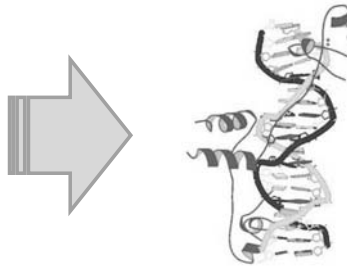


```

>1D66:A|PDBID|CHAIN|SEQUENCE
MKLLSSIEQACDICRLKKLKCSKEPKCAKCLKN
NWECRYSPKTKRSPLTRAHLTEVESRLERLEF
>1D66:B|PDBID|CHAIN|SEQUENCE
MKLLSSIEQACDICRLKKLKCSKEPKCAKCLKN
NWECRYSPKTKRSPLTRAHLTEVESRLERLEF
>1D66:D|PDBID|CHAIN|SEQUENCE
CCGGAGGACAGTCTCCGG
>1D66:E|PDBID|CHAIN|SEQUENCE
CCGGAGGACTGTCTCCGG

```



# Databases for Protein Structure

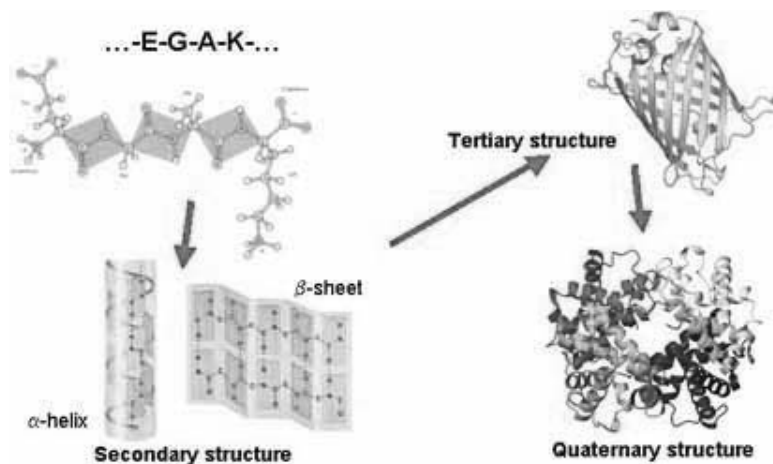
呂平江

國立清華大學

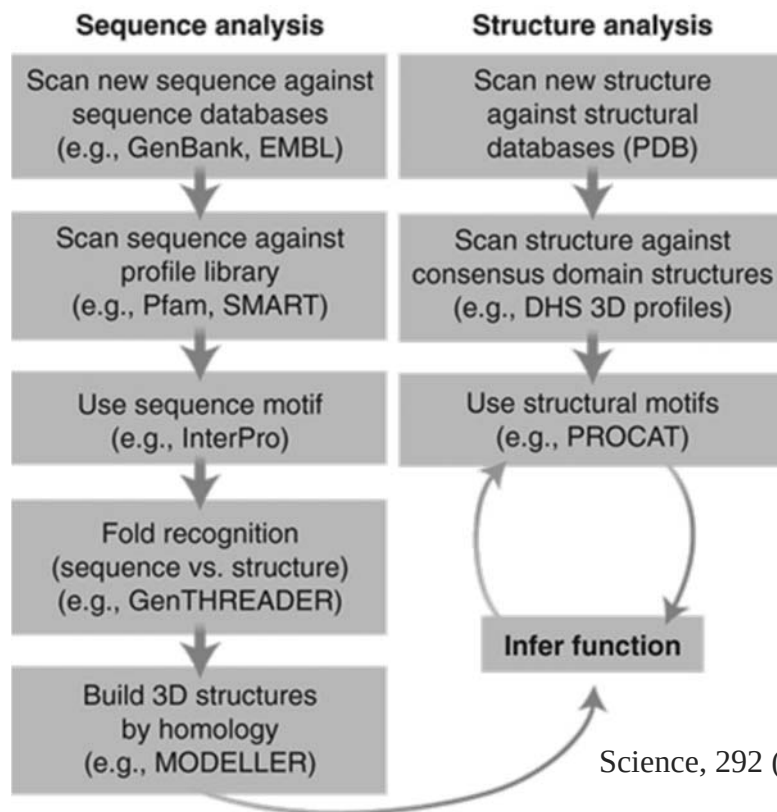
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2012/06/27

## From Sequence to Structure



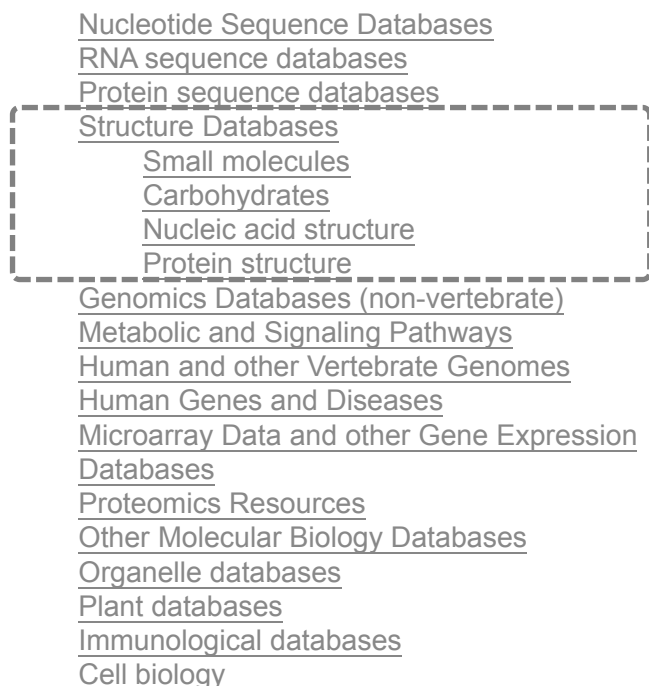
# From sequence and structure to function



Science, 292 (5524): 2095-2097  
(2001)

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- [PIDD](#)
- [PMDB - Protein Model Database](#)
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- ❑ Structure data determined by X-ray crystallography and NMR
- ❑ The data include the atom coordinate, reference, sequence, secondary structure, disulfide bond .....etc.



**The number of protein structure and the last update date**

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In our genome, it takes thousands of DNA nucleotides to encode the information for each protein, and even more to encode the information for the regulatory information. So, when a cell needs to regulate a process, it has to manage long, long stretches of DNA. As you might imagine, this is not easy in the chaotic environment of the cell.

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**Protein Structure Initiative Featured System**  
**Anthrax Stealth Siderophores**

Researchers at MCGS have reconstructed the structure of an essential synthetic enzyme in the pathway.

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**Organism**

**Exp. Method**

**Release Date**

**Taxonomy**

**X-ray Resolution**

**Release Time**

**Organism**

- Homo sapiens (20160)
- Escherichia coli (4603)
- Mus musculus (3541)

**SMILES**

- Has exact structure C1c1cccc1
- Has sub-structure C1c1cccc1
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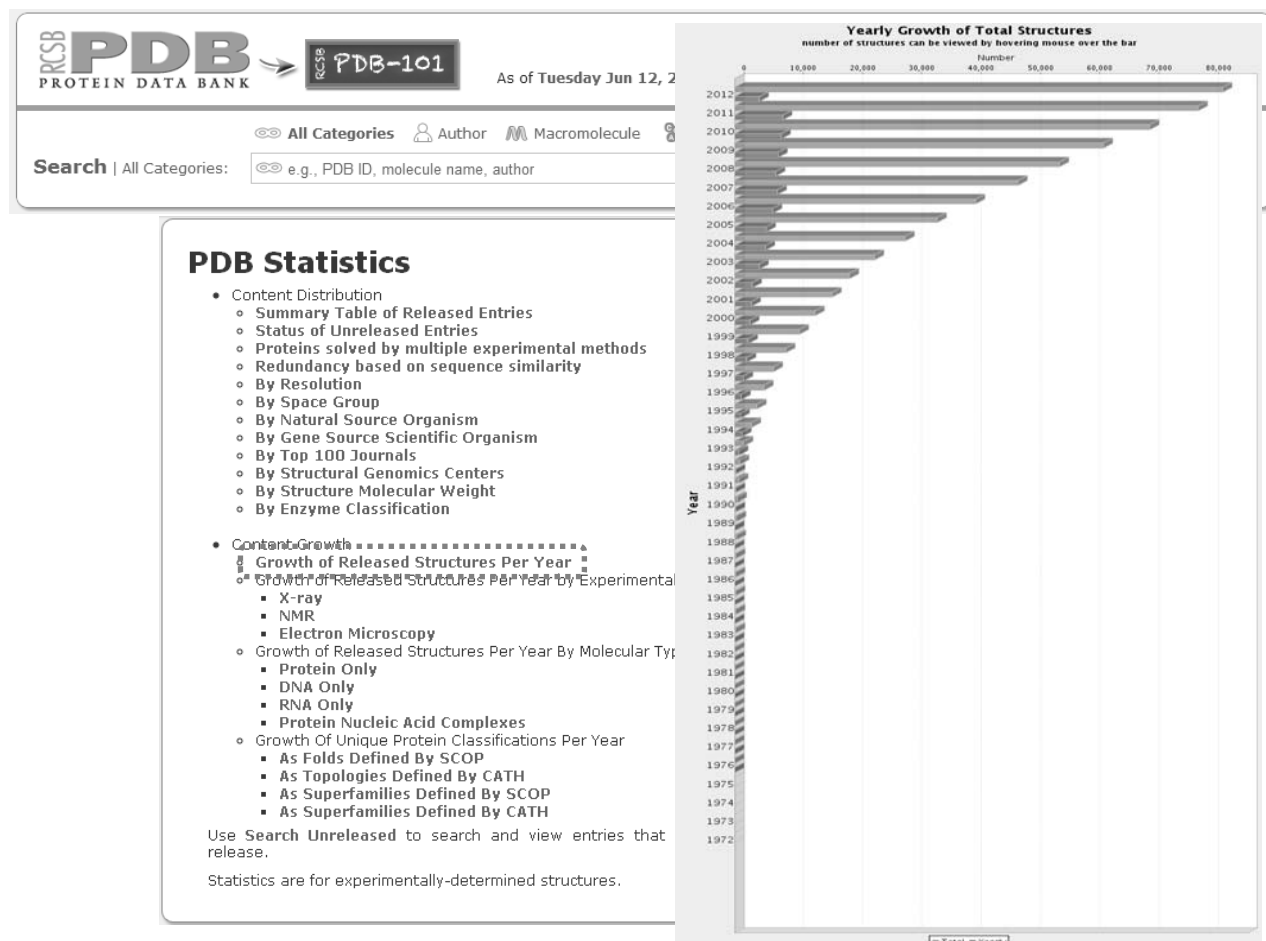
Easily perform substructure, exact structure, or similar structure searches. [more](#)

**Molecule of the Month** reaches 150

**Tour the PDB with Drill-down Pie Charts**

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**SMILES**  
 • Has exact structure C1c1cccc1  
 • Has sub-structure C1c1cccc1  
 • Is very similar (95%) with C1c1ccc  
 • Is similar (70%) with C1c1cccc1  
 • Super-structure of C1c1cccc1  
 Easily perform substructure, exact structure, or similar structure searches. [more](#)

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[Full Article](#)

**Protein Structure Initiative Featured System**  
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**Organism**  
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 • Escherichia coli (4603)  
 • Mus musculus (3541)

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  - UniProtKB Accession Number(s)
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  - Structure Description
  - Macromolecule Name
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Protein Synthesis



#### Molecule of the Month Sliding Clamps

In our genome, it takes thousands of DNA nucleotides to encode the information for each protein, and even more to store all the regulatory information. So, when a cell needs to copy this information, it has to manage long, long stretches of DNA. As you might imagine, this is not easy in the chaotic environment of the cell.

Full Article

#### Protein Structure Initiative Featured System Anthrax Stealth Siderophores

Researchers at MCSG have reconstructed the biosynthetic pathway for the stealth siderophore petrobactin, and determined the structure of an essential synthetic enzyme in the pathway.

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- Organism Taxonomy
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## Organism

- Homo sapiens (20160)
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Top Bar SMILES String Searching

☐ C1ccc1cc1

### SMILES

- Has exact structure C1ccc1cc1
- Has sub-structure C1ccc1cc1
- Is very similar (95%) with C1ccc1cc1
- Is similar (70%) with C1ccc1cc1
- Super-structure of C1ccc1cc1

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**DNA RECOGNITION BY GAL4: STRUCTURE OF A PROTEIN/DNA COMPLEX**

DOI: 10.2210/pdb1d66/pdb    NDB ID: PD0003

**Primary Citation**

DNA recognition by GAL4: structure of a protein-DNA complex.  
Harmorestein, R., Carey, M., Plasman, M., Harrison, S.C.,  
**Journal:** (1992) Nature 356: 408-414  
**PubMed:** 1557122 ☐  
**DOI:** 10.1038/356408a0 ☐  
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**PubMed Abstract:**  
A specific DNA complex of the 65-residue, N-terminal fragment of the yeast transcriptional activator, GAL4, has been analysed at 2.7 Å resolution by X-ray crystallography. The protein binds as a dimer to a symmetrical 17-base-pair sequence. A small, Zn(2+)-containing domain... [[Read More & Search PubMed Abstracts](#)]

| Molecular Description                                                                       |                      |                   |
|---------------------------------------------------------------------------------------------|----------------------|-------------------|
| <b>Classification:</b> Transcription/dna.                                                   |                      |                   |
| <b>Structure Weight:</b> 27737.04                                                           |                      |                   |
| <b>Molecule:</b> DNA (5'-D(C)*C*(G)*G*(A)*G*(G)*A*(C)*A*(G)*T*(C)*G*(T)*C*(C)*A*(G)*(G)*3') | <b>Type:</b> dna     | <b>Length:</b> 19 |
| <b>Chains:</b> D                                                                            |                      |                   |
| <b>Molecule:</b> DNA (5'-D(C)*C*(G)*G*(A)*G*(G)*A*(C)*A*(G)*T*(C)*G*(T)*C*(C)*A*(G)*(G)*3') | <b>Type:</b> dna     | <b>Length:</b> 19 |
| <b>Polymers:</b> 2                                                                          |                      |                   |
| <b>Chains:</b> E                                                                            |                      |                   |
| <b>Molecule:</b> PROTEIN (GAL4)                                                             | <b>Type:</b> protein | <b>Length:</b> 66 |
| <b>Polymers:</b> 3                                                                          |                      |                   |
| <b>Chains:</b> A, B                                                                         |                      |                   |
| <b>Organism:</b> Saccharomyces cerevisiae ☐                                                 |                      |                   |
| <b>UniprotKB:</b> P04319 ☐                                                                  |                      |                   |

| Source                                             |                            |                                              |
|----------------------------------------------------|----------------------------|----------------------------------------------|
| <b>Polymer: 1</b>                                  |                            |                                              |
| <b>Scientific Name:</b> Synthetic construct        | <a href="#">Taxonomy</a> ☐ |                                              |
| <b>Polymer: 2</b>                                  |                            |                                              |
| <b>Scientific Name:</b> Synthetic construct        | <a href="#">Taxonomy</a> ☐ |                                              |
| <b>Polymer: 3</b>                                  |                            |                                              |
| <b>Scientific Name:</b> Saccharomyces cerevisiae ☐ | <a href="#">Taxonomy</a> ☐ | <b>Common Name:</b> Baker's yeast            |
|                                                    |                            | <b>Expression System:</b> Escherichia coli ☐ |

| Ligand Chemical Component |                |                                 |
|---------------------------|----------------|---------------------------------|
| <b>Identifier</b>         | <b>Formula</b> | <b>Name</b>                     |
| CD                        | Cd             | CADMIUM ION                     |
| <b>Search:</b> ☐          |                |                                 |
| <b>Download:</b> ☐        |                | <a href="#">Ligand Explorer</a> |

**External Domain Annotations**

- SCOP Classification v1.75: 4 Domains - data from SCOP ☐
- CATH Classification v3.4.0: 3 Domains - data from CATH ☐
- PFAM Classification: 4 Domains - data from PFAM ☐

**Structural Biology Knowledgebase Data**

Information from the Structural Biology Knowledgebase ☐

- Models from the Protein Model Portal: 40 models ☐
- Related Biological Annotations: >18 annotations ☐
- Related Clones from PSI-Biology Materials Repository: 0 clones ☐
- Related Targets & Protocols from TargetTrack: 0 targets ☐

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Biological assembly 1 assigned by authors

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**Authors:** Harmorestein, R., Carey, M., Plasman, M., Harrison, S.C.,  
**Date:** 1992-03-06  
**Release:** 1992-03-06  
**Last Modified (REVSTAT):** 2009-02-24

**Experimental Details** Hide

**Method:** X-RAY DIFFRACTION  
**Exp. Data:** NA  
**Resolution(Å):** 2.70  
**R-Value:** 0.230 (obs.)  
**R-Free:** n/a  
**Space Group:** P 4<sub>3</sub> 2<sub>1</sub> 2  
**Unit Cell:**  
**Length (Å)**  
a = 80.85  
b = 80.85  
c = 73.70  
**Angles (°)**  
α = 90.00  
β = 90.00  
γ = 90.00

The RCSB PDB is managed by two members of the RCSB: Rutgers and UCSD, and is funded by NSF, NIHGS, DOE, NLM, NCI, NINDS, and NIDDK.

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# DNA recognition by GAL4: structure of a protein–DNA complex

Ronen Marmorstein, Michael Carey\*, Mark Ptashne & Stephen C. Harrison†

Harvard University, Department of Biochemistry and Molecular Biology, and †Howard Hughes Medical Institute, 7 Divinity Avenue, Cambridge, Massachusetts 02138, USA

A specific DNA complex of the 65-residue, N-terminal fragment of the yeast transcriptional activator, GAL4, has been analysed at 2.7 Å resolution by X-ray crystallography. The protein binds as a dimer to a symmetrical 17-base-pair sequence. A small, Zn<sup>2+</sup>-containing domain recognizes a conserved CCG triplet at each end of the site through direct contacts with the major groove. A short coiled-coil dimerization element imposes 2-fold symmetry. A segment of extended polypeptide chain links the metal-binding module to the dimerization element and specifies the length of the site. The relatively open structure of the complex would allow another protein to bind coordinately with GAL4.

THE yeast protein GAL4 activates transcription of genes required for catabolism of galactose and melibiose<sup>1–3</sup>. The DNA sequences recognized by GAL4 are 17 base pairs (bp) in length<sup>4–6</sup>, and each site binds a dimer of the protein<sup>7</sup>. Four such sites, similar but not identical in sequence, are found in the upstream activating sequence (UAS<sub>G</sub>) that mediates GAL4 activation of the GAL1 and GAL10 genes, for example<sup>8</sup>.

Functions have been assigned to various parts of the 881-amino-acid GAL4 protein (Fig. 1a), including DNA binding

(1–65) is a monomer in the absence of DNA. The open features of the complex, in which a long stretch of DNA at the centre of the 17-bp site is accessible in the major groove, suggest that another protein may be able to bind coordinately with GAL4.

## Structure determination

Crystals in space group *P*<sub>4</sub><sub>3</sub><sub>2</sub><sub>1</sub>2 were prepared as described in the legend to Table 1. The structure of a Cd<sup>2+</sup>-containing complex was determined and refined, because the crystals were of better quality than the isomorphous crystals containing Zn<sup>2+</sup>. Isomorphous derivatives were obtained either by replacing Cd<sup>2+</sup> with Zn<sup>2+</sup> or Hg<sup>2+</sup>, or by preparing duplex DNA in which 5-iodo-uridine was substituted for thymidine in selected positions (Fig. 1; Table 1).

The structure of the cadmium-containing complex was initially determined to 3.2 Å by multiple isomorphous replacement (MIR) using phase information from one Hg<sup>2+</sup> and four 5-iodo-uridine derivatives (Table 1). Locations of the heavy atom derivations confirmed that there was one complete protein–DNA complex per asymmetric unit, and that the protein bound the consensus DNA site as a homodimer. The initial MIR map showed clear density for B-form DNA, and the highest peaks in the map confirmed earlier spectroscopic experiments indicating that each protein monomer bound two closely spaced metal ions<sup>10</sup>. But the protein chain could not be traced. The map was improved by non-crystallographic averaging about a dyad relating the two protein–DNA half-sites<sup>19</sup>. The initial dyad was calculated using heavy-atom positions. Base pairs with ideal B-DNA geometry were built into the twofold averaged map using the model-building program FRODO<sup>20</sup>. The DNA model

## View Structure : 1D66

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**DNA RECOGNITION BY GAL4: STRUCTURE OF A PROTEIN/DNA COMPLEX**

DOI:10.2210/pdb1d66/pdb NDB ID: PDT003

**Primary Citation**

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Journal: (1992) Nature 356: 408–414

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**Molecular Description**

Classification: Transcription/dna

Structure Weight: 27737.04

| Molecule                                                        | Polymer                  | Type    | Length |
|-----------------------------------------------------------------|--------------------------|---------|--------|
| DNA (5'-D(CP*CP*GP*GP*AP*GP*GP*AP*GP*TP*CP*CP*TP*CP*P*GP*G)-3') | 1                        | dna     | 19     |
| Chains:                                                         | D                        |         |        |
| DNA (5'-D(CP*CP*GP*GP*AP*GP*GP*AP*GP*TP*CP*CP*TP*CP*P*GP*G)-3') | 2                        | dna     | 19     |
| Chains:                                                         | E                        |         |        |
| Protein (GAL4)                                                  | 3                        | protein | 66     |
| Chains:                                                         | A, B                     |         |        |
| Organism                                                        | Saccharomyces cerevisiae |         |        |
| UniProtKB:                                                      | P04386                   |         |        |

**Biological Assembly**

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Other Viewers Protein Workshop

Biological assembly 1 assigned by authors

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**Deposition Summary**

Authors: Marmorstein, R., Carey,

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# DNA RECOGNITION BY GAL4: STRUCTURE OF A PROTEIN/DNA COMPLEX

## Sequence Display

The sequence display provides a graphical representation of the UniProtKB, PDB - ATOM and PDB - SEQRES sequences. Different 3rd party annotations can be graphically mapped on the sequence and displayed in the Jmol viewer.

The structure **1D66** has in total 4 chains. Out of these 3 are sequence-unique.

Currently viewing **unique chains** only. show all chains

Chain A : PROTEIN (GAL4)

FASTA | Sequence & DSSP | Image

Polymer 3

Length: 66 residues

Chain Type: polypeptide(L)

Reference: [UniProtKB P04386](#)

### Sequence & Structure Relationships

[Display Jmol](#)

Enable Jmol to view annotations in 3D.

### Display Parameters

Identical chains: ☐ show all chains

show polypeptide chains only

Currently displayed: **SEORES**

sequence.

Display external (UniProtKB)

sequence

Mouse over an annotation to see more details.

### Annotations

Add Annotations

Domain Assignment: **SCOP**

[hide] [reference]

**01d66a1** Gal4: 41 residues

**01d66a2** CD2-Gal4: 16 residues

34% helical (3 helices; 23 residues)

Secondary Structure: **DSSP**

[hide] [reference]

Structural Feature: **Protein Modification** 0252: Metal coordination, CD

[hide] [reference] [reference]

SCOP

DSSP

Protein Modification

PER **0252** Metal coordination, CD

Legend: Metal coordination, CD

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Biology and Chemistry Report

Structure Details

Structure Keywords

Keywords
TRANSCRIPTION/DNA  
Text
PROTEIN-DNA COMPLEX, DOUBLE HELIX, TRANSCRIPTION/DNA COMPLEX

Polymeric Molecules

Chain D

Description
DNA (5'-D(\*CP\*CP\*GP\*GP\*AP\*GP\*GP\*AP\*CP\*AP\*GP\*TP\*CP\*CP\*TP\*CP\*CP\*GP\*G)-3')  
Nonstandard Linkage
no  
Nonstandard Monomers
no  
Polymer Type
polydeoxyribonucleotide  
Formula Weight
5831.8  
Source Method
synthetic

Chain E

Description
DNA (5'-D(\*CP\*CP\*GP\*GP\*AP\*GP\*GP\*AP\*CP\*TP\*GP\*TP\*CP\*CP\*TP\*CP\*CP\*GP\*G)-3')  
Nonstandard Linkage
no  
Nonstandard Monomers
no  
Polymer Type
polydeoxyribonucleotide  
Formula Weight
5822.8  
Source Method
synthetic

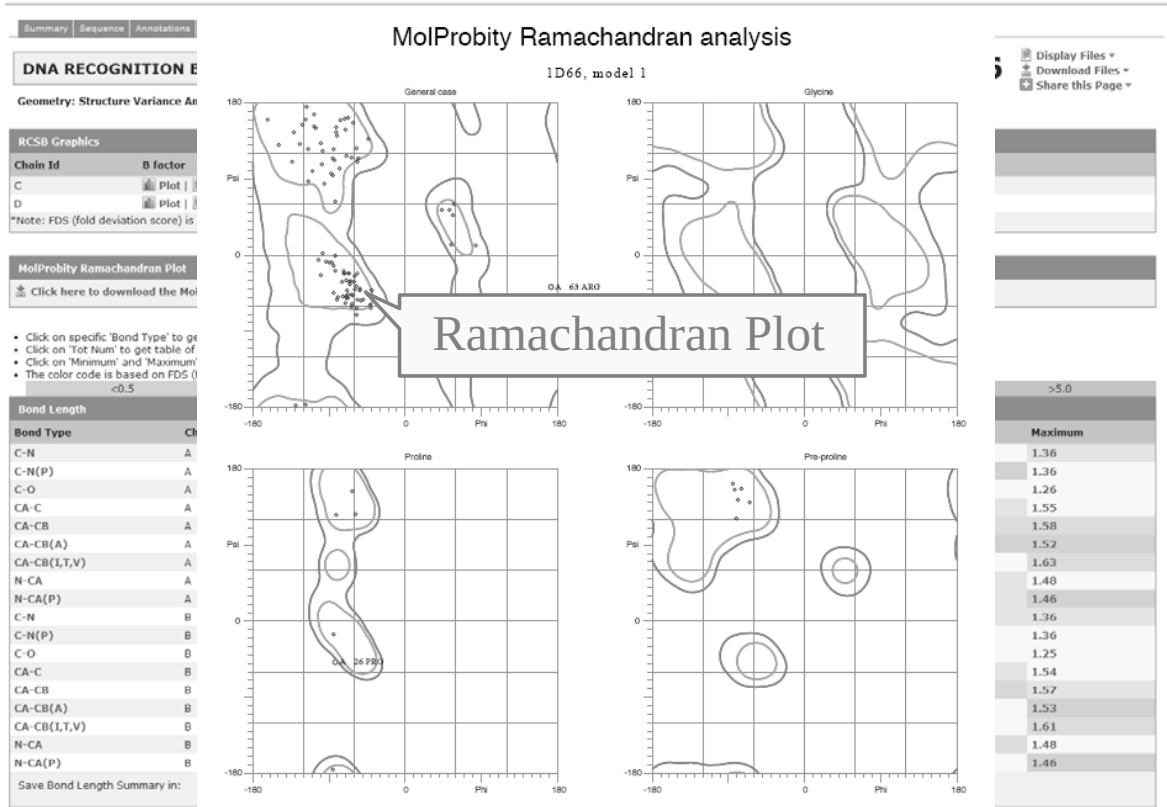
Chain A,B

Description
PROTEIN (GAL4)  
Nonstandard Linkage
no  
Nonstandard Monomers
no  
Polymer Type
polypeptide(L)  
Formula Weight
7816.4  
Source Method
genetically manipulated

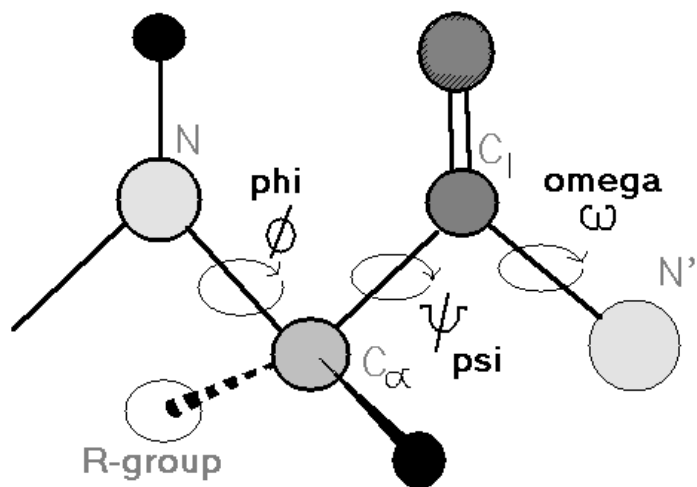
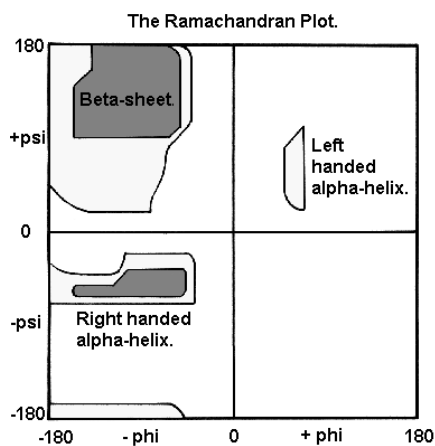
Ligands and Prosthetic Groups

| ID | Name        | Chemical Formula | Weight | Ligand Structure |
|----|-------------|------------------|--------|------------------|
| CD | CADMIUM ION | Cd               | 112.41 | View             |

## Geometry



## Ramachandran plot



**β-strand:**

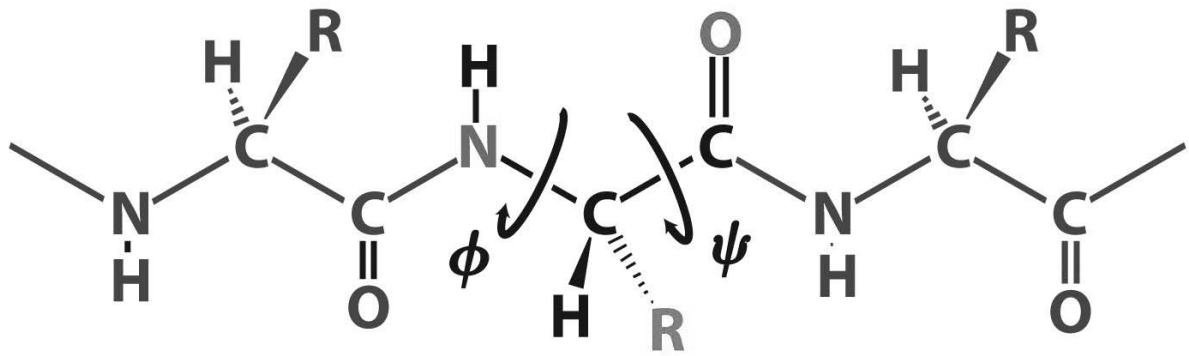
$$-180 < \phi < -60$$

$$180 > \phi > 60$$

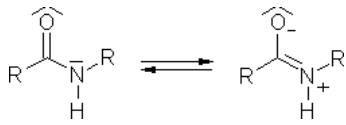
**α-helix:**

$$\phi: \sim -60$$

**Φ (phi, Cα-N bond) vs. Ψ (psi, Cα-C(O) bond)**

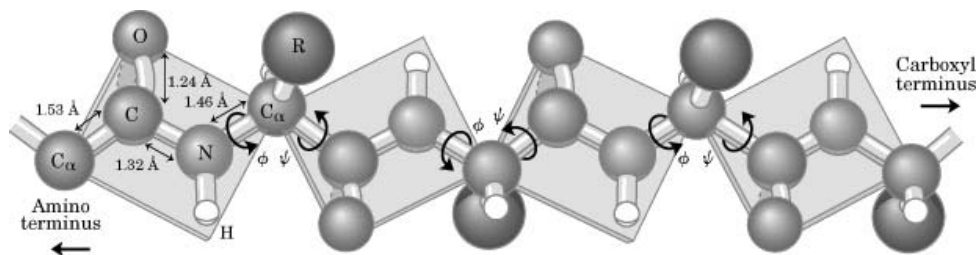


**Figure 2.22a**  
*Biochemistry, Seventh Edition*  
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"partial" double bond character

- Peptide bond N–C–O atoms and atoms attached to them lie all in the same plane
  - Peptide bond is planar !
- Only 2 bonds can freely rotate
  - C $\alpha$ –N bond and C $\alpha$ –C(O) bond



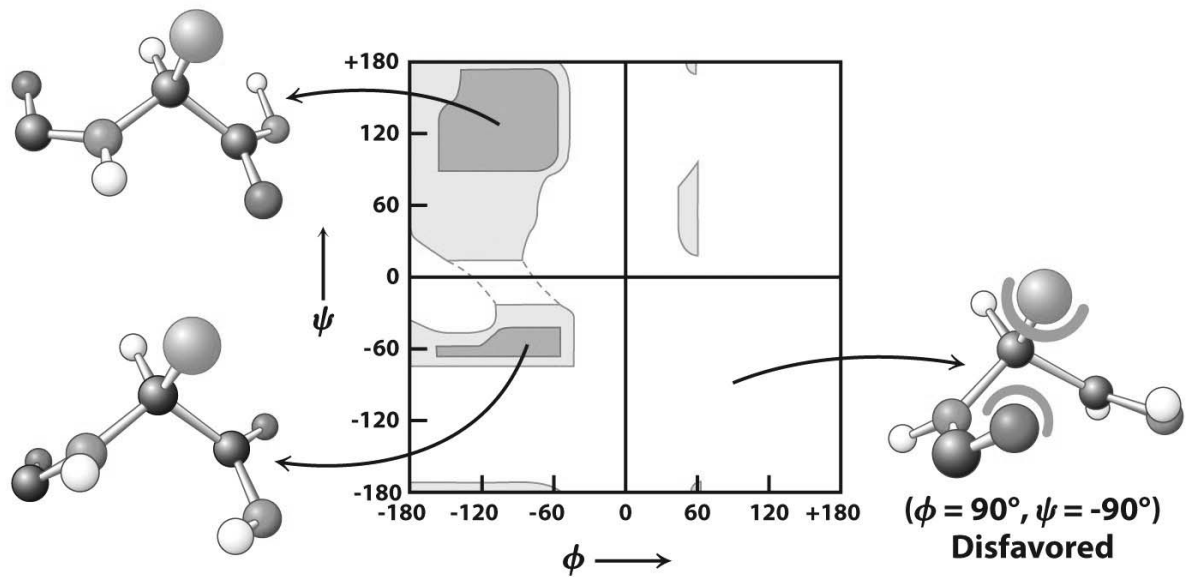
**Limit amount of free rotations possible** (high torsion barriers)

Specified by the **torsion angles  $\Phi$**  (phi, C $\alpha$ –N bond) and  **$\Psi$**  (psi, C $\alpha$ –C(O) bond)

Possible  $\Phi$  and  $\Psi$  values are **constrained** by the structure of adjacent amino acid residues

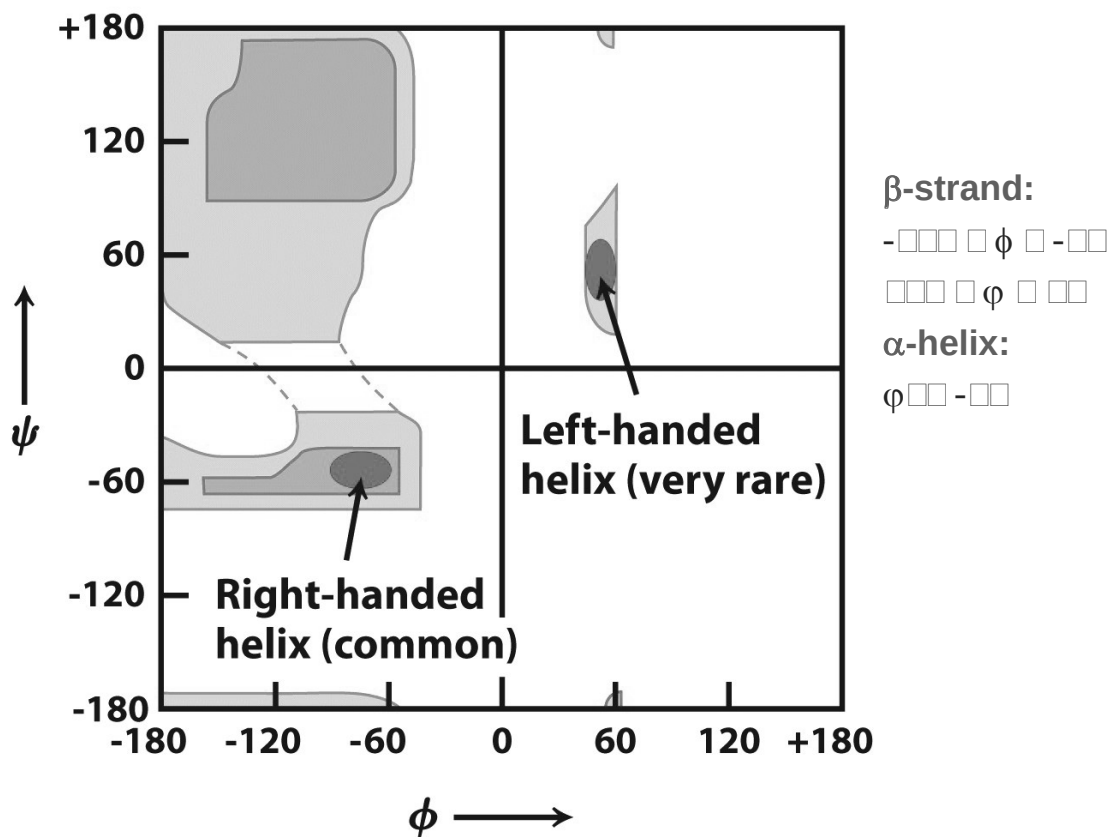
繞N-C $\alpha$ 鍵旋轉的角度稱為phi( $\psi$ )，而繞C $\alpha$ -C'鍵旋轉的角度則稱為psi( $\Psi$ )。因此，每一胺基酸的phi( $\psi$ ) & psi( $\Psi$ )兩個角度決定主鏈原子的型態。

# Ramachandran plot



**Figure 2.23**  
*Biochemistry, Seventh Edition*  
 © 2012 W. H. Freeman and Company

Shaded areas: allowed  $\Phi$  and  $\Psi$  angles  
 White areas: sterically disallowed  
 Disfavored region:  $(\phi = 90^\circ, \psi = -90^\circ)$



**Figure 2.26**  
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Geometry: Structure Variance Analysis Results

Bond Angle

| Bond Angle | Chain Id | Tot Num | Cal Ave | Cal StdDev | Std Val | Std StdDev | Minimum | Maximum |
|------------|----------|---------|---------|------------|---------|------------|---------|---------|
| Chi1 g(+)  | A        | 22      | -73.90  | 17.794     | -66.7   | 15.0       | -117.20 | -22.80  |
| Chi1 g(-)  | A        | 12      | 56.52   | 17.006     | 64.1    | 15.7       | 30.00   | 84.80   |
| Chi1 trans | A        | 20      | 193.05  | 20.939     | 183.6   | 16.8       | 167.50  | 236.20  |
| Omega      | A        | 56      | 176.15  | 20.302     | 180     | 5.8        | 29.10   | 188.30  |
| Phi        | A        | 30      | -66.85  | 66.876     | -65.3   | 11.9       | -132.20 | 172.60  |
| Phi helix  | A        | 23      | -67.03  | 15.678     | -65.3   | 11.9       | -100.70 | -41.90  |
| Phi(P)     | A        | 3       | -68.67  | 10.253     | -65.4   | 11.2       | -83.00  | -59.60  |
| Psi        | A        | 33      | 93.14   | 78.415     | -39.4   | 11.3       | -176.50 | 176.10  |
| Psi helix  | A        | 23      | -38.39  | 19.054     | -39.4   | 11.3       | -70.80  | 3.90    |
| Chi1 g(+)  | B        | 25      | -74.08  | 18.861     | -66.7   | 15.0       | -112.50 | -36.50  |
| Chi1 g(-)  | B        | 14      | 63.87   | 20.734     | 64.1    | 15.7       | 35.80   | 113.10  |
| Chi1 trans | B        | 15      | 196.39  | 16.726     | 183.6   | 16.8       | 173.60  | 229.00  |
| Omega      | B        | 56      | 176.54  | 23.547     | 180     | 5.8        | 6.00    | 196.40  |
| Phi        | B        | 29      | -79.58  | 52.756     | -65.3   | 11.9       | -163.30 | 57.00   |
| Phi helix  | B        | 24      | -67.62  | 14.287     | -65.3   | 11.9       | -103.40 | -35.80  |
| Phi(P)     | B        | 3       | -84.83  | 1.443      | -65.4   | 11.2       | -86.00  | -82.80  |
| Psi        | B        | 32      | 91.02   | 87.488     | -39.4   | 11.3       | -177.60 | 167.20  |
| Psi helix  | B        | 24      | -37.06  | 16.801     | -39.4   | 11.3       | -60.40  | -0.40   |

Save Dihedral Angle Summary in:

CSV (Excel) Format

Save Report

|                |   |    |        |       |       |     |        |        |
|----------------|---|----|--------|-------|-------|-----|--------|--------|
| N-CA-C         | B | 54 | 109.75 | 4.621 | 111.2 | 2.8 | 97.25  | 120.74 |
| N-CA-C(P)      | B | 3  | 115.34 | 2.966 | 111.8 | 2.5 | 111.14 | 117.47 |
| N-CA-CB        | B | 46 | 109.83 | 2.540 | 110.5 | 1.7 | 104.36 | 116.35 |
| N-CA-CB(A)     | B | 3  | 110.38 | 3.615 | 110.4 | 1.5 | 107.50 | 115.48 |
| N-CA-CB(L,T,V) | B | 5  | 109.94 | 3.726 | 111.5 | 1.7 | 104.85 | 114.36 |
| N-CA-CB(P)     | B | 3  | 102.17 | 0.739 | 103.0 | 1.1 | 101.27 | 103.08 |
| O-C-N          | B | 53 | 121.77 | 2.344 | 123.0 | 1.6 | 115.70 | 126.06 |
| O-C-N(P)       | B | 3  | 121.96 | 1.735 | 122.0 | 1.4 | 119.51 | 123.31 |

Save Bond Angle Summary in:

CSV (Excel) Format

Save Report

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FASTA Sequence  
PDB File (Text)  
PDB File (gz)  
mmCIF File  
mmCIF File (gz)  
PDBML/XML File  
PDBML/XML File (gz)  
Biological Assembly (gz) (A)

Biological assembly assigned by authors

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```
HEADER TRANSCRIPTION REGULATION 06-MAR-92 1D66 1D66 2
COMPND GAL4 (RESIDUES 1 - 65) COMPLEX WITH 19MER DNA 1D66 3
SOURCE (SACCHAROMYCES $CEREVISIAE) OVEREXPRESSED IN (ESCHERICHIA 1D66 4
SOURCE 2 $COLI) 1D66 5
AUTHOR R.MARMORSTEIN,S.HARRISON 1D66 6
REVDAT 1 15-APR-93 1D66 7
JRNL 1D66 8
JRNL 6 9
JRNL 1D66 10
JRNL 1D66 11
JRNL 1D66 12
REMARK 1D66 13
REMARK 1D66 14
REMARK 1D66 15
REMARK 1D66 16
REMARK 1D66 17
REMARK 1D66 18
REMARK 1D66 19
REMARK 1D66 20
REMARK 1D66 21
REMARK 1D66 22
REMARK 1D66 23
REMARK 1D66 24
REMARK 1D66 25
REMARK 1D66 26
REMARK 1D66 27
REMARK 1D66 28
REMARK 1D66 29
REMARK 1D66 30
REMARK 1D66 31
REMARK 1D66 32
REMARK 1D66 33
REMARK 1D66 34
REMARK 1D66 35
```

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是否要開啟或儲存這個檔案?

名稱: 1D66.pdb  
類型: Brookhaven Protein Databank File  
從: www.pdb.org

開啟舊檔 (O) 儲存 (S) 取消

雖然來自網際網路的檔案可能是有用的，但是某些檔案有可能會傷害您的電腦。如果您不信任其來源，請不要開啟或儲存這個檔案。有什麼樣的風險?

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mmCIF File (gz)  
PDBML/XML File  
PDBML/XML File (gz)  
Biological Assembly (gz) (A)

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```
HET CD 41 1 CADMIUM 1D66 68
HET CD 42 1 CADMIUM 1D66 69
FORMUL 5 CD 4(CD1) 1D66 70
FORMUL 6 HOH *51(H2 O1) 1D66 71
HELIX 1 H1A CYS A 11 LYS A 18 1 RESIDUE 18 HAS POSITIVE PHI 1D66 72
HELIX 2 H2A CYS A 28 ASN A 35 1 RESIDUE 35 HAS POSITIVE PHI 1D66 73
HELIX 3 H3A THR A 50 LEU A 64 1 1D66 74
HELIX 4 H1B CYS B 11 LYS B 18 1 RESIDUE 18 HAS POSITIVE PHI 1D66 75
HELIX 5 H2B CYS B 28 ASN B 35 1 RESIDUE 35 HAS POSITIVE PHI 1D66 76
HELIX 6 H3B THR B 50 LEU B 64 1 1D66 77
CRYST1 80.850 80.850 73.700 90.00 90.00 90.00 P 43 21 2 8 1D66 78
ORIGX1 1.000000 0.000000 0.000000 0.00000 1D66 79
ORIGX2 0.000000 1.000000 0.000000 0.00000 1D66 80
ORIGX3 0.000000 0.000000 1.000000 0.00000 1D66 81
SCALE1 0.012369 0.000000 0.000000 0.00000 1D66 82
SCALE2 0.000000 0.012369 0.000000 0.00000 1D66 83
SCALE3 0.000000 0.000000 0.013569 0.00000 1D66 84
MTRIX1 1 0.969990 0.014680 -0.242700 7.19246 1 1D66 85
MTRIX2 1 0.014290 -0.999900 -0.003900 83.38941 1 1D66 86
MTRIX3 1 -0.242710 -0.000190 0.970100 82.87497 1 1D66 87
ATOM 1 O5* C D 1 23.081 73.401 36.511 1.00 44.77 1D66 88
ATOM 2 C5* C D 1 24.340 73.259 35.792 1.00 46.46 1D66 89
ATOM 3 C4* C D 1 24.267 72.789 34.262 1.00 42.04 1D66 90
ATOM 4 O4* C D 1 25.550 72.957 33.595 1.00 41.08 1D66 91
ATOM 5 C3* C D 1 23.957 71.289 34.142 1.00 38.19 1D66 92
ATOM 6 O3* C D 1 23.249 71.081 32.947 1.00 33.45 1D66 93
ATOM 7 C2* C D 1 25.339 70.690 33.983 1.00 35.90 1D66 94
ATOM 8 C1* C D 1 26.031 71.694 33.078 1.00 39.17 1D66 95
ATOM 9 N1 C D 1 27.530 71.609 33.190 1.00 38.42 1D66 96
ATOM 10 C2 C D 1 28.318 71.429 32.033 1.00 32.78 1D66 97
ATOM 11 O2 C D 1 27.833 71.357 30.908 1.00 30.98 1D66 98
ATOM 12 N3 C D 1 29.661 71.362 32.174 1.00 28.51 1D66 99
ATOM 13 C4 C D 1 30.215 71.469 33.389 1.00 30.53 1D66 100
ATOM 14 N4 C D 1 31.535 71.390 33.519 1.00 28.65 1D66 101
```

# PDB File Title Section

|        |                                                                                        |        |                                                                                                                                                 |
|--------|----------------------------------------------------------------------------------------|--------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| HEAD   | First line of the entry, contains PDB ID code, classification, and date of deposition. | HELIX  | Identification of helical substructures.                                                                                                        |
| COMPND | Description of macromolecular contents of the entry.                                   | CRYST1 | Unit cell parameters, space group, and Z.                                                                                                       |
| SOURCE | Biological source of macromolecules in the entry.                                      | ORIGXn | Transformation from orthogonal coordinates to the submitted coordinates (n = 1, 2, or 3). 由直角(orthogonal)座標系，轉換到 submitted座標系，座標系之間的轉換          |
| AUTHOR | List of contributors.                                                                  | SCALEn | Transformation from orthogonal coordinates to fractional crystallographic coordinates (n = 1, 2, or 3).由直角座標系，轉換到晶圖(□□s□□□□□phi□)座標系，座標系之間的轉換值。 |
| REVDAT | Revision date and related information.                                                 | MTRIXn | Transformations expressing non-crystallographic symmetry (n = 1, 2, or 3). There may be multiple sets of these records. 非晶圖對稱的轉換                |
| JRNL   | Literature citation that defines the coordinate set.                                   | ATOM   | Atomic coordinate records for standard groups.                                                                                                  |
| REMARK | General remarks, some are structured and some are free form.                           | HETATM | Atomic coordinate records for heterogens.                                                                                                       |
| SEQRES | Primary sequence of backbone residues.                                                 | TER    | Chain terminator.                                                                                                                               |
| FORMUL | Chemical formula of non-standard groups.                                               | END    | Last record in the file.                                                                                                                        |

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- Protein Interfaces, Surfaces and Assemblies (PISA)
- Molecular Modeling Database (NCBI/Entrez) (MMDb)
- PDBsum
- Jena Library
- PDBWiki
- Proteopedia
- OCA Browser (OCA)
- PDB\_SEDO : No external link available

STRUCTURE FEATURES

- Homology derived Secondary Structure of Proteins (HSSP)
- Analysis of Ligand-Protein Contacts (LPC)
- Analysis of Interatomic Contacts of Structural Units (CSU)
- Computed Atlas of Surface Topography of proteins (CASTp)
- Gaussian Network Model (GNM)
- HIV Sequence/Structure Function Analyzer (HIVToolbox) : No external link available

LIGAND FEATURES

- BindingDB : No external link available
- Ligand-Expo
- Chem-BLAST
- PubChem
- DrugBank

STRUCTURE CLASSIFICATION AND COMPARISON

- Structural Classification of Proteins (SCOP)
- Protein Structure Classification (CATH)
- Vector Alignment Search Tool (VAST)
- Flexible structure Alignment by Chaining Aligned fragment pairs allowing Twists (FATCAT)
- DALI
- SUPERFAMILY

SECONDARY STRUCTURE

- Secondary Structure Assignments (DSSP)

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NO EXTERNAL LINK IN EXPERIMENTAL DATA

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- IEDB : No external link available

PATHWAYS

- METACYC : No external link available

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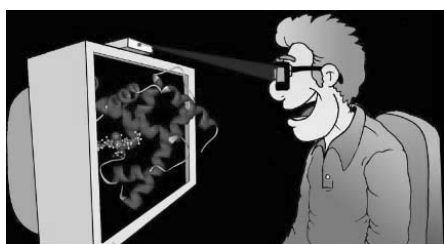
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- WHAT\_CHECK (WHAT IF)
- PROCHECK

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- PyMOL
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- Swiss PDB viewer
- MOLMOL
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- WebLabViewer



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| Today      | 98    |
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週四, 23 十月 2008 11:27 管理者

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2. [Rasmol Help File \(rasmol.hlp\) \(Command mode\)](#)
3. [Rasmol Help File \(raswin.hlp\) \(Windows HELP file\)](#)
4. [MDL Chime SP6](#)
5. [Swiss-pdb viewer](#)
6. [Cn3D](#)
7. [Pymol](#)
8. [蛋白質結構下載: 1D66](#)

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2. [FTP: FFFTP&Tutorial](#)

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2. [Flash MX 2004 中文試用版](#)
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