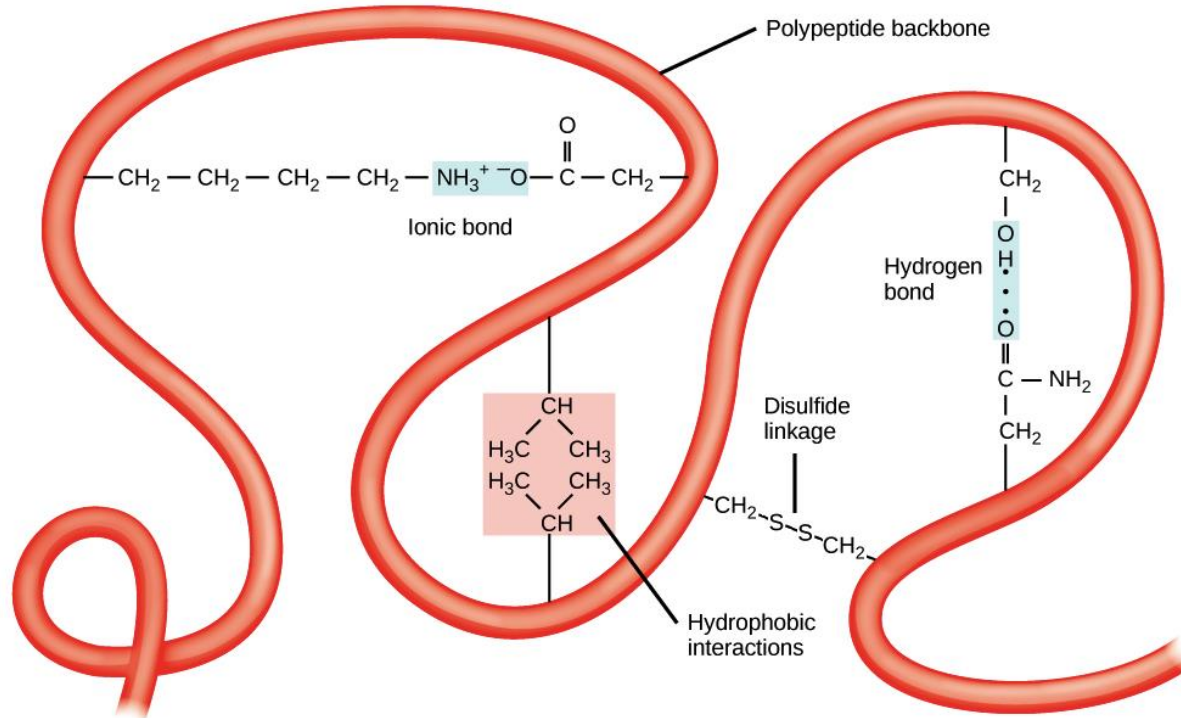
# Proteinlerin tersiyer yapısı

## ➤ Hidrofobik etkileşimler:

Polar olmayan yan zincire sahip amino asitler diğer hidrofobik aa lerle birleşerek polipeptid molekülünün iç tarafında yer almaya çalışırlar.

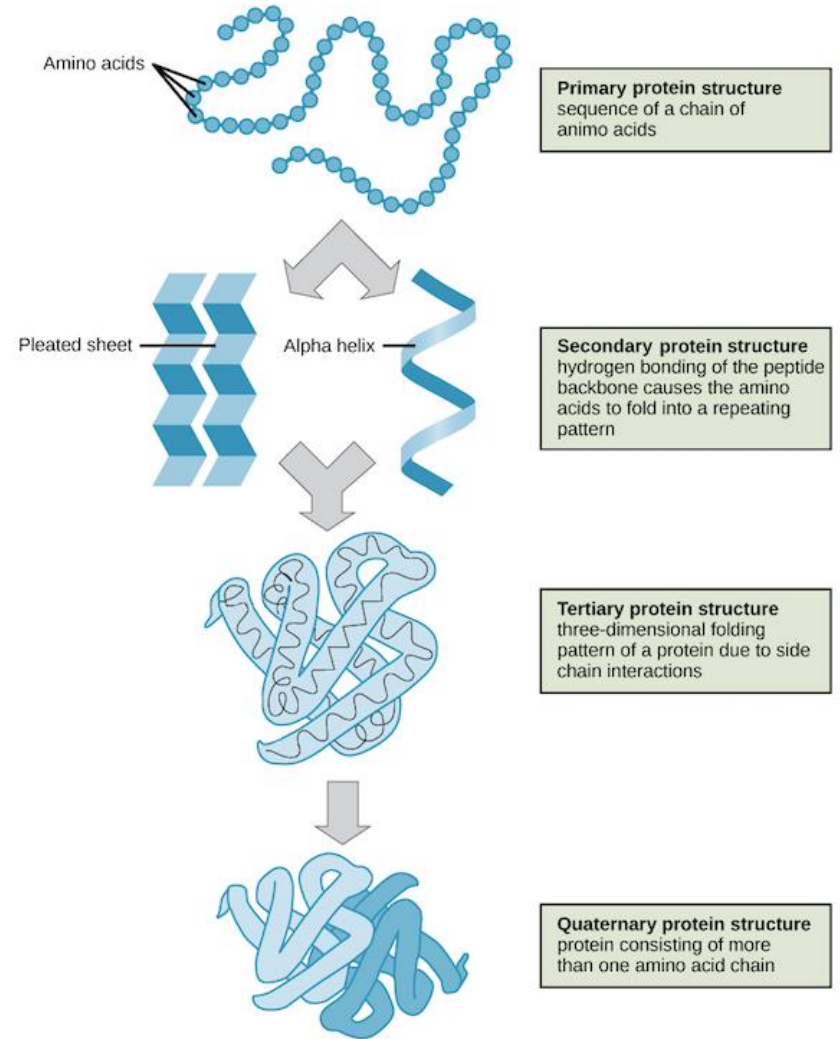
## ➤ İyonik etkileşimler:

Aspartat veya glutamatın yan zincirindeki karboksil grupları gibi negatif yüklü gruplar, lizinin yan zincirindeki amino grubu gibi pozitif yüklü gruplarla reaksiyona girer.



# Proteinlerin kuaterner yapısı

- Birçok protein tek polipeptid zincirinden meydana gelir. Bunlar monomerik proteinlerdir.
- Bir çoğu da yapısal olarak benzer veya tamamen ilgisiz bir yada daha fazla polipeptid zincirinden oluşur.
- Bu polipeptid zincirlerinin düzenlenmesine proteinin **kuaterner yapısı** denir.
- Subuniteler hidrofobik etkileşimler, hidrojen bağları ve iyonik bağlar gibi kovalent olmayan etkileşimlerde biraraya gelirler.



Bu dördüncül yapılanmaya göre düşünüldüğünde proteinler uzun bloklar olarak yapılanmış **fibriler proteinler** ve yuvarlak biçimlerde katlanmış **globular proteinler** olarak sınıflandırılmaktadırlar.

➤ **Fibriler proteinler:**

- tek tip sekonder yapı içerirler.
- destek, yapı, koruma, dayanıklılık ve esneklik ( keratin, kolajen, ipek) sağlarlar.

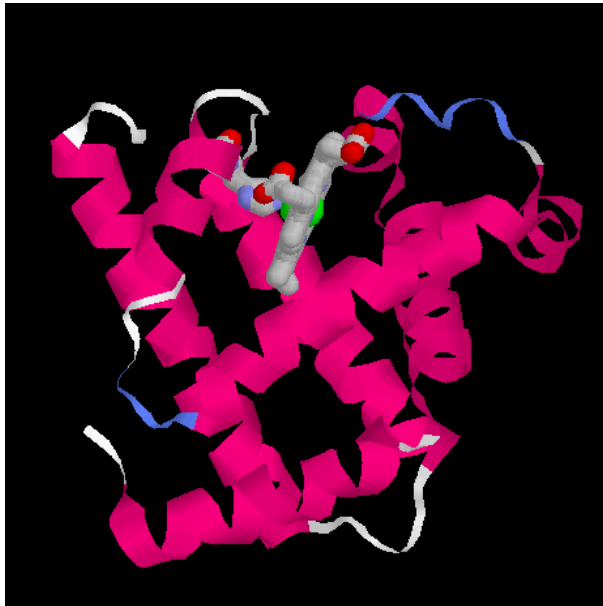
**Kolajen:** tendon, kırıkta kemik gibi bağ dokular, göz kornea tabakası

**Keratin:** Saç, tırnak, odun, boynuz, kirpi oku

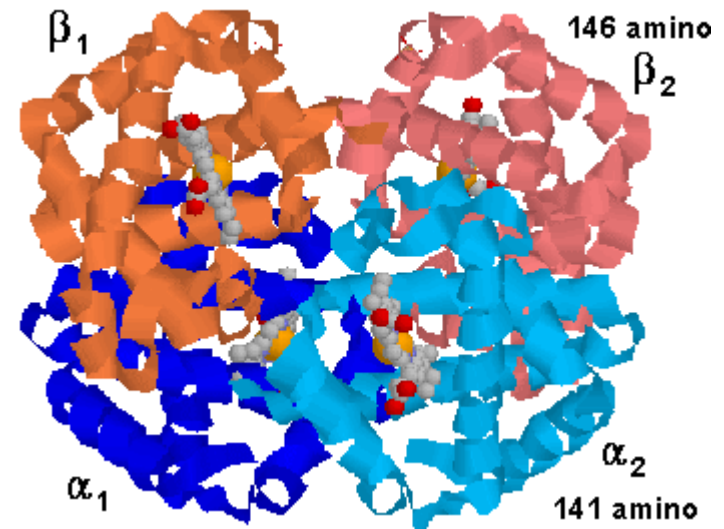
- iç kısmında ve yüzeyde yer alan hidrofobik aa lerden dolayı suda çözünmezler.
- polipeptid zincirleri arasındaki kovalant çapraz bağlarla (disülfid bağı) dayanıklılıkları arttırırlar.

## ➤ Globular proteinler:

- Bir polipeptidin farklı segmentleri ya da birden fazla polipeptid zinciri katlanarak paketlenmiş sıkı bir yapı oluşturur.
- Katlanma sayesinde artan yapısal çeşitlilik farklı biyolojik fonksiyonların gerçekleşebilmesi için de önemlidir.
- Birden fazla sekonder yapı içerir.
- enzimler, düzenleyici proteinler, transport proteinler, motor proteinler, immunoglobulinler vb.



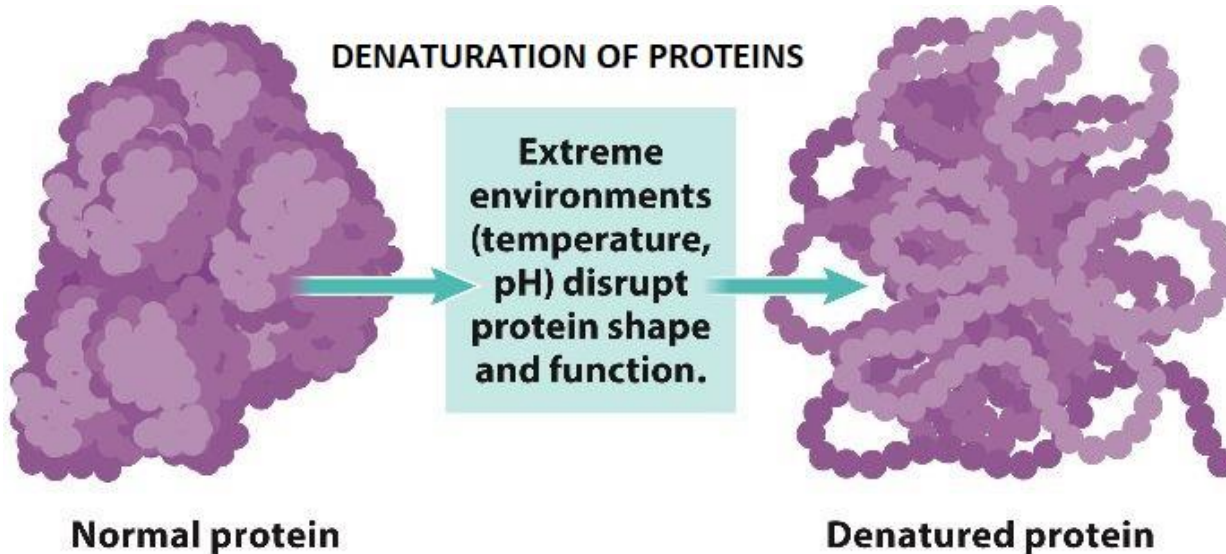
myoglobinin ribbon yapısı



İnsan hemoglobini

# Protein Denaturasyonu

- Üç boyutlu bir yapıya sahip olan ve biyolojik bakımdan aktif olan proteinlere yapısı bozunmamış anlamına gelen doğal proteinler adı verilmektedir.
- Peptit bağları koparılmadan bir proteinin üç boyutlu yapısının bozulmasına ve aktivitenin kaybolması olayına ise **denaturasyon** adı verilmektedir.
- Bir proteinde biyolojik aktivitenin bozulması ve çözünürlüğün değişmesi, denaturasyon için bir kriter olarak kabul edilmektedir.





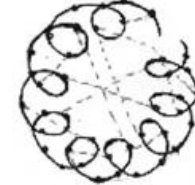
# Protein Denaturasyonu

Proteinler genellikle aşağıdaki koşullar altında denature olmaktadır.

1- Proteinler 50-60 °C'ın üstündeki sıcaklıklarda denature olmaktadır.

2- Proteinler pH 4'ün altında ve pH 10'un üzerinde denature olmaktadır.

3- Proteinler alkol, aseton ve eter gibi organik çözücülerle veya üre,  $\beta$ -merkaptoetanol ve guanidin HCl gibi bileşiklerle muamele edildiklerinde denature olmaktadır.

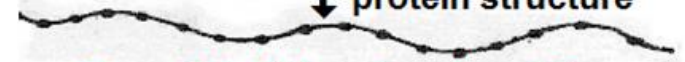


**Native conformation/tertiary structure of protein-stabilized by non-covalent bonds (Biologically active/functional protein)**

**Heat** ↓ Uncoiling and Disruption of protein structure



**Heat** ↓ Uncoiling and Disruption of protein structure



**Coagulated/denatured protein with unaltered primary structure (Biologically inactive protein)**

**Fig. 6.10: Heat coagulation**

# Protein Denaturasyonu

Eğer protein kuaterner bir yapıya sahipse denaturasyon koşulları altında iki türlü değişme ortaya çıkmaktadır.

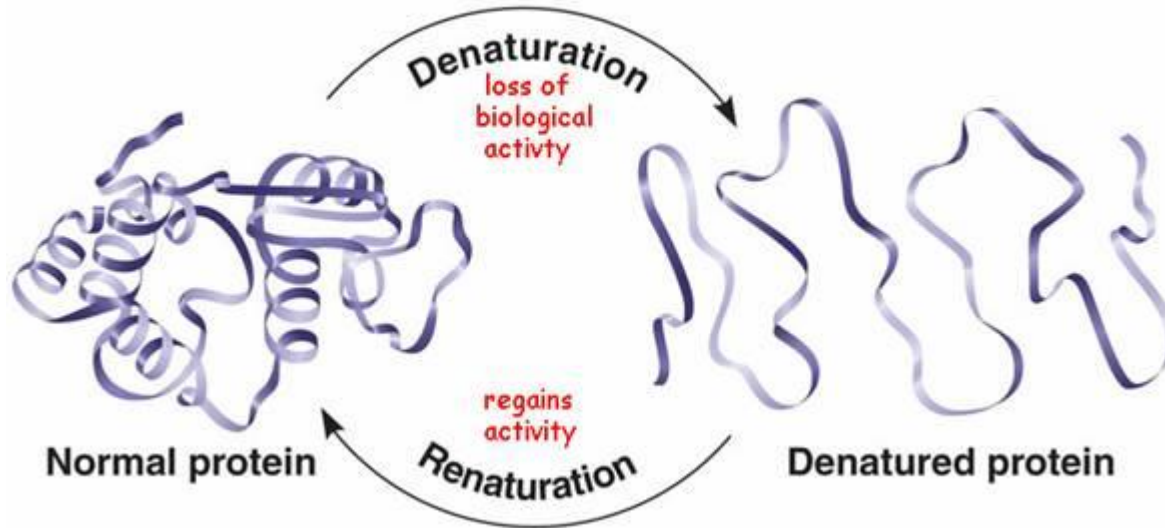
1- Proteinin subüniteleri birbirinden ayrılmaktadır.

2- Her bir subünitenin ve tersiyer yapıya sahip tek polipeptit zincirlerinin konformasyonu, yani üç boyutlu yapısı bozularak tesadüfi kıvrılmalar ve bükülmeler meydana gelmektedir.



# Protein Denaturasyonu

- Denaturasyon eğer ılımlı koşullarda gerçekleştirilmiş ise bazen kuaterner yapıya sahip proteinlerin sadece subuniteleri birbirinden ayrılmakta; fakat tersiyer yapıları bozulmamaktadır.
- Böyle durumlarda denature edici faktör ortadan kalktığında protein eski konformasyonunu, dolayısıyla aktivitesini geri kazanabilir.
- Proteinler, bozulmuş durumda iken tekrar üç boyutlu yapılarını kazanmaları ve yeniden biyolojik aktivite göstermeleri olayına **renaturasyon** adı verilmektedir.



# Protein DataBank

The image shows a screenshot of the RCSB PDB website. At the top, there is a navigation bar with links for Deposit, Search, Visualize, Analyze, Download, Learn, and More. A search bar is located on the right side of the header. The main content area features a 'Welcome' message, a 'Deposit' button, and a section titled 'A Structural View of Biology' which describes the database's mission. To the right, there is a 'June Molecule of the Month' section featuring a 3D model of the SARS-CoV-2 Spike protein. Below this, there are sections for 'Latest Entries', 'Features & Highlights', and 'News'. A callout box on the left side of the page contains the text: 'Protein Data Bank Home Page https://www.rcsb.org/'.

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Welcome

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**Protein Data Bank Home Page**  
<https://www.rcsb.org/>

**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.

Upon the data by creating tools and resources for in molecular biology, structural biology, computational

**June Molecule of the Month**

SARS-CoV-2 Spike

**VIRUS**

**Latest Entries** As of Tue, Jun 16, 2020

**Features & Highlights**

- Sequence Motif Searching  
Use Advanced Search to find short sequence patterns in PDB structures
- Enter the Coronavirus CellPAINT Contest  
Show us how you can illustrate coronavirus with a new version of CellPAINT
- Announcement: Legacy MyPDB Will

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From careful biocuration of important drug targets to releasing new website functionality, RCSB PDB supports research and education during this public health crisis. 06/16/2020

Coronavirus CellPAINT Contest Winners 06/16/2020

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### A Structural View of Biology

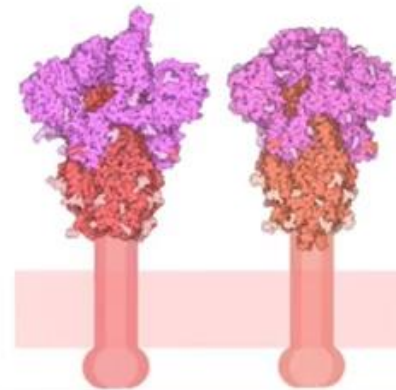
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The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.



### June Molecule of the Month



SARS-CoV-2 Spike

### Latest Entries

As of Tue Jun 16 2020



### Features & Highlights



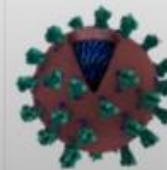
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### News

Publications



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Enter search term(s)



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### A Structural View of Biology

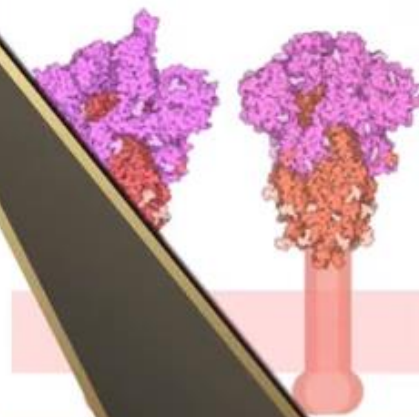
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The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.



### June Molecule of the Month



Type the protein name in the search box (LasR)

### Latest Entries

As of Tue Jun 16 2020



### Features & Highlights



Sequence Motif Searching Use Advanced Search to find short sequence patterns in PDB structures



Enter the Coronavirus CellPAINT Contest Show us how you can illustrate coronavirus with a new version of CellPAINT



Announcement: Legacy MyPDB Will Be Discontinued October 2020



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cular Structures  
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nd Education



NUCLEIC ACID  
DATABASE



Worldwide  
Protein Data Bank  
Foundation

## Structural View of Bio

orce is powered by the Protein  
s of proteins, nucleic acids, an  
nd researchers understand al  
in synthesis to health and dise  
iber of the wwPDB, the RCSB  
3 PDB builds upon the data by  
and education in molecular bio  
nd beyond.

lasR



*in Polymer Entity Description*

Transcriptional regulator **LasR**

Transcriptional activator protein **lasR**

Transcriptional activator protein **LasR**

*in Gene Name*

**lasR**

*in Citation Title*

**LasR-OC12 HSL complex**

of Non-native Agonists of the **LasR** Quorum-Sensing Receptor Reveal

*in Structure Description*

Transcriptional regulator **LasR**

Transcriptional activator protein **lasR**

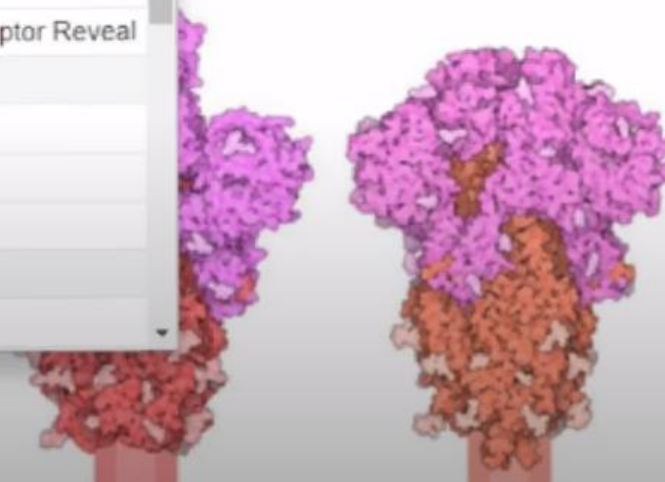
Transcriptional activator protein **LasR**

*in Structure Title*

**LasR-TP1 complex**



## Molecule of the Month



Search History Browse Annotations MyPDB Help

QUERY: Polymer Entity Description CONTAINS PHRASE "Transcriptional regulator LasR"

Open In Query Builder MyPDB Login

Advanced Search Query Builder

Refinements Clear All

Summary Gallery Compact -- Tabular Report --

Score

Download Selected Files

Select All

SCIENTIFIC NAME OF SOURCE ORGANISM Clear

Pseudomonas aeruginosa UCBPP-PA14 (6)

TAXONOMY Clear

Bacteria (6)

EXPERIMENTAL METHOD Clear

X-RAY DIFFRACTION (6)

POLYMER ENTITY TYPE Clear

Protein (6)

RESOLUTION Clear

1.5 - 2.0 (3)

2.0 - 2.5 (2)

2.5 - 3.0 (1)

RELEASE DATE Clear

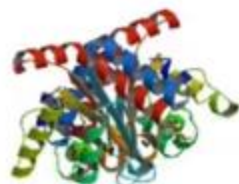
2015 - 2019 (6)

ENZYME CLASSIFICATION NAME Clear

MEMBRANE PROTEIN NAME Clear

Displaying 1 to 6 of 6 Structures Page 1 of 1

Display 25 per page



3D View

6MVN

LasR LBD L130F:3OC10HSL complex

Bassler, B.L., Paczkowski, J.E.

(2019) Proc Natl Acad Sci U S A 116: 245-254

Released 2019-01-16

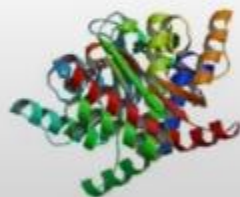
Method X-RAY DIFFRACTION 2.2 Å

Organisms Pseudomonas aeruginosa UCBPP-PA14

Macromolecule Transcriptional regulator LasR (protein)

Unique Ligands 3M5

Download File View File



3D View

6MVM

LasR LBD L130F:3OC14HSL complex

Paczkowski, J.E., Bassler, B.L.

(2019) ACS Chem Biol 14: 378-389

Released 2019-01-16

Method X-RAY DIFFRACTION 1.895 Å

Organisms Pseudomonas aeruginosa UCBPP-PA14

Macromolecule Transcriptional regulator LasR (protein)

Unique Ligands K4G

Download File View File

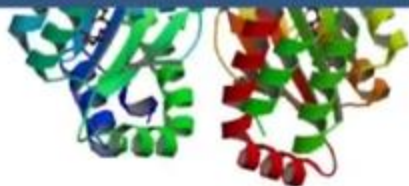


6MWW

LasR LBD:BB0126 complex

Bassler, B.L., Paczkowski, J.E.

Download File View File



3D View: [Structure](#) | [Electron Density](#) | [Ligand Interaction](#)

Global Symmetry: Cyclic - C2 (3D View)  
Global Stoichiometry: Homo 2-mer - A2

[Find Similar Assemblies](#)

Biological assembly 1 assigned by authors and generated by PISA (software)

#### Macromolecule Content

- Total Structure Weight: 79.94 kDa
- Atom Count: 5891
- Residue Count: 660
- Unique protein chains: 1

Mutation(s): No

Deposited: 2007-03-08 Released: 2007-03-27

Deposition Author(s): Bottomley, M.J., Muraglia, E., Bazzo, R., Carfi, A.

#### Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 1.80 Å

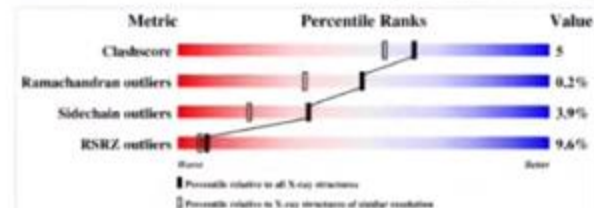
R-Value Free: 0.254

R-Value Work: 0.209

R-Value Observed: 0.211

#### wwPDB Validation

[3D Report](#) [Full Report](#)



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

#### Literature

[Download Primary Citation](#)

Molecular Insights Into Quorum Sensing in the Human Pathogen *Pseudomonas Aeruginosa* from the Structure of the Virulence Regulator<sub>1</sub>Lasr Bound to its Autoinducer.

[Bottomley, M.J., Muraglia, E., Bazzo, R., Carfi, A.](#)

(2007) *J Biol Chem* **282**: 13592

PubMed: [17363368](#) [Search on PubMed](#)

DOI: 10.1074/jbc.M700556200

[Structures With Same Primary Citation](#)

#### PubMed Abstract:

Many Gram-negative bacteria communicate via molecules called autoinducers to coordinate the activities of their populations. Such communication is termed quorum sensing and can regulate pathogenic virulence factor production and antimicrobial resista ...

#### Macromolecules

Find similar proteins by: [Sequence](#) | [Structure](#)

Entity ID: 1

Molecule	Chain	Sequence Length	Organism	Details
----------	-------	-----------------	----------	---------



Structure Summary

3D View

Annotations

Sequence

Experiment

Display Files

Download Files

Biological Assembly 1

# 2UV0

Structure of the *P. aeruginosa* LasR ligand-binding domain bound to its autoinducer

DOI: 10.2210/pdb2UV0/pdb

Classification: TRANSCRIPTION

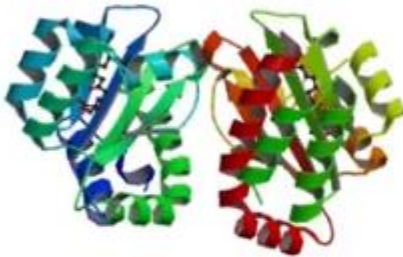
Organism(s): *Pseudomonas aeruginosa* PAO1

Expression System: *Escherichia coli* BL21(DE3)

Mutation(s): No

Deposited: 2007-03-08 Released: 2007-03-27

Deposition Author(s): Bottomley, M.J., Muraglia, E., Bazzo, R., Carfi, A.



## Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 1.80 Å

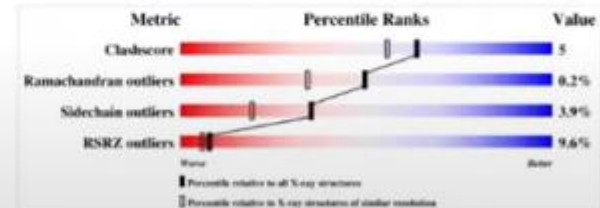
R-Value Free: 0.254

R-Value Work: 0.209

R-Value Observed: 0.211

## wwPDB Validation

3D Report Full Report



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

## Literature

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Molecular Insights Into Quorum Sensing in the Human Pathogen *Pseudomonas Aeruginosa* from the Structure of the Virulence Regulator Lasr Bound to its Autoinducer.

3D View: Structure | Electron Density | Ligand Interaction

Global Symmetry: Cyclic - C2 (3D View)

Global Stoichiometry: Homo 2-mer - A2

Find Similar Assemblies

Biological assembly 1 assigned by authors and generated by PISA (software)

## Macromolecule Content

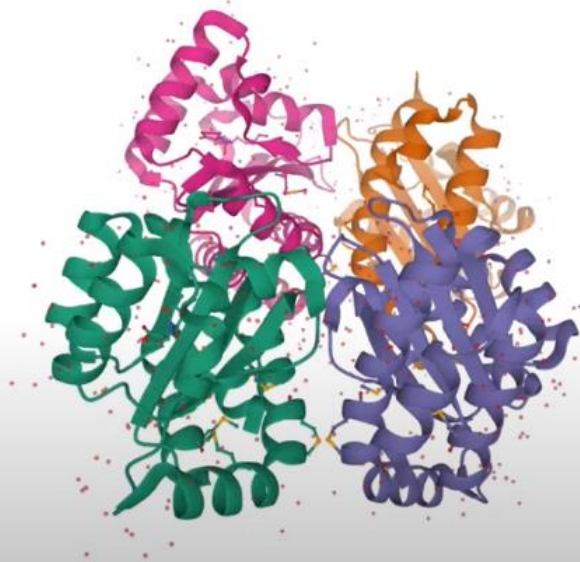
Total Structure Weight: 79.94 kDa



1: TRANSCRIP... A [auth E]

15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150

KLEWDAIQKKAEDLOFDFKILFOLLPRDQDYENAFIVGHYPAARREYDIAVYAPYDPTVSEHCTQGVLPDPWEPDIYQTRAGHEFFESABAAGLVYGLTKPLGARGELGALSLVYEAENRAEAMRFKESVLPFLMKLEDAVLQGGAGLAFFEPVSE



### Structure

2UVD | Structure of the P. aeruginosa

Type Model

Nothing Focused

#### Measurements

#### Components

Preset + Add

Polymer Cartoon

Ligand Ball & Stick

Non-standard Ball & Stick

Water Ball & Stick

Unit Cell  $a \ 1 \ 21 \ 1$

#### Density

#### Assembly Symmetry

19 20 30 40 50 60 70 80 90 100 110 120 130 140 150  
HLEHSAIQKXASDGLDFSKILFOLLFFDSQCYENAFIGVHNYPAARRENTDRAQYARVDFVSHCTQGVLPFIPWEPQIYQTRKQHEFFTEASALGLVYGLTXPLNGARDELGALSLSVEAENRAEANRFCEVSLPLWGLKFDIALQDQAGLAFESHFVSR

Structure

2UV0 | Structure of the P. aeruginosa

Type Model

Nothing Focused

Measurements

Components

Preset + Add

Polymer Cartoon

Ligand Ball & Stick

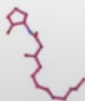
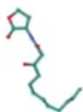
Non-standard Ball & Stick

Water Ball & Stick

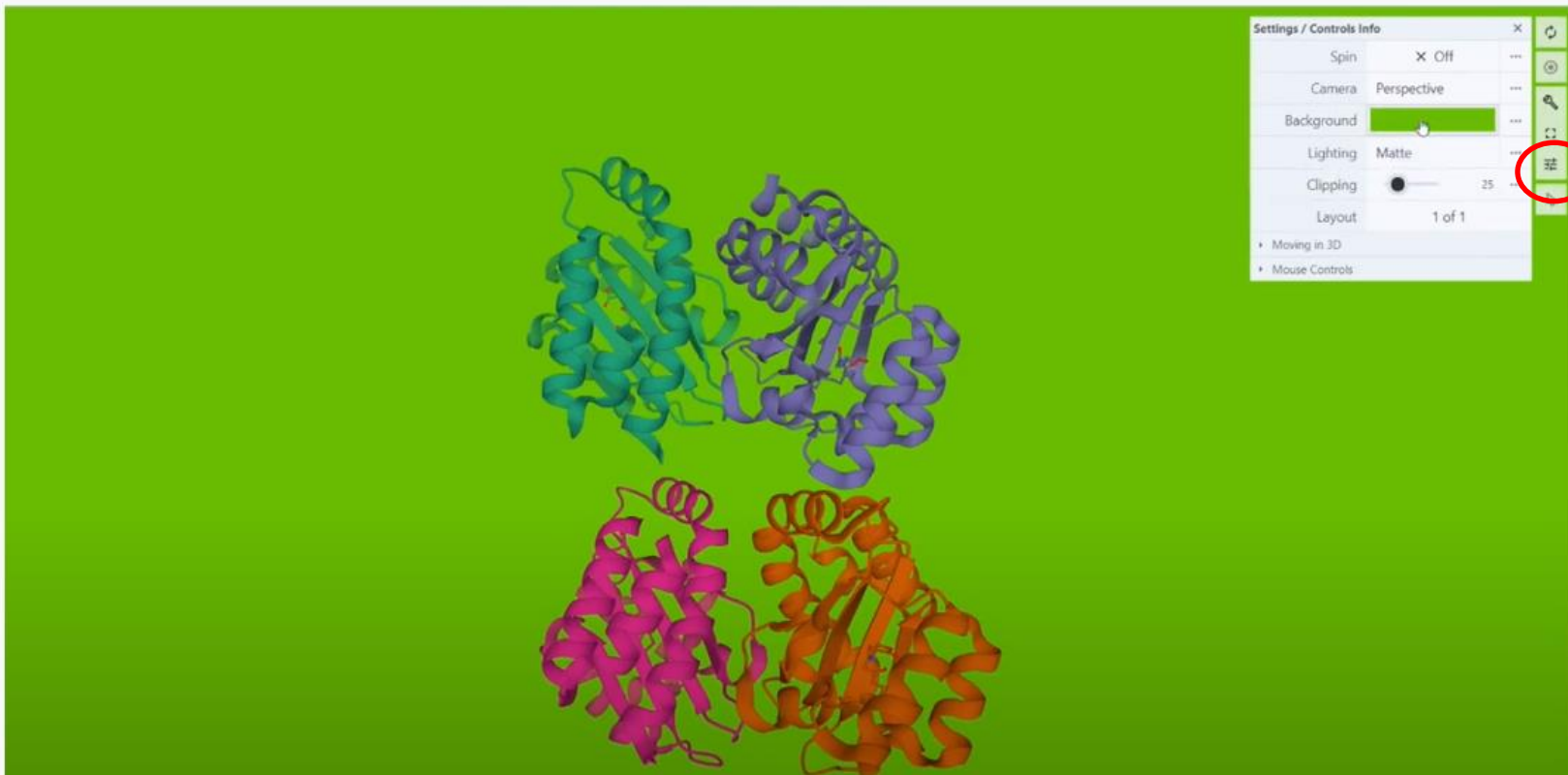
Unit Cell P 1 21 1

Density

Assembly Symmetry



1: TRANSCRIP... A [auth E]  
10 20 30 40 50 60 70 80 90 100 110 120 130 140 150  
IKLENSAILQKXASDLOGPSKILFOLLPEIQOVENAFIVGHVFAHREHYDRAQVAVDPTVSRCTQVLPWFHPSIYQTRQHEFFREASALGLVGLKPLGARGELGALSLQVEAHRASANRFXESVLPCLMKLFDYALQDAGLAFEPVSR



Settings / Controls Info

Spin	Off
Camera	Perspective
Background	[Green]
Lighting	Matte
Clipping	25
Layout	1 of 1

• Moving in 3D  
• Mouse Controls

Structure

ZUV0 | Structure of the P. aeruginosa

Type Model

Nothing Focused

Measurements

Components

Preset	+ Add
polymer	Cartoon
Ligand	Ball & Stick
Non-standard	Ball & Stick
Water	Ball & Stick

Unit Cell P 1 21 1

Density

Assembly Symmetry



# 2UV0

Display Files Download Files

Structure of the *P. aeruginosa* LasR ligand-binding domain bound to its autoinducer

## Domain Annotation: CATH

[CATH Database \(version 4.2.0\) Homepage](#)

Chain	Domain	Class	Architecture	Topology	Homology
A	3.30.450.80	Alpha Beta	2-Layer Sandwich	Beta-Lactamase	Transcription factor LuxR-like, autoinducer-binding domain
B	3.30.450.80	Alpha Beta	2-Layer Sandwich	Beta-Lactamase	Transcription factor LuxR-like, autoinducer-binding domain
C	3.30.450.80	Alpha Beta	2-Layer Sandwich	Beta-Lactamase	Transcription factor LuxR-like, autoinducer-binding domain
D	3.30.450.80	Alpha Beta	2-Layer Sandwich	Beta-Lactamase	Transcription factor LuxR-like, autoinducer-binding domain

## Protein Family Annotation

[Pfam Database Homepage](#)

Chains	Accession	Identifier	Description	Comments	Source
A, B, C, D	PF03472	Autoinducer binding domain (Autoind_bind)	Autoinducer binding domain	This domain is found a a large family of transcriptional regulators. This domain specifically binds to autoinducer molecules.	Domain
A, B, C, D	PF00196	Bacterial regulatory proteins, luxR family (GerE)	Bacterial regulatory proteins, luxR family	-	Domain

## Gene Product Annotation

[Gene Product Annotation](#)

Chains	Polymer	Molecular Function	Biological Process	Cellular Component
E, F, G, H	TRANSCRIPTIONAL ACTIVATOR PROTEIN LASR	<ul style="list-style-type: none"> <li>DNA-binding transcription factor activity</li> <li>transcription regulator activity</li> </ul>	<ul style="list-style-type: none"> <li>pathogenesis</li> <li>interspecies interaction between organisms</li> </ul>	<ul style="list-style-type: none"> <li>protein-containing complex</li> <li>protein-DNA complex</li> </ul>



The graphical representation below shows this entry's sequences as reported in UniProtKB, in the sample (SEQRES), or as observed in the experiment (ATOM). Different 3rd party annotations can be graphically mapped on the sequence and displayed in the Jmol viewer. Read more about the sequence display on our help pages.

The structure 2UV0 has in total 4 chains. These are represented by 1 sequence-unique entity.

Show all chains

Sequence & Structure Relationships. Enable Jmol to view annotations in 3D.

Display Jmol

Chain E: TRANSCRIPTIONAL ACTIVATOR PROTEIN LASR

Chain Downloadable Files

- Download FASTA File
- View Sequence & DSSP Image
- Download Sequence Chain Image

Chain Info

Polymer: 1  
 Length: 175 residues  
 Chain Type: polypeptide(L)  
 Reference: UniProtKB (P25084)  
 Up-to-date UniProt IDs are provided by the SIFTS project

Display Parameters

Identical Chains

Show F chain Show G chain Show H chain

Show all chains

Currently displayed

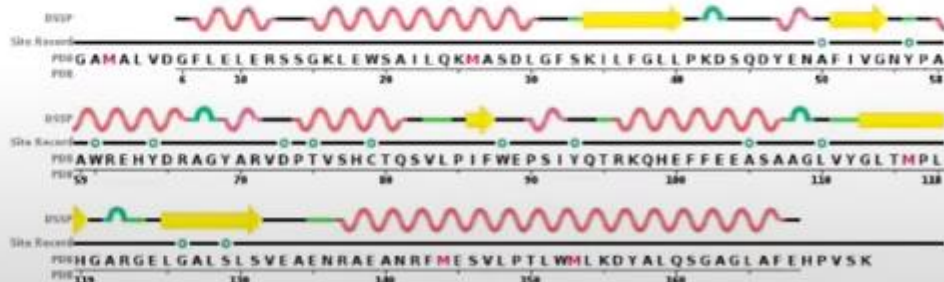
**SEQRES** sequence.

Display external (UniProtKB) sequence

Mouse over an annotation to see more details. Click on any annotation to enable Jmol.

Annotations	Details
Secondary Structure: <b>DSSP</b> [hide] [reference]	52% helical (9 helices; 91 residues) 15% beta sheet (5 strands; 27 residues)
Structural Feature: <b>Site Record</b> [hide] [reference]	<b>2UV0 E: ACT 1A</b> BINDING SITE FOR RESIDUE OHN E1169 (Software)

Sequence Chain View



```

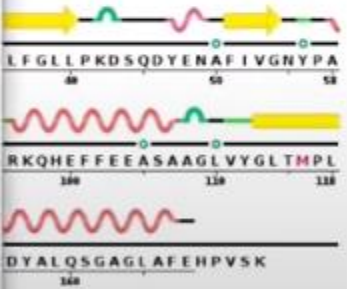
2UN0_E.fasta.txt - Notepad
File Edit Format View Help
>2UN0::E|PDBID|CHAIN|SEQUENCE
GAMALVDGFLELERSSGKLENSAILQKMASDLGFSKILFGLLPKDSQDYENAFIVGNYPAAAMREHYDRAGYARVDPTVSH
CTQSVLPITFWEP$IVOTRKHQHEFFEASAAGLVYGLTMPLHGARGELGALSLSVEAENRAEANRFMESVLPITLWMLKDYA
LQSGAGLAFEHPV$
    
```

Structure Relationships. Enable Jmol to view structures in 3D.

Parameters

Show G chain Show H chain

Unfolded sequence (UniProtKB) sequence



Enter search term(s)

[Advanced Search](#) | [Browse Annotations](#)



- Structure Summary
- 3D View
- Annotations
- Sequences
- Experiment

# 2UV0

[Display Files](#) [Download Files](#)

Structure of the *P. aeruginosa* LasR ligand-binding domain bound to its autoinducer

## X-RAY DIFFRACTION

### Crystallization

Crystallization Experiments				
ID	Method	pH	Temperature	Details
1		7.3		20% W/V PEG 4000, 80 MM CALCIUM ACETATE, 40 MM HEPES PH 7.3, 5 MM DTT AND 50 MICROMOLAR N-3-OXO-DODECANOYL-HOMOSERINE LACTONE.

Crystal Properties	
Matthew coefficient	Solvent content
2.22	44.6

### Crystal Data

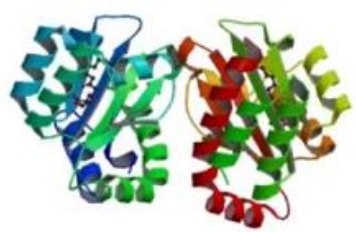
Unit Cell	
Length (Å)	Angle (°)
a = 53.82	α = 90
b = 85.33	β = 95.82
c = 75.51	γ = 90

Symmetry	
Space Group	P 1 2 1 1



Structure Summary 3D View Annotations Sequence Experiment

Biological Assembly 1



3D View: Structure | Electron Density | Ligand Interaction

Global Symmetry: Cyclic - C2 (3D View)  
Global Stoichiometry: Homo 2-mer - A2

Find Similar Assemblies

Biological assembly 1 assigned by authors and generated by PISA (software)

Macromolecule Content

# 2UV0

Structure of the *P. aeruginosa* LasR ligand-binding domain bound to its autoinducer

DOI: 10.2210/pdb2UV0/pdb

Classification: TRANSCRIPTION

Organism(s): *Pseudomonas aeruginosa* PAO1

Expression System: *Escherichia coli* BL21(DE3)

Mutation(s): No

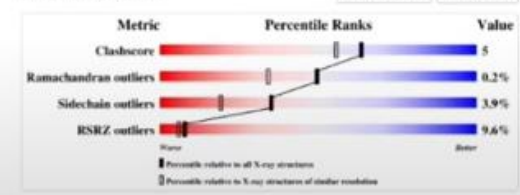
Deposited: 2007-03-08 Released: 2007-03-27

Deposition Author(s): Bottomley, M.J., Muraglia, E., Bazzo, R., Carfi, A.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION  
Resolution: 1.80 Å  
R-Value Free: 0.254  
R-Value Work: 0.209  
R-Value Observed: 0.211

wwPDB Validation



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

Literature

Download Primary Citation

Molecular Insights Into Quorum Sensing in the Human Pathogen *Pseudomonas Aeruginosa* from the Structure of the Virulence Regulator LasR Bound to its Autoinducer

Enter search term(s)



Advanced Search | Browse Annotations

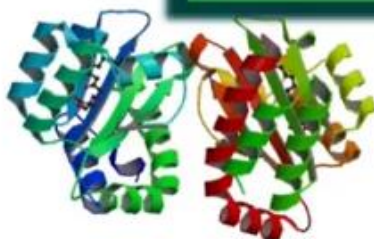


Structure Summary

Biological

# Download file

Download Files



Classification: TRANSCRIPTION

Organism(s): *Pseudomonas aeruginosa* PAO1

Expression System: *Escherichia coli* BL21(DE3)

Mutation(s): No

Deposited: 2007-03-08 Released: 2007-03-27

Deposition Author(s): Bottomley, M.J., Muraglia, E., Bazzo, R., Carli, A.

### Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 1.80 Å

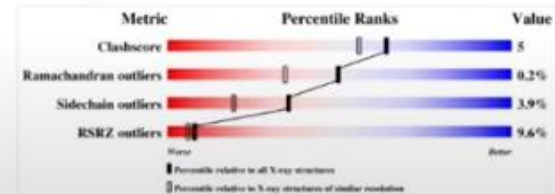
R-Value Free: 0.254

R-Value Work: 0.209

R-Value Observed: 0.211

### wwPDB Validation

3D Report Full Report



3D View: Structure | Electron Density | Ligand Interaction

Global Symmetry: Cyclic - C2 (3D View)

Global Stoichiometry: Homo 2-mer - A2

Find Similar Assemblies

Biological assembly 1 assigned by authors and generated by PISA (software)

### Macromolecule Content

Total Structure Weight: 79.94 kDa

ing domain bound to its autoinducer

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

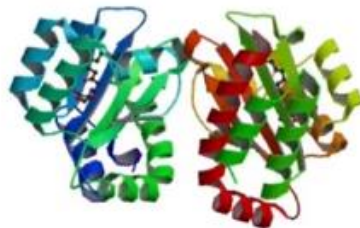
### Literature

Download Primary Citation

Molecular Insights Into Quorum Sensing in the Human Pathogen *Pseudomonas Aeruginosa* from the Structure of the Virulence Regulator LasR Bound to its Autoinducer.

Structure Summary 3D View Annotations Sequence Experiment

Biological Assembly 1



3D View: Structure | Electron Density | Ligand Interaction

Global Symmetry: Cyclic - C2 (3D View) | Global Stoichiometry: Homo 2-mer - A2

Find Similar Assemblies

Biological assembly 1 assigned by authors and generated by PISA (software)

Macromolecule Content

# 2UV0

Structure of the *P. aeruginosa* LasR ligand-binding domain b

DOI: 10.2210/pdb2UV0/pdb

Classification: TRANSCRIPTION

Organism(s): *Pseudomonas aeruginosa* PAO1

Expression System: *Escherichia coli* BL21(DE3)

Mutation(s): No

Deposited: 2007-03-08 Released: 2007-03-27

Deposition Author(s): Bottomley, M.J., Muraglia, E., Bazzo, R., Carfi, A.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION

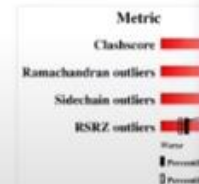
Resolution: 1.80 Å

R-Value Free: 0.254

R-Value Work: 0.209

R-Value Observed: 0.211

wwPDB Validation



Display Files Download Files

FASTA Sequence

PDB Format

PDB Format (gz)

PDBx/mmCIF Format

PDBx/mmCIF Format (gz)

PDBML/XML Format (gz)

Biological Assembly 1

Biological Assembly 2

Structure Factors (CIF)

Structure Factors (CIF - gz)

1fo-1c Map (DSN6)

2fo-1c Map (DSN6)

Map Coefficients (MTZ format)

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

Literature

Download Primary Citation

Molecular Insights Into Quorum Sensing in the Human Pathogen *Pseudomonas Aeruginosa* from the Structure of the Virulence Regulator LasR Bound to its Autoinducer.

# Kaynaklar

- Emel ORDU, Protein Kimyası, Yıldız Teknik Üniversitesi, Moleküler Biyoloji ve Genetik Bölümü, 2015
- [https://acikders.ankara.edu.tr/pluginfile.php/26753/mod\\_resource/content/0/1.%20PROTE%C4%BONLER%C4%BON%20TEME L%20YAPI%20VE%20C3%96ZELL%C4%BOKLER%C4%B0.pdf](https://acikders.ankara.edu.tr/pluginfile.php/26753/mod_resource/content/0/1.%20PROTE%C4%BONLER%C4%BON%20TEME L%20YAPI%20VE%20C3%96ZELL%C4%BOKLER%C4%B0.pdf)
- [http://eczacilik.anadolu.edu.tr/bolumSayfalari/belgeler/Peptit%20ve%20protein%20I.%20\\_20140402061928.pdf](http://eczacilik.anadolu.edu.tr/bolumSayfalari/belgeler/Peptit%20ve%20protein%20I.%20_20140402061928.pdf)
- [https://acikders.ankara.edu.tr/pluginfile.php/33107/mod\\_resource/content/1/Kiralite%20ve%20optik%20izomeri.pdf](https://acikders.ankara.edu.tr/pluginfile.php/33107/mod_resource/content/1/Kiralite%20ve%20optik%20izomeri.pdf)
- <https://embnet.vital-it.ch/CoursEMBnet/Pages3D07/documents/3Dintro07.pdf>
- [https://www.angelo.edu/faculty/kboudrea/index\\_2353/Chapter\\_09\\_2SPP.pdf](https://www.angelo.edu/faculty/kboudrea/index_2353/Chapter_09_2SPP.pdf)
- p.c. Champe, R.A. Harvey, Biyokimya, Nobel tıp Kitabevi, 1997.
- [http://eczacilik.anadolu.edu.tr/bolumSayfalari/belgeler/03%20Amino%20asitler,%20Peptitler%20ve%20Proteinler%20II\\_20140404062844.pdf](http://eczacilik.anadolu.edu.tr/bolumSayfalari/belgeler/03%20Amino%20asitler,%20Peptitler%20ve%20Proteinler%20II_20140404062844.pdf)
- [https://acikders.ankara.edu.tr/pluginfile.php/1003/mod\\_resource/content/1/7.%20Proteinler.pdf](https://acikders.ankara.edu.tr/pluginfile.php/1003/mod_resource/content/1/7.%20Proteinler.pdf)
- <https://www.youtube.com/watch?v=tDHBNxqUr94>