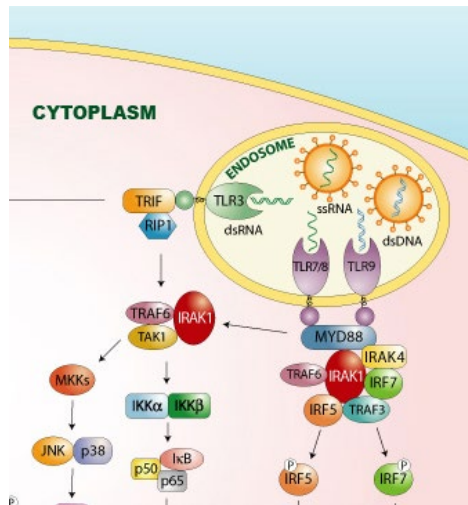


# 生物信息学

## 蛋白质三维结构预测 1

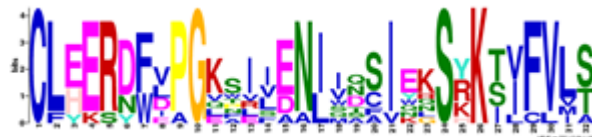
# 蛋白质结构



功能



结构

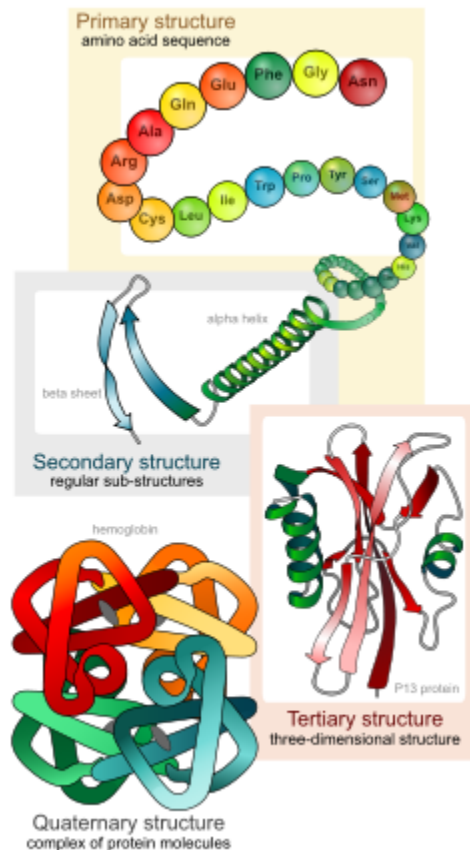


序列



# 蛋白质结构

蛋白质结构分四级：



一级结构

氨基酸序列

二级结构

周期性的局部结构构象

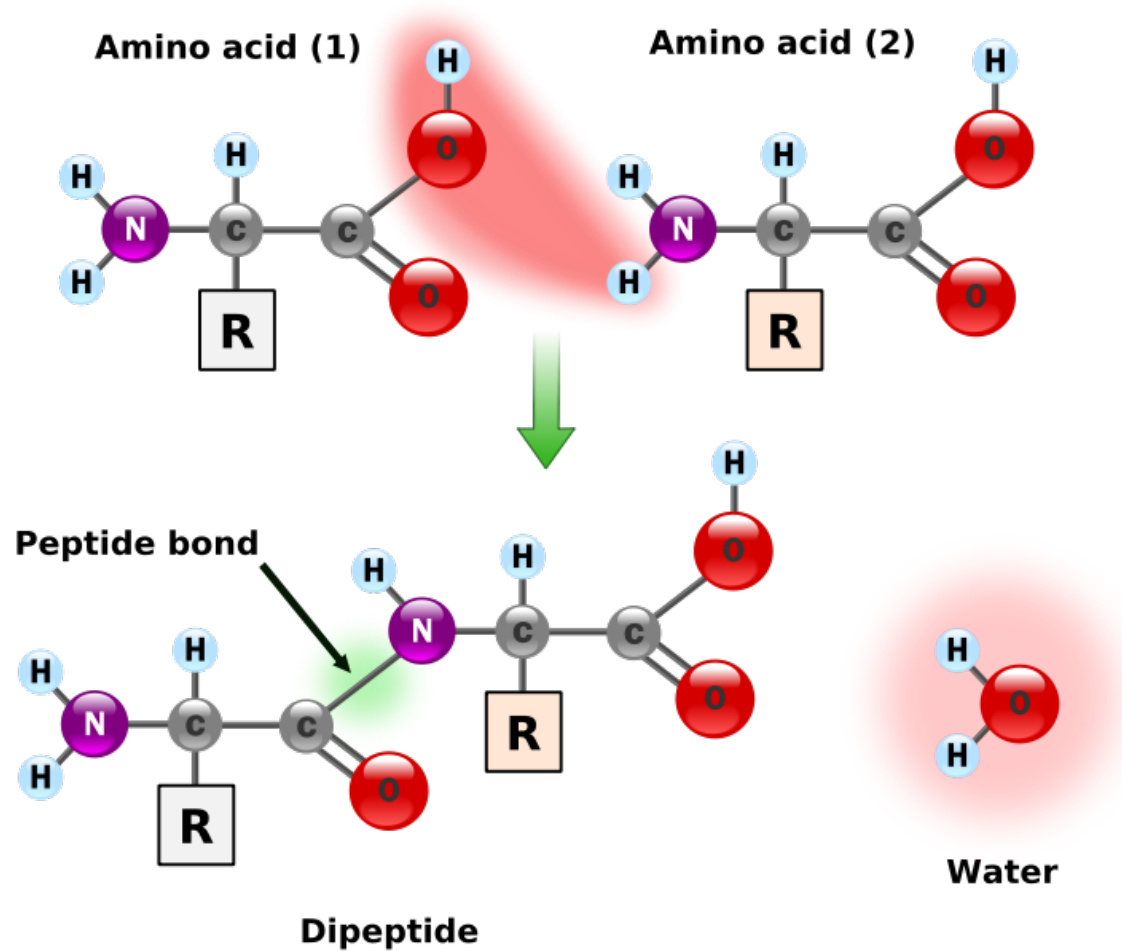
三级结构

三维空间结构

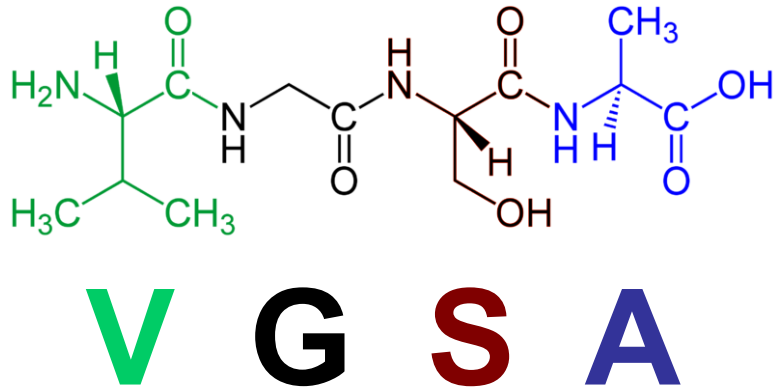
四级结构

几个蛋白质分子形成的复合体或含有多结构域单个蛋白质分子

# 蛋白质结构



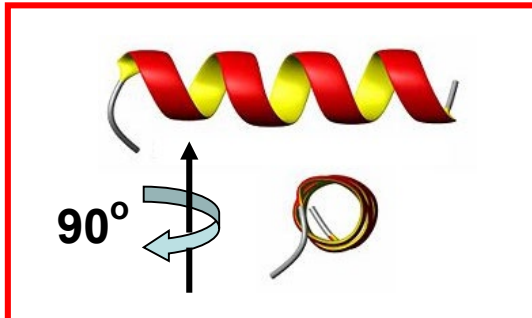
# 蛋白质结构 --- 一级结构



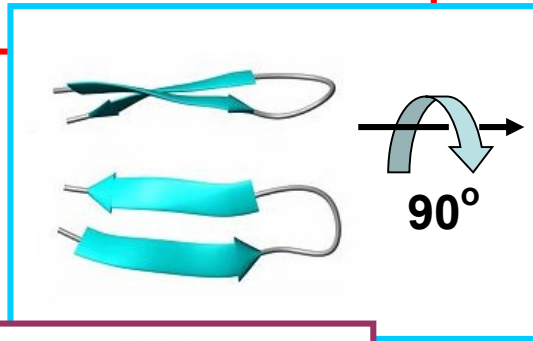
一级结构 – 蛋白质的氨基酸序列

```
>sp|P06968|DUT_ECOLI  
MKKIDVKILDPRVGKEFPLPTYATSGSAGLDLRACLNDAVELAPGDTTLVPTGL  
AIHIADPSLAAMMLPRSGLGHKHGIVLGNLVGLIDSDYQGQLMISVWNRGQDSF  
TIQPGERIAQMIFVPVVQAEFNLVEDFDATDRGEGGFHGHSGRQ
```

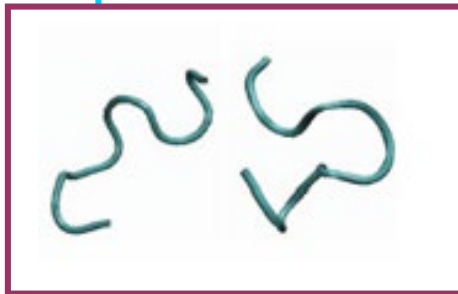
# 蛋白质结构 --- 二级结构



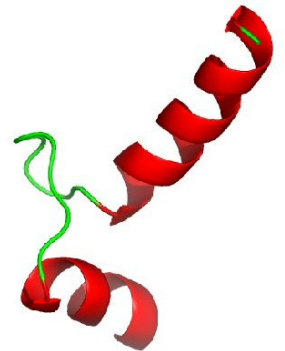
螺旋: 最常见的就是 $\alpha$ 螺旋。



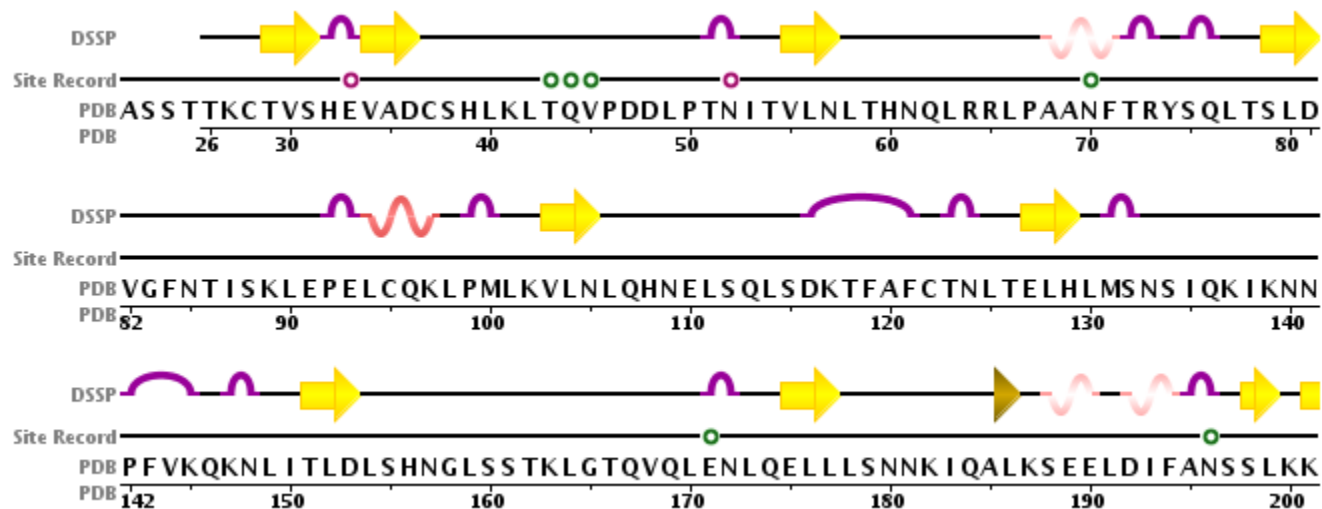
**$\beta$ 折叠 ( $\beta$  sheet)**:  $\beta$ 折叠由 $\beta$ 折片 ( $\beta$  strand) 平行排列而成。



**无规卷曲 (loop)**: 无规律松散结构.  
**转角 (turn)**: 如果肽链发生了急转弯 (角度大于 $90^\circ$ ), 这个转弯结构叫转角。



# 蛋白质结构 --- 二级结构



1	ASSTTKCTVS	HEVADCSHLK	LTQVPDDLPT	NITVLNLTHN	QLRRLPAANF
	EEE	TTEE	SS	SS	SSS T T SEEE SS GGGG
51	TRYSQLTSLD	VGFNTISKLE	PELCQKLPML	KVLNLQHNEL	SQLSDKTFAF
	TT TT SEEE	SS	TTHHHH TT	EEE SS	TTTTT
101	CTNLTELHLM	SNSIQIKNN	PFVKQKNLIT	LDLSHNGLS	TKLGTQVQLE
	TT SEEE T TS	S	TTTT TT E EE SS	SSS T	
151	NLQELLSNN	KIQALKSEEL	DIFANSSLKK	LELSSNQIKE	FSPGCFHAIG
	T EEE SS	B GGGT	GGGT EEE EE S	B TTTTTSS	
201	RLFGLFLNNV	QLGPSLTEKL	CLELANTSIR	NLSLSNSQLS	TTSNTTFLGL
	EE EEE TT	HHHHHHH	HHHTTS	EEE TTS	EE TTTTGGG
251	KWTNLTMLDL	SYNNLNWVG	DSFAWLPQLE	YFFLEYNNIQ	HLFSHSLHGL
	GGG	EEE TTS	EE T TTTT TT	EEE S B	EE TTTTT

# 蛋白质结构 --- 三级结构

三级结构是指整条多肽链的三维空间结构，即，包括骨架和侧链在内的所有原子的空间排列。

第一个蛋白质的三维空间结构是1958 由英国的Kendrew和Perutz博士用 X-射线晶体衍射法测定的。



X射线衍射法  
X-ray Crystallography



核磁共振法  
Nuclear Magnetic Resonance (NMR)

>130000

>12000



Max Ferdinand  
Perutz (1914-2002)  
nobel prize 1962

John Cowdery  
Kendrew (1917-1997)  
nobel prize 1962





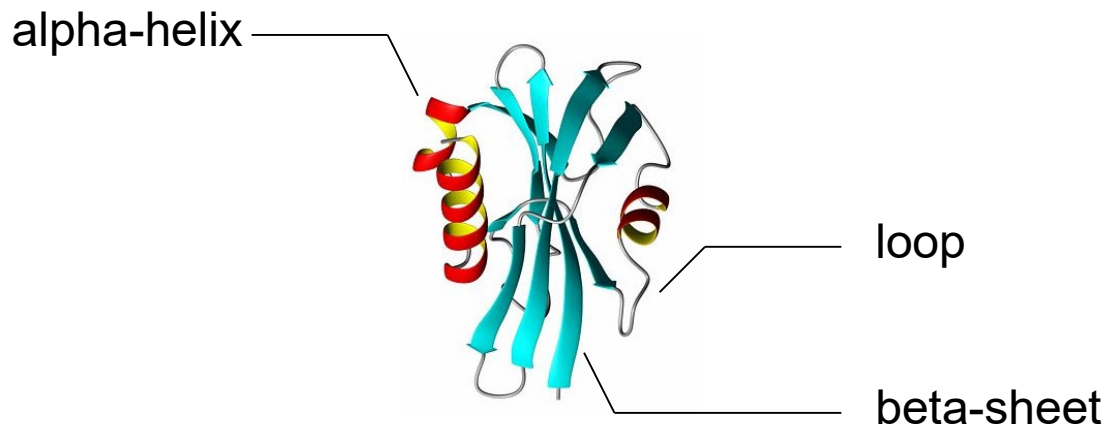
# 蛋白质结构 --- 二级结构的获取

如何获得蛋白质的二级结构

## 1. PDB/DSSP – 对于结构已知的蛋白质

**DSSP (Definition of Secondary Structure of Proteins)**，即，蛋白质二级结构词典。DSSP并不预测二级结构，而是根据二级结构的定义对已经测定结构的蛋白质的各个位置指出是哪种二级结构。

主页：<http://swift.cmbi.ru.nl/gv/dssp>



# 蛋白质结构 --- 二级结构获取

如何获得蛋白质的二级结构

## 1. PDB/DSSP – 对于结构已知的蛋白质

66	92	A	P	T	>>	S+	0	0	32	0, 0.0	3, -1.3	0, 0.0
67	93	A	E	H	>>	S+	0	0	79	1, -0.3	4, -3.1	2, -0.2
68	94	A	L	H	<>	S+	0	0	13	-3, -1.3	4, -1.4	1, -0.3
69	95	A	b	H	<4	S+	0	0	4	-3, -1.3	6, -0.3	-4, -0.4
70	96	A	Q	H	<<	S+	0	0	3	-3, -0.7	-2, -0.2	-4, -0.7
71	97	A	I	H	<	S+	0	0	00	-4, -3.1	-1, -0.2	1, -0.3
72	98	A	L	S	><	S+	0	0	6	-4, -1.4	3, -1.2	-5, -0.4
73	99	A	P	T	3	S+	0	0	67	0, 0.0	25, -0.2	0, 0.0
74	100	A	L	T	3	+	0	0	88	-23, -0.2	2, -0.6	-25, -0.2
75	101	A	L		<	+	0	0	7	-3, -1.2	-22, -0.2	-6, -0.3
76	102	A	K			+	0	0	83	-24, -3.2	24, -3.1	-2, -0.6
77	103	A	V	E		-de	53	101A	31	-25, -1.3	-23, -0.7	23, -0.2
78	104	A	L	E		-de	54	102A	6	23, -2.0	25, -1.3	-2, -0.6
79	105	A	N	E		+de	55	103A	17	-25, -1.9	-23, -1.9	-2, -0.4
80	106	A	L		>	+	0	0	0	23, -2.8	3, -0.9	-2, -0.4
81	107	A	Q	T	3	+	0	0	23	1, -0.2	-23, -2.2	24, -0.1

二级结构

一个DSSP文件的一部分

# 蛋白质结构 --- 二级结构获取

如何获得蛋白质的二级结构

## 1. PDB/DSSP – 对于结构已知的蛋白质

66	92	A	P	T	>>	S+	0	0	32	0, 0.0	3, -1.3	0, 0.0
67	93	A	E	H	>>	S+	0	0	79	1, -0.3	4, -3.1	2, -0.2
68	94	A	L	H	<>	S+	0	0	13	-3, -1.3	4, -1.4	1, -0.3
69	95	A	b	H	<4	S+	0	0	4	2, -1.2	6, -0.3	-4, -0.4
70	96	A	Q	H	<<	S+					-2, -0.2	-4, -0.7
71	97	A	I	H	<	S+						
72	98	A	L	S	><	S+						
73	99	A	P	T	3	S+						
74	100	A	L	T	3	+						
75	101	A	L		<	+						
76	102	A	K			+						
77	103	A	V	E		-de						
78	104	A	L	E		-de						
79	105	A	N	E		+de						
80	106	A	L		>	+						
81	107	A	Q	T	3	+						



### 二级结构

- H = alpha helix
- B = residue in isolated beta-bridge
- E = extended strand, participates in beta ladder
- G = 3-helix (3/10 helix)
- I = 5 helix (pi helix)
- T = hydrogen bonded turn
- S = bend
- Blank = loop or irregular

# 蛋白质结构 --- 二级结构获取

## 如何获得蛋白质的二级结构

### 1. PDB/DSSP – 对于结构已知的蛋白质

LAY-OUT	DSSP
<div><a href="#">Introduction</a> <a href="#">Output short</a> <a href="#">Explanation</a> <a href="#">Usage</a> <a href="#">Download</a></div>	<div><p>In 2011 Maarten Hekkelman has written new software that produces the same output as the original DSSP, but that deals better with the many exceptions life and the PDB throw at us. And the new software is much faster and easier to maintain in the future too. To not confuse the topic too much, we call this new software DSSP. The original DSSP will be referred to as DSSPold. In 2012 the determination of <math>\pi</math>-helices (I prefer to call them <math>\alpha</math>-bulges) has been implemented in DSSP strictly following the original description by Kabsch and Sander. Output from the new version (2.1.0) therefore deviates a bit from output from the original DSSP (that now is called DSSPold). We believe that the newest DSSP version is 'better' than all previous versions.</p><p><b>Obtaining the software</b></p><p>Under 'Download' you find access to DSSP. The package comes with everything in, on, and at it (including source code), and it comes under the <a href="#">Boost license</a>.</p><p>There is no license agreement or anything like that. If you are a commercial entity, the same rules hold for the new DSSP. So, as of 'now' (July 8 2011) DSSP is free of cost, free of license restrictions, and free of costs for everybody.</p><p><b>Using DSSP</b></p><p>We provide a series of DSSP related facilities that are explained partly in these DSSP pages, and partly elsewhere in the <a href="#">PDBfacilities</a> pages.</p><ul style="list-style-type: none"><li>• <a href="#">MRS</a> can be used to obtain DSSP files for PDB entries; alternatively, you can use <a href="#">MRS</a> to obtain <a href="#">PDBfinder</a> entries that also contain the DSSP derived secondary structure information.</li><li>• In case a DSSP file doesn't exist and you do not understand why not, please feel free to look at the <a href="#">Why Not</a> pages to see what "is going on".</li><li>• Under "Download" (a few pages down) we explain how you can get all DSSP files on your in-house computer.</li><li>• A <a href="#">web server</a> can be used to obtain individual DSSP files for your private PDB files.</li><li>• Feel free to look at the <a href="#">WSDL</a> that explains how you can use the DSSP web service.</li></ul></div>
<div><b>Miscellaneous</b> <a href="#">DSSP Article(s)</a> <a href="#">License agreement</a> <a href="#">Distribution</a></div>	
<div><b>Pointers</b> <a href="#">MRS</a> <a href="#">PDBFINDER</a> <a href="#">HSSP</a> <a href="#">WHAT IF</a> <a href="#">WHYNOT</a></div>	

# 蛋白质结构 --- 二级结构获取

如何获得蛋白质的二级结构

## 1. PDB/DSSP – 对于结构已知的蛋白质

**RCSB PDB** PROTEIN DATA BANK  
149886 Biological Macromolecular Structures  
Enabling Breakthroughs in Research and Education

Search by PDB ID, author, macromolecule, sequence, or ligand **Go**

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


**PDB-101** **WORLDWIDE PDB** **EMDataResource** **ndb** **NUCLEIC ACID DATABASE** **Worldwide Protein Data Bank Foundation**

[Structure Summary](#) [3D View](#) [Annotations](#) [Sequence](#) [Sequence Similarity](#) [Structure Similarity](#) [Experiment](#)

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

**3H6X**  
Crystal structure of dUTPase from Streptococcus mutans  
DOI: [10.2210/pdb3H6X/pdb](https://doi.org/10.2210/pdb3H6X/pdb)  
Classification: [HYDROLASE](#)  
Organism(s): [Streptococcus mutans serotype c \(strain ATCC 700610 / UA159\)](#)  
Expression System: [Escherichia coli BL21\(DE3\)](#)  
Deposited: 2009-04-24 Released: 2010-05-05  
Deposition Author(s): [Li, G.L.](#), [Wang, K.T.](#), [Liu, X.](#), [Li, L.F.](#), [Su, X.D.](#)

Experimental Data Snapshot      wwPDB Validation      [3D Report](#) [Full Report](#)



# 蛋白质结构 --- 二级结构获取

如何获得蛋白质的二级结构

## 2. 预测软件 – 对于结构未知的蛋白质

已知一个蛋白质的氨基酸序列，预测其二级结构。

常用软件：PSIPRED, Jpred, APSSP2, NNPREICT, PREDICTPROTEIN

PSIPRED: <http://bioinf.cs.ucl.ac.uk/psipred>



Jpred: <http://www.compbio.dundee.ac.uk/www-jpred>

# 蛋白质结构 --- 二级结构获取

如何获得蛋白质的二级结构

## 2. 预测软件 – 对于结构未知的蛋白质

**UCL Department Of Computer Science**  
**Bioinformatics Group**

Search Group UCL Home >> Departments of Computer Science >> Bioinformatics Group >> psipred

Site Navigation

Server Navigation

- PSIPRED Server
- PSIPRED help
- Server Overview
- Server Citation
- News
- History
- Software Download
- Login

## The PSIPRED Protein Structure Prediction Server

The PSIPRED Protein Structure Prediction Server aggregates several of our structure prediction methods into submit a protein sequence, perform the prediction of their choice and receive the results of the prediction via three prediction methods to apply to your sequence:

PSIPRED - a highly accurate method for protein secondary structure prediction

MEMSAT and MEMSAT-SVM - our widely used transmembrane topology prediction method

and one of GenTHREADER, pGenTHREADER and pDomTHREADER - sequence profile based fold recognition me

**Choose Prediction Method**

- ☒ Predict Secondary Structure (PSIPRED v3.0)
- ☐ Predict Transmembrane Topology (MEMSAT3 & MEMSAT-SVM)
- ☐ SVM Prediction of TM Topology and Helix Packing (MEMPACK) - **NEW!**
- ☐ Fold Recognition (GenTHREADER - quick)
- ☐ Fold Recognition (pGenTHREADER - with profiles and predicted secondary structure)
- ☐ Fold Recognition (pDomTHREADER - annotates multiple domain on chains)

[Help...](#)

# 蛋白质结构 --- 二级结构获取

如何获得蛋白质的二级结构

## 2. 预测软件 – 对于结构未知的蛋白质

Input Sequence (single letter amino acid code)

>3CIG:A|PDBID|CHAIN|SEQUENCE  
QCTVRYNVADCSHLKLTHIPDDLPSNITVLNLTHNQLRRLPPTNFTRYSQLAILDAGFNSISKLEPELCQILPLLKVLNI  
QHNELSQISDQTFVFCNTLTDLMSNSIHKIKSNPFKNQKNLIKLDLSHNGLSSTKLGTGVQLENLQELLAKNKILAL  
TFSGLKWTNLTQLDLSYNNLHDVGNGSFSYLPRLRYLSLEYNNIQRLSPRSFYGLSNLRYLSLKRAFTKQSVSLASHPNI

3cig.fasta

Filtering Options

☒ Mask low complexity regions ☐ Mask transmembrane helices ☐ Mask coiled-coil regions

Warning: No sequence filters are applied when running MEMSAT or MEMPACK

Submission Details

Email Address for job completion alert (optional)  
gongj@informatik.uni-muenchen.de

Password (only required for licenced commercial e-mail addresses)

Short identifier for submission  
3cig

Predict Clear form

结果会发送到给入的邮箱里，也可以在线等待，大约需要30分钟。

**注意：**不支持免费的大众邮箱，比如：hotmail，gmail。



# 蛋白质结构 --- 二级结构获取

如何获得蛋白质的二级结构

2. 预测软件 – 对于结构未知的蛋白质

网页显示的预测结果

## Results for psipred job 305290

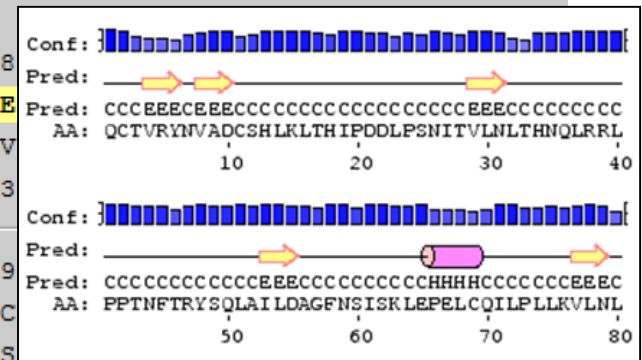
### Output for PSIPRED predictions

#### Psipred Residue Predictions

Conf: Confidence 0 =low 9 =high  
Pred: Predicted secondary structure H =helix E =strand C =coil  
AA: Target sequence

```
Conf: 9 8 3 2 2 0 4 7 9 8 4 6 8 9 9 9 8 6 8 9 8 8 5 8 6 9 7 5 8  
Pred: C C C E E E C E E E C C C C C C C C C C C C C C C E  
AA: Q C T V R Y N V A D C S H L K L T H I P D D L P S N I T V  
1 0 2 0 3
```

```
Conf: 9 9 6 7 9 3 3 4 2 4 9 9 6 5 8 5 8 8 7 2 2 8 8 4 8 8 8 8 9  
Pred: C C C C C H H H C C C C C C C E E E C C C C C C C C  
AA: I S K L E P E L C Q I L P L L K V L N L Q H N E L S Q I S  
7 0 8 0 9 0
```



Click to download these results in plain text format

# 蛋白质结构 --- 二级结构获取

如何获得蛋白质的二级结构

## 2. 预测软件 – 对于结构未知的蛋白质

发送至邮箱的预测结果

```
# PSIPRED HFORMAT (PSIPRED V3.0)
```

```
Conf: 9832204798468999868988586975888227869989998886898897
Pred: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
AA: QCTVRYNVADCSHLKLTHIPDDLPSNITVLNLTHNQLRRLPPTNFTRYSQLAILDAGFNS
      10      20      30      40      50      60
```

```
Conf: 996793342499658588722884888891014799988999840654884599888888
Pred: CCCCCHHHHCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
AA: ISKLEPELCQILPLLKVLNLQHNELSQISDQTFVFCNTLTELDMNSIHKIKSNPFKNQ
      70      80      90     100     110     120
```

```
Conf: 777679677883886899979899998989810886986786821237999746999538
Pred: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
AA: KNLIKLDLSHNGLSSTKLGTGVQLENLQELLLAKNKILALRSEELEFLGNSSLRKLDLSS
      130     140     150     160     170     180
```

```
Conf: 989888996367899886998768879902257652016999859799227838978921
Pred: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
AA: NPLKEFSPGCFQTIGKLFALLNNAQLNPHLTEKLCWELSNTSIQNLSLANNQLLATSES
      190     200     210     220     230     240
```

**Subject:** Psipred results for job ID:305293/3cig  
**From:** psipred@cs.ucl.ac.uk  
**Date:** Sat, October 1, 2011 5:49 am  
**To:** gongj@informatik.uni-muenchen.de  
**Priority:** Normal  
**Signature:** Unsigned  
**Options:** [View Full Header](#) | [View Printable Version](#) | [!](#)

# 蛋白质结构 --- 二级结构获取

如何获得蛋白质的二级结构

DSSP

2. 预测软件 – 对于结构未知的蛋白质

PSIPRED

```
51  LAILDAGFNSISKLEPELCQILPLLKVLNLQHNELSQISDQTFVFCTNLT
    CSEEECCSSCCCCCCTHHHHHSTTCSEEECTTCCCCCCTTSTTSCCSCC
    COEEECSCCCCCCCCCCHHHHCCCCCCCCSEEECCCCCCCCCCCCCCCCC

101 ELDLMSNSIHKIKSNPFKNQKNLIKLDLSHNGLSSTKLGTGVQLENLQEL
    EEECTTSCCCCCCSCTTTTCTTCSEEECCSSCCCCCCCCSSSCCTTCCEE
    EEEECSCCCCCCCCCCCCCCCCCCCCCCEEECCCCCCCCCCCCCCCCCEE

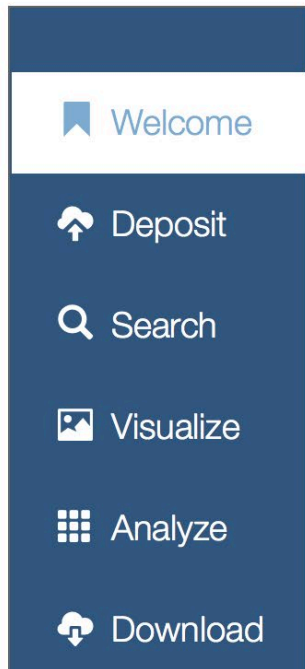
151 LLAKNKILALRSEELEFLGNSSLRKLDLSSNPLKEFSPGCFQTIGKLFAL
    ECCSSCCCEECSSGGGGGGTTCEESEEECCSCCCCEECTTTTTTSSEECCE
    EEECCCCCCCCCCCCCCCCCCCCCCCCCEEECCCCCCCCCCCCCCCCCEE
```

准确率超过90%

# 蛋白质结构 --- 三级结构

蛋白质结构数据库PDB

<https://www.rcsb.org>

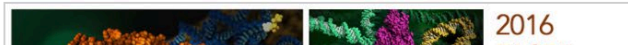


## A Structural View of Biology

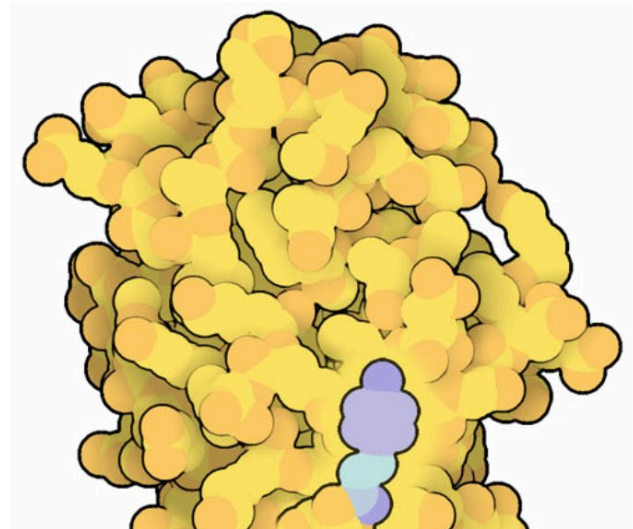
This resource is powered by the Protein Data Bank archive-information about the 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease.

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.

## A Molecular View of HIV Therapy



## March Molecule of the Month



# 蛋白质结构 --- 三级结构

蛋白质结构数据库PDB

<https://www.rcsb.org>

Advanced Search Interface

Sequence (BLAST/FASTA/PSI-BLAST) ▼

Sequence search (BLAST or FASTA)

Structure Id

Chain Id

Sequence

Search Tool  ▼

Mask Low  ▼

Complexity

E Cut Off

?

**85 Structures**

Add Search Criteria +

☐ Remove Similar Sequences at 90% ▼ Identity ?

Match  ▼ of the above conditions.

pdb.fasta

## 浏览dUTPase蛋白质的三级结构

Summary3D ViewSequenceAnnotationsSeq. Similarity3D SimilarityLiteratureBiol. & Chem.MethodsLinks

Crystal structure of dUTPase from Streptococcus mutans

DOI:10.2210/pdb3h6x/pdb

Primary Citation

Structure and activity analysis of dUTP nucleotidohydrolase from Streptococcus mutans

Li, G.L., Wang, K.T., Liu, X., Li, L.F., Su, X.D.

Journal: To be Published

3H6X.pdb - 记事本

文件(F) 编辑(E) 格式(O) 查看(V) 帮助(H)

HEADER HYDROLASE 24-APR-09 3H6X  
TITLE CRYSTAL STRUCTURE OF DUTPASE FROM STREPTOCOCCUS MUTANS  
COMPND MOL\_ID: 1;  
COMPND 2 MOLECULE: DUTPASE;  
COMPND 3 CHAIN: A, B, C;  
COMPND 4 EC: 3.6.1.23;  
COMPND 5 ENGINEERED: YES  
SOURCE MOL\_ID: 1;  
SOURCE 2 ORGANISM\_SCIENTIFIC: STREPTOCOCCUS MUTANS;  
SOURCE 3 ORGANISM\_TAXID: 1309;  
SOURCE 4 GENE: DUT;  
SOURCE 5 EXPRESSION\_SYSTEM: ESCHERICHIA COLI;  
SOURCE 6 EXPRESSION\_SYSTEM\_TAXID: 469008;  
SOURCE 7 EXPRESSION\_SYSTEM\_STRAIN: BL21 (DE3);  
SOURCE 8 EXPRESSION\_SYSTEM\_VECTOR\_TYPE: PLASMID;  
SOURCE 9 EXPRESSION\_SYSTEM\_PLASMID: PET28A  
KEYWDS JELLY-ROLL BETA-BARREL, HYDROLASE

3H6X.pdb  
345 KB - 已完成

148

3H6X

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FASTA Sequence  
PDB File (Text)  
PDB File (gz)  
mmCIF File  
mmCIF File (gz)  
PDBML/XML File  
PDBML/XML File (gz)  
Structure Factor (Text)  
Structure Factor (gz)  
Biological Assembly (gz) (A+S)

Hide

3D View: JSmol or PV More Images

Symmetry: C3 view  
Stoichiometry: Homo 3-mer - A3  
Biological assembly 1 assigned by authors and generated by PISA (software)

看看一个3D结构是怎么存在数据库里的?

## 浏览dUTPase蛋白质的三级结构

```
HEADER      HYDROLASE                      24-APR-09   3H6X
TITLE       CRYSTAL STRUCTURE OF DUTPASE FROM STREPTOCOCCUS MUTANS
COMPND      MOL_ID: 1;
.....
COMPND      5 ENGINEERED: YES
SOURCE      MOL ID: 1;
.....
SOURCE      9 EXPRESSION_SYSTEM_PLASMID: PE
KEYWDS      JELLY-ROLL BETA-BARREL, HYDRO
EXPDTA      X-RAY DIFFRACTION
AUTHOR      G. L. LI, K. T. WANG, X. LIU, L. F. LI, X
REVDAT      1   05-MAY-10 3H6X   0
JRNL        AUTH   G. L. LI, K. T. WANG, X. LIU
.....
JRNL        REFN
REMARK      2
REMARK      2 RESOLUTION.      1.70 ANGSTROMS.
REMARK      3
REMARK      3 REFINEMENT.
```

### 基本信息部分

这部分对蛋白质进行了基本描述，  
包括以下索引词：

**HEADER, OBSLTE, TITLE,  
SPLIT, CAVEAT, COMPND,  
SOURCE, KEYWDS, EXPDTA,  
AUTHOR, REVDAT, SPRSDE,  
JRNL, REMARK.**



## 浏览dUTPase蛋白质的三级结构

HEADER	HYDROLASE	24-APR-09	3H6X
--------	-----------	-----------	------

TITLE CRYSTAL STRUCTURE OF DUTPASE FROM STREPTOCOCCUS MUTANS

COMPND MOL\_ID: 1;

COMPND 2 MOLECULE: DUTPASE;

COMPND 3 CHAIN: A, B, C;

COMPND 4 EC: 3.6.1.23;

COMPND 5 ENGINEERED: YES

SOURCE MOL\_ID: 1;

SOURCE 2 ORGANISM\_SCIENTIFIC: STREPTOCOCCUS MUTANS;

SOURCE 3 ORGANISM\_TAXID: 1309;

SOURCE 4 GENE: DUT;

SOURCE 5 EXPRESSION\_SYSTEM: ESCHERICHIA COLI;

SOURCE 6 EXPRESSION\_SYSTEM\_TAXID: 469008;

SOURCE 7 EXPRESSION\_SYSTEM\_STRAIN: BL21 (DE3);

SOURCE 8 EXPRESSION\_SYSTEM\_VECTOR\_TYPE: PLASMID;

SOURCE 9 EXPRESSION\_SYSTEM\_PLASMID: PET28A

KEYWDS JELLY-ROLL BETA-BARREL, HYDROLASE

**HEADER : 分子类别,  
日期, 数据库编号**



## 浏览dUTPase蛋白质的三级结构

HEADER	HYDROLASE	24-APR-09	3H6X
TITLE	CRYSTAL STRUCTURE OF DUTPASE FROM STREPTOCOCCUS MUTANS		
COMPND	MOL_ID: 1;		
COMPND	2 MOLECULE: DUTPASE;		
COMPND	3 CHAIN: A, B, C;		
COMPND	4 EC: 3.6.1.23;		
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SOURCE	MOL_ID: 1;		
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SOURCE	7 EXPRESSION_SYSTEM_STRAIN: BL21 (DE3);		
SOURCE	8 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;		
SOURCE	9 EXPRESSION_SYSTEM_PLASMID: PET28A		
KEYWDS	JELLY-ROLL BETA-BARREL, HYDROLASE		

**TITLE:** 题目，一般就是相关文献的题目。

## 浏览dUTPase蛋白质的三级结构

```
HEADER      HYDROLASE                                24-APR-09   3H6X
TITLE       CRYSTAL STRUCTURE OF DUTPASE FROM STREPTOCOCCUS MUTANS
COMPND      MOL_ID: 1;
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COMPND      4 EC: 3.6.1.23;
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SOURCE      MOL_ID: 1;
SOURCE      2 ORGANISM_SCIENTIFIC: STREPTOCOCCUS MUTANS;
SOURCE      3 ORGANISM_TAXID: 1309;
SOURCE      4 GENE: DUT;
SOURCE      5 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE      6 EXPRESSION_SYSTEM_TAXID: 469008;
SOURCE      7 EXPRESSION_SYSTEM_STRAIN: BL21 (DE3);
SOURCE      8 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
SOURCE      9 EXPRESSION_SYSTEM_PLASMID: PET28A
KEYWDS      JELLY-ROLL BETA-BARREL, HYDROLASE
```

**COMPND:** 对各个分子的描述。

## 浏览dUTPase蛋白质的三级结构

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HEADER      HYDROLASE                                24-APR-09   3H6X
TITLE       CRYSTAL STRUCTURE OF DUTPASE FROM STREPTOCOCCUS MUTANS
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: DUTPASE;
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COMPND      4 EC: 3.6.1.23;
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SOURCE      2 ORGANISM_SCIENTIFIC: STREPTOCOCCUS MUTANS;
SOURCE      3 ORGANISM_TAXID: 1309;
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SOURCE      9 EXPRESSION_SYSTEM_PLASMID: PET28A
KEYWDS      JELLY-ROLL BETA-BARREL, HYDROLASE
```

**SOURCE:** 结构中包括的每一个分子的来源（生物学/化学）。

## 浏览dUTPase蛋白质的三级结构

```
HEADER      HYDROLASE                                24-APR-09   3H6X
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SOURCE      3 ORGANISM_TAXID: 1309;
SOURCE      4 GENE: DUT;
SOURCE      5 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE      6 EXPRESSION_SYSTEM_TAXID: 469008;
SOURCE      7 EXPRESSION_SYSTEM_STRAIN: BL21 (DE3);
SOURCE      8 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
SOURCE      9 EXPRESSION_SYSTEM_PLASMID: PET28A
KEYWDS      JELLY-ROLL BETA-BARREL, HYDROLASE
```

**KEYWDS:** 一系列关键词，可用于数据库搜索。

浏览dUTPase蛋白质的三级结构

SOURCE	8	EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;	
SOURCE	9	EXPRESSION_SYSTEM_PLASMID: PET28A	
KEYWDS		JELLY-ROLL BETA-BARREL, HYDROLASE	
EXPDTA		X-RAY DIFFRACTION	
AUTHOR		G. L. LI, K. T. WANG, X. LIU, L. F. LI, X. D. SU	
REVDAT	1	05-MAY-10 3H6X	0
JRNL		AUTH	G.
JRNL		TITL	ST
JRNL		TITL 2	FR
JRNL		REF	TO
JRNL		REFN	
REMARK	2		
REMARK	2	RESOLUTION	
REMARK	3		
REMARK	3	REFINEMENT	
REMARK	3	PROGRAM	
REMARK	3	AUTHORS	

**EXPDTA: 测定结构所用的实验方法:**

**X-RAY DIFFRACTION** X-射线衍射

**FIBER DIFFRACTION** 光纤点衍射

**NEUTRON DIFFRACTION** 中子粉末衍射

**ELECTRON CRYSTALLOGRAPHY** 电子晶体学

**ELECTRON MICROSCOPY** 电子显微镜

**SOLID-STATE NMR** 固态核磁共振

**SOLUTION NMR** 液态核磁共振

**SOLUTION SCATTERING** 液态散射

HYDROLASE

## 浏览dUTPase蛋白质的三级结构

SOURCE 8 EXPRESSION\_SYSTEM\_VECTOR\_TYPE: PLASMID;

SOURCE 9 EXPRESSION\_SYSTEM\_PLASMID: PET28A

KEYWDS JELLY-ROLL BETA-BARREL, HYDROLASE

EXPDTA X-RAY DIFFRACTION

**AUTHOR: 结构测定者**

AUTHOR G. L. LI, K. T. WANG, X. LIU, L. F. LI, X. D. SU

REVDAT 1 05-MAY-10 3H6X 0

JRNL AUTH G. L. LI, K. T. WANG, X. LIU, L. F. LI, X. D. SU

JRNL TITL STRUCTURE AND ACTIVITY ANALYSIS OF DUTP NUCLEOTIDOHYDROLASE

JRNL TITL 2 FROM STREPTOCOCCUS MUTANS

JRNL REF TO BE PUBLISHED

JRNL REFN

REMARK 2

REMARK 2 RESOLUTION. 1.70 ANGSTROMS.

REMARK 3

REMARK 3 REFINEMENT.

REMARK 3 PROGRAM : PHENIX (PHENIX.REFINE)

REMARK 3 AUTHORS : PAUL ADAMS, PAVEL AFONINE, VICENT CHEN, IAN

## 浏览dUTPase蛋白质的三级结构

SOURCE 8 EXPRESSION\_SYSTEM\_VECTOR\_TYPE: PLASMID;  
SOURCE 9 EXPRESSION\_SYSTEM\_PLASMID: PET28A  
KEYWDS JELLY-ROLL BETA-BARREL, HYDROLASE  
EXPDTA X-RAY DIFFRACTION  
AUTHOR G. L. LI, K. T. WANG, X. LIU, L. F. LI, X. D. SU

**REVDAT:** 历史上  
曾经对该数据库记  
录进行过的修改。

REVDAT 1 05-MAY-10 3H6X 0

JRNL AUTH G. L. LI, K. T. WANG, X. LIU, L. F. LI, X. D. SU

JRNL TITL STRUCTURE AND ACTIVITY ANALYSIS OF DUTP NUCLEOTIDOHYDROLASE

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REMARK 3 REFINEMENT.

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## 浏览dUTPase蛋白质的三级结构

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KEYWDS JELLY-ROLL BETA-BARREL, HYDROLASE  
EXPDTA X-RAY DIFFRACTION  
AUTHOR G. L. LI, K. T. WANG, X. LIU, L. F. LI, X. D. SU  
REVDAT 1 05-MAY-10 3H6X 0

**JRNL:** 发表这个  
结构的文献信息。

JRNL AUTH G. L. LI, K. T. WANG, X. LIU, L. F. LI, X. D. SU  
JRNL TITL STRUCTURE AND ACTIVITY ANALYSIS OF DUTP NUCLEOTIDOHYDROLASE  
JRNL TITL 2 FROM STREPTOCOCCUS MUTANS  
JRNL REF TO BE PUBLISHED  
JRNL REFN

REMARK 2  
REMARK 2 RESOLUTION. 1.70 ANGSTROMS.  
REMARK 3  
REMARK 3 REFINEMENT.  
REMARK 3 PROGRAM : PHENIX (PHENIX.REFINE)  
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## 浏览dUTPase蛋白质的三级结构

```
SOURCE      8 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;  
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KEYWDS      JELLY-ROLL BETA-BARREL, HYDROLASE  
EXPDTA      X-RAY DIFFRACTION  
AUTHOR      G. L. LI, K. T. WANG, X. LIU, L. F. LI, X. D. SU  
REVDAT      1   05-MAY-10 3H6X   0  
JRNL        AUTH    G. L. LI, K. T. WANG, X. LIU, L. F. LI, X. D. SU  
JRNL        TITL    STRUCTURE AND ACTIVITY ANALYSIS OF DUTP NUCLEOTIDOHYDROLASE  
JRNL        TITL 2  FROM STREPTOCOCCUS MUTANS  
JRNL        REF     TO BE PUBLISHED  
JRNL        REFN
```

**REMARK:** 注释,  
关于这个蛋白质的  
各种注释信息,  
这些信息无法归  
入其他部分, 所  
以就都放这里了。

```
REMARK      2  
REMARK      2 RESOLUTION.      1.70 ANGSTROMS.  
REMARK      3  
REMARK      3 REFINEMENT.  
REMARK      3   PROGRAM      : PHENIX (PHENIX.REFINE)  
REMARK      3   AUTHORS      : PAUL ADAMS, PAVEL AFONINE, VICENT CHEN, IAN
```

## 浏览dUTPase蛋白质的三级结构

```
REMARK 525      HOH A 616          DISTANCE =  5.29  ANGSTROMS
REMARK 525      HOH A 677          DISTANCE =  5.20  ANGSTROMS
DBREF  3H6X A      1    148  UNP      Q8DVY3  Q8DVY3_STRMU      1    148
DBREF  3H6X B      1    148  UNP      Q8DVY3  Q8DVY3_STRMU      1    148
DBREF  3H6X C      1    148  UNP      Q8DVY3  Q8DVY3_STRMU      1    148
SEQRES   1 A  148  MSE MSE LYS THR ARG GLY PHE GLU LEU ILE THR ASP TYR
SEQRES   2 A  148  THR ASP GLU ASN LEU LEU PRO LYS ARG GLU THR ALA HIS
SEQRES   3 A  148  ALA ALA GLY TYR ASP LEU LYS
SEQRES   4 A  148  ILE SER ALA GLY ALA ILE VAL
.....
SEQRES   9 C  148  ASN MSE THR ASP GLN THR VAL
SEQRES  10 C  148  ARG VAL VAL GLN GLY VAL PHE
SEQRES  11 C  148  ASP GLY ASP LYS ALA THR GLY
SEQRES  12 C  148  GLY SER THR GLY GLY
MODRES 3H6X MSE A    56  MET  SELENOMETHIONINE
MODRES 3H6X MSE A   103  MET  SELENOMETHIONINE
MODRES 3H6X MSE A   106  MET  SELENOMETHIONINE
MODRES 3H6X MSE A   125  MET  SELENOMETHIONINE
.....
```

### 一级结构信息部分

这部分包括大分子（蛋白质）各个残基的信息，包括以下索引词：

**DBREF, SEQADV,  
SEQRES, MODRES**

## 浏览dUTPase蛋白质的三级结构

```
REMARK 525      HOH A 616          DISTANCE =  5.29  ANGSTROMS
REMARK 525      HOH A 677          DISTANCE =  5.20  ANGSTROMS
DBREF  3H6X A      1    148  UNP      Q8DVY3    Q8DVY3_STRMU      1    148
DBREF  3H6X B      1    148  UNP      Q8DVY3    Q8DVY3_STRMU      1    148
DBREF  3H6X C      1    148  UNP      Q8DVY3    Q8DVY3_STRMU      1    148
SEQRES   1 A   148  MSE MSE LYS THR ARG GLY PHE GLU LEU ILE THR ASP TYR
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SEQRES   9 C   148  ASN MSE THR ASP GLN THR VAL
SEQRES  10 C   148  ARG VAL VAL GLN GLY VAL PHE MSE PRO PHE LEU LEU ILE
SEQRES  11 C   148  ASP GLY ASP LYS ALA THR GLY THR ARG THR GLY GLY PHE
SEQRES  12 C   148  GLY SER THR GLY GLY
MODRES  3H6X MSE A    56  MET  SELENOMETHIONINE
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MODRES  3H6X MSE A   106  MET  SELENOMETHIONINE
MODRES  3H6X MSE A   125  MET  SELENOMETHIONINE
.....
```

**DBREF:** 其他蛋白质序列数据库的有关记录。

## 浏览dUTPase蛋白质的三级结构

```
REMARK 525      HOH A 616          DISTANCE =  5.29  ANGSTROMS
REMARK 525      HOH A 677          DISTANCE =  5.20  ANGSTROMS
DBREF  3H6X A      1    148  UNP      Q8DVY3    Q8DVY3_STRMU      1    148
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SEQRES   4 A  148  ILE SER ALA GLY ALA ILE VAL LEU VAL PRO THR GLY VAL
.....
SEQRES   9 C  148  ASN MSE THR ASP GLN THR VAL VAL LEU GLU ALA GLY GLU
SEQRES  10 C  148  ARG VAL VAL GLN GLY VAL PHE MSE PRO PHE LEU LEU ILE
SEQRES  11 C  148  ASP GLY ASP LYS ALA THR GLY THR ARG THR GLY GLY PHE
SEQRES  12 C  148  GLY SER THR GLY GLY
MODRES 3H6X MSE A    56  MET  SELENOMETHIONINE
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MODRES 3H6X MSE A   106  MET  SELENOMETHIONINE
MODRES 3H6X MSE A   125  MET  SELENOMETHIONINE
.....
```

**SEQRES:** 氨基酸序列。

## 浏览dUTPase蛋白质的三级结构

```
REMARK 525      HOH A 616          DISTANCE =  5.29  ANGSTROMS
REMARK 525      HOH A 677          DISTANCE =  5.20  ANGSTROMS
DBREF  3H6X A      1    148  UNP      Q8DVY3  Q8DVY3_STRMU      1    148
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.....
SEQRES   9 C  148  ASN MSE THR ASP GLN THR VAL VAL LEU GLU ALA GLY GLU
SEQRES  10 C  148  ARG VAL VAL GLY
SEQRES  11 C  148  ASP GLY ASP LYS ALA THR GLY THR ARG THR GLY GLY PHE
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MODRES 3H6X MSE A   103  MET  SELENOMETHIONINE
MODRES 3H6X MSE A   106  MET  SELENOMETHIONINE
MODRES 3H6X MSE A   125  MET  SELENOMETHIONINE
.....
```

**MODRES: 对标准残基上的修饰。**

蛋氨酸 → 硒代蛋氨酸

## 浏览dUTPase蛋白质的三级结构

```
HET      MSE  B   56          8
HET      MSE  B  103          8
HET      MSE  B  106          8
HET      MSE  B  125          8
HET      MSE  C   56          8
HET      MSE  C  103          8
HET      MSE  C  106          8
HET      MSE  C  125          8
HETNAM          MSE SELENOMETHIONINE
FORMUL      1  MSE      12(C5 H11 N 02 SE)
FORMUL      4  HOH     *688(H2 O)
```

非标准残基部分，包括以下索引词：  
**HET:** 非标准残基及位置  
**HETNAM:** 非标准残基的化学名称  
**FORMUL:** 非标准残基的化学式

## 浏览dUTPase蛋白质的三级结构

二级结构部分，  
包括以下索引词：

**HELIX: 螺旋**

**SHEET: 折片**

**TURN: 转角**

Protein Data Bank (PDB) File Format											
HELIX	1	1	ASP	A	15	LEU	A	19	5		
HELIX	2	2	SER	A	68	GLY	A	75	1		
HELIX	3	3	ASP	B	15	LEU	B	19	5		
HELIX	4	4	SER	B	68	GLY	B	75	1		
HELIX	5	5	ASP	C	15	LEU	C	19	5		
HELIX	6	6	SER	C	68	GLY	C	75	1		
SHEET	1	A	2	GLY	A	6	LEU	A	9	0	
SHEET	2	A	2	VAL	A	52	TYR	A	55	-1	0
SHEET	1	B	4	TYR	A	30	LYS	A	33	0	
SHEET	2	B	4	ARG	A	118	PRO	A	126	-1	0
SHEET	3	B	4	GLU	A	60	ASP	A	66	-1	N
SHEET	4	B	4	VAL	A	82	ILE	A	85	-1	0
SHEET	1	C	2	THR	A	38	ILE	A	40	0	
SHEET	2	C	2	VAL	A	111	LEU	A	113	-1	0
SHEET	1	D	3	ILE	A	45	PRO	A	49	0	

5  
8  
5  
8  
5  
8

## 浏览dUTPase蛋白质的三级结构

**LINK:** 残基间化学键，  
比如氢键，二硫键等。

LINK	C	MSE	A	106	N	THR	A	107	1555	1555	1.32
LINK	C	PHE	A	124	N	MSE	A	125	1555	1555	1.33
LINK	C	MSE	A	125	N	PRO	A	126	1555	1555	1.34
LINK	C	TYR	B	55	N	MSE	B	56	1555	1555	1.33
LINK	C	MSE	B	56	N	GLN	B	57	1555	1555	1.33
LINK	C	GLN	B	102	N	MSE	B	103	1555	1555	1.33
LINK	C	MSE	B	103	N	LYS	B	104	1555	1555	1.33
LINK	C	ASN	B	105	N	MSE	B	106	1555	1555	1.34
LINK	C	MSE	B	106	N	THR	B	107	1555	1555	1.33
LINK	C	PHE	B	124	N	MSE	B	125	1555	1555	1.34
LINK	C	MSE	B	125	N	PRO	B	126	1555	1555	1.34
LINK	C	TYR	C	55	N	MSE	C	56	1555	1555	1.33
LINK	C	MSE	C	56	N	GLN	C	57	1555	1555	1.33
LINK	C	GLN	C	102	N	MSE	C	103	1555	1555	1.33
LINK	C	MSE	C	103	N	LYS	C	104	1555	1555	1.33



浏览dUTPase蛋白质的三级结构

ATOM: 原子坐标

	ATOM: 原子坐标					3D坐标			温度因子		元素符号
	原子号	原子名	残基名	分子链	残基号	X轴	Y轴	Z轴	占有率	温度因子	
ATOM	134	N	PRO	A	20	6.147	-10.140	21.368	1.00	10.34	N
ATOM	135	CA	PRO	A	20	7.611	-10.161	21.225	1.00	10.95	C
ATOM	136	C	PRO	A	20	8.320	-11.125	22.163	1.00	11.53	C
ATOM	137	O	PRO	A	20	7.895	-11.335	23.310	1.00	11.87	O
ATOM	138	CB	PRO	A	20	8.022	-8.719	21.567	1.00	9.74	C
ATOM	139	CG	PRO	A	20	6.790	-7.890	21.271	1.00	10.92	C
ATOM	140	CD	PRO	A	20	5.638	-8.787	21.670	1.00	7.65	C
ATOM	141	N	LYS	A	21	9.412	-11.701	21.670	1.00	11.67	N
ATOM	142	CA	LYS	A	21	10.297	-12.480	22.521	1.00	12.81	C
ATOM	143	C	LYS	A	21	11.732	-12.080	22.223	1.00	11.21	C
ATOM	144	O	LYS	A	21	12.020	-11.451	21.190	1.00	12.10	O
ATOM	145	CB	LYS	A	21	10.098	-13.978	22.289	1.00	16.83	C
ATOM	146	CG	LYS	A	21	10.533	-14.470	20.914	1.00	24.79	C
ATOM	147	CD	LYS	A	21	10.280	-15.970	20.773	1.00	30.83	C
ATOM	148	CE	LYS	A	21	10.625	-16.476	19.371	1.00	31.96	C
ATOM	149	NZ	LYS	A	21	10.319	-17.928	19.240	1.00	44.03	N

## 浏览dUTPase蛋白质的三级结构

```
CONNECT 390 400
CONNECT 400 390 401
CONNECT 401 400 402 404
CONNECT 402 401 403 408
CONNECT 403 402
CONNECT 404 401 405
CONNECT 405 404 406
CONNECT 406 405 407
CONNECT 407 406
CONNECT 408 402
CONNECT 765 772
CONNECT 772 765 773
CONNECT 773 772 774 776
CONNECT 774 773 775 780
CONNECT 775 774
```

**CONNECT: 原子间化学键连接**

## 浏览dUTPase蛋白质的三级结构

```
CONNECT 2940 2949
CONNECT 2949 2940 2950
CONNECT 2950 2949 2951 2953
CONNECT 2951 2950 2952 2957
CONNECT 2952 2951
CONNECT 2953 2950 2954
CONNECT 2954 2953 2955
CONNECT 2955 2954 2956
CONNECT 2956 2955
CONNECT 2957 2951
```

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**END:** 结束符

```
MASTER      385      0      12      6      33      0      0      6 3696      3      120      36
END
```

## 浏览dUTPase蛋白质的三级结构

Summary

3D

Crystal structure

DOI:10.2210/pdb

Primary Citation

Structure and a

Li, G.L. , Wan

Journal: To be

PubMed ID is n

↓ Molecular D

Classification:

Structure Weig

Molecule:

Polymer:

Chains:

EC#:

Organism:

Gene Name:

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mutans

3H6X

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Biological Assembly ?



 3D View: JSmol or PV [More Images](#)

Symmetry: **C3** view




Stoichiometry: **Homo 3-mer - A3**

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

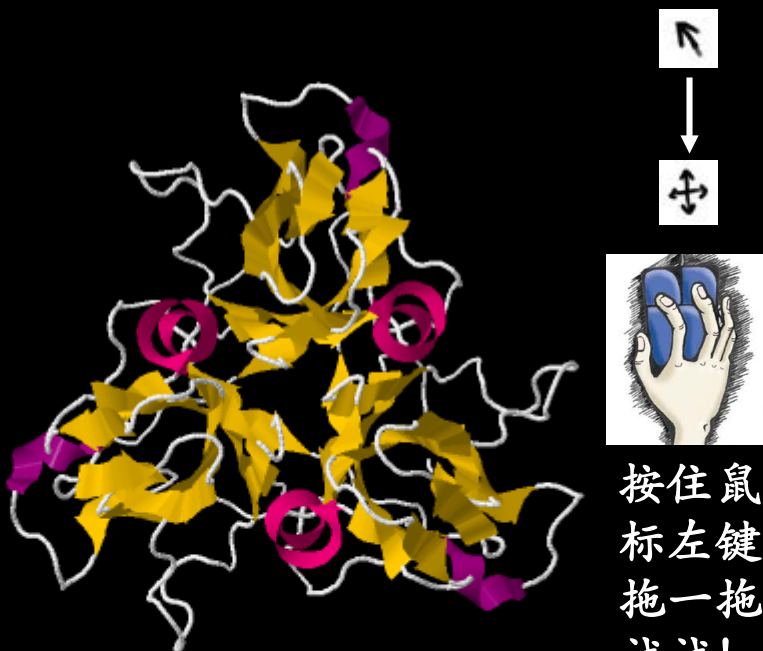
[Summary](#)[3D View](#)[Sequence](#)[Annotations](#)[Seq. Similarity](#)[3D Similarity](#)[Literature](#)[Biol. & Chem.](#)[Methods](#)[Geometry](#)[Links](#)

## Crystal structure of dUTPase from Streptococcus mutans

**3H6X**

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### Structure Details ?

Structure Biological Assembly 1 ▾

Symmetry Type Global Symmetry ▾

Symmetry C3

Stoichiometry A3

#### Select Orientation

<< Front C3 axis >>

#### Select Display Mode ?

Secondary Structure

Symmetry

Subunit

Custom View

#### Custom View options

Style Cartoon ▾

Color Secondary Structure ▾

Surface None ▾

Jmol mode HTML5 (beta) ▾

☐ H-Bonds

☐ SS Bonds

☐ Rotation

☒ Black Background




☐ Polyhedron


☐ Axes

[Summary](#)[3D View](#)[Sequence](#)[Annotations](#)[Seq. Similarity](#)[3D Similarity](#)[Literature](#)[Biol. & Chem.](#)[Methods](#)[Geometry](#)[Links](#)

## Crystal structure of dUTPase from Streptococcus mutans

**3H6X**

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




### Structure Details

Structure Biological Assembly 1 ▾Symmetry Type Global Symmetry ▾

Symmetry C3

Stoichiometry A3

Select Orientation

<< *Front C3 axis* >>Select Display Mode 

操作

旋转

放大/缩小

选择

Jmol菜单

Secondary Structure

Symmetry

按住鼠标左键拖拽

按住Shift + 鼠标左键拖拽 或者利用鼠标中键

点击鼠标左键

点击鼠标右键

☐ Polyhedron☐ Axes

[Summary](#)[3D View](#)[Sequence](#)[Annotations](#)[Seq. Similarity](#)[3D Similarity](#)[Literature](#)[Biol. & Chem.](#)[Methods](#)[Geometry](#)[Links](#)

## Crystal structure of dUTPase from Streptococcus mutans

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Structure Biological Assembly 1 ▾Symmetry Type Global Symmetry ▾

Symmetry C3

Stoichiometry A3

### Select Orientation

<< *Front C3 axis* >>

### Select Display Mode ?

Secondary Structure

Symmetry

Subunit

Custom View




#### Custom View options


Style Cartoon ▾Color Secondary Structure ▾Surface None ▾Jmol mode HTML5 (beta) ▾☐ H-Bonds☐ SS Bonds☐ Rotation☒ Black Background☐ Polyhedron☐ Axes

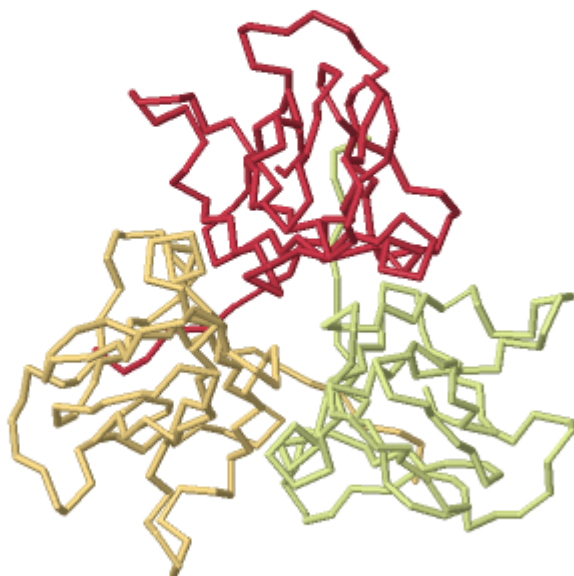
[Summary](#)**[3D View](#)**[Sequence](#)[Annotations](#)[Seq. Similarity](#)[3D Similarity](#)[Literature](#)[Biol. & Chem.](#)[Methods](#)[Geometry](#)[Links](#)

## Crystal structure of dUTPase from Streptococcus mutans

**3H6X**

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



### Structure Details

Structure Biological Assembly 1 ▾Symmetry Type Global Symmetry ▾

Symmetry C3

Stoichiometry A3

#### Select Orientation

<< *Front C3 axis* >>

#### Select Display Mode

Secondary Structure

Symmetry

Subunit

Custom View

#### Custom View options

Style Backbone ▾Color Subunit ▾Surface None ▾Jmol mode HTML5 (beta) ▾☐ H-Bonds☐ SS Bonds☐ Rotation☐ Black Background☐ Polyhedron☐ Axes