

Protein databases

PDB database

- From the class website
- External Links/Structure Databases/PDB database

The screenshot shows the RCSB Protein Data Bank (PDB) homepage. At the top, the header includes the PDB logo, the text "An Information Portal to Biological Macromolecular Structures", and a status bar indicating "As of Tuesday Sep 15, 2009" with "60173 Structures" and links to "PDB Statistics". A search bar is prominently displayed with a "Search" button and a link to "Advanced Search". The left sidebar contains navigation links under "Home", "Deposition", and "Search". The main content area features a section titled "A Resource for Studying Biological Macromolecules" with a brief description of the PDB archive and its role in curating and annotating protein structures. Below this, a "Molecule of the Month" section highlights "Xanthine Oxidoreductase" (PDB entry 1fo4), accompanied by a 3D ribbon diagram of the protein structure. The right sidebar includes a "News" section with links to "Complete News", "Newsletter", "Discussion Forum", and "Job Listings", and a specific news item dated "15-September-2009" titled "New Tool For Exploring Sequence and Structure Alignments" which mentions the "RCSB PDB Comparison Tool".

RCSB Protein Data Bank

MyPDB Login

A MEMBER OF THE PDB

An Information Portal to Biological Macromolecular Structures

As of Tuesday Sep 15, 2009 there are 60173 Structures | PDB Statistics

WHAT'S NEW | HELP | PRINT

PDB ID or keyword Search Advanced Search

Home

- News & Publications
- Policies
- FAQ
- Contact
- Feedback
- About Us

Deposition

- All Deposit Services
- Electron Microscopy
- NMR
- Validation Server
- BioSync Beamline
- Related Tools

Search

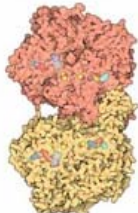
- Advanced Search
- Latest Release
- Latest Publications
- Sequence Search
- Ligand Search
- Unreleased Entries
- Browse Database
- Histograms

A Resource for Studying Biological Macromolecules

The PDB archive contains information about experimentally-determined structures of proteins, nucleic acids, and complex assemblies. As a member of the [wwPDB](#), the RCSB PDB curates and annotates PDB data according to agreed upon standards.

The RCSB PDB also provides a variety of tools and resources. Users can perform simple and advanced searches based on annotations relating to sequence, structure and function. These molecules are visualized, downloaded, and analyzed by users who range from students to specialized scientists.

Molecule of the Month: Xanthine Oxidoreductase



Our diet includes a wide variety of different molecules. Many of these molecules are broken down completely and used to generate the metabolic energy that powers our cells. Others are disassembled piece-by-piece and recycled to build our own proteins and nucleic acids. The ones that are left over are broken down and discarded. Xanthine oxidoreductase, shown here from PDB entry [1fo4](#), is the last stop for extra purine nucleotides (ATP and GTP) in our cells. Purines are broken down in several steps, ultimately yielding uric acid, which is excreted from the body.

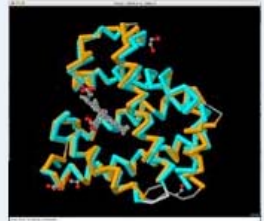
[Read more ...](#) [Previous Features](#)

News

- Complete News
- Newsletter
- Discussion Forum
- Job Listings

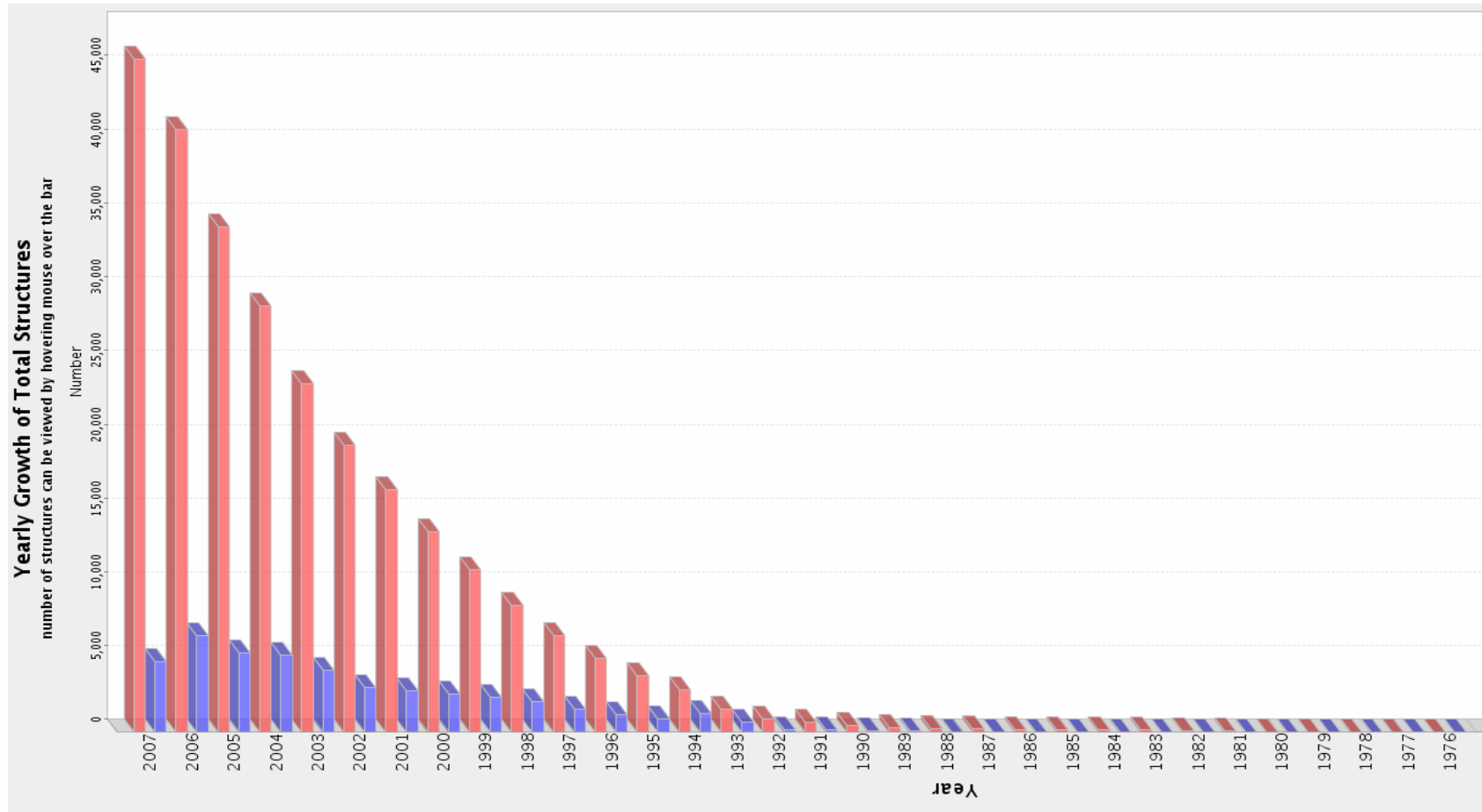
15-September-2009

New Tool For Exploring Sequence and Structure Alignments



The new **RCSB PDB Comparison Tool** can calculate pairwise sequence

What's in this database



A range of contents

- PDB code (simplest, and most common)
- Advanced search: molecule name
 - Hemoglobin (449 hits)
 - Histone acetylase (7 hits)
- Select one (Click on pdb code)

RCSB PDB : Query Results

RCSB PDB
PROTEIN DATA BANK

A MEMBER OF THE **PDB**

An Information Portal to Biological Macromolecular Structures

As of Tuesday Sep 15, 2009 there are 60173 Structures | PDB Statistics

WHAT'S NEW | HELP | PRINT

PDB ID or keyword Search ? | Advanced Search


449 Structure Hits 29 Unreleased Structures 191 Citations 86 Ligand Hits 91 Web Page Hits GO Hits SCOP Hits CATH Hits

Advanced Keyword Query for: HEMOGLOBIN

[1] 2 3 4 5 .. 45

Sort by: Results per Page:

☒ **3A59**
Structure of Hemoglobin from flightless bird (*Struthio camelus*)



Characteristics Release Date: 18-Aug-2009 Exp. Method: X-RAY DIFFRACTION
Resolution: 3.41 Å

Classification **Oxygen Storage** **Oxygen Transport**

Compound Molecule: Hemoglobin subunit alpha-A Length: 141
Polymer: 1 Type: polypeptide(L)
Chains: A, C, E, G

Molecule: Hemoglobin subunit beta Length: 146
Polymer: 2 Type: polypeptide(L)
Chains: B, D, F, H

Authors Jaimohan, S.M., Naresh, M.D., Mandal, A.B.

☒ **3DUT**
The high salt (phosphate) crystal structure of deoxy hemoglobin E (GLU26LYS) at physiological pH (pH 7.35)

Release Date: 04-Aug-2009 Exp. Method: X-RAY DIFFRACTION

What's to see

- “View in Jmol”
 - (Viewer option, Java based)
- “Display files”
 - PDB file
 - Straight text file with coordinates of lots of atoms
- “Download Files”
 - Bring file to your own computer
 - Note “Biological Unit gz”
 - Zipped file
 - Only one molecule to look at (or one protein with its subunits)

Methods Geometry Links

1wum

- Display Files ▼
- Download Files ▼
- Print this Page
- Share this Page

Structure Image



More Images...

[View in Jmol](#) SimpleViewer Protein Workshop Other Viewers ▼

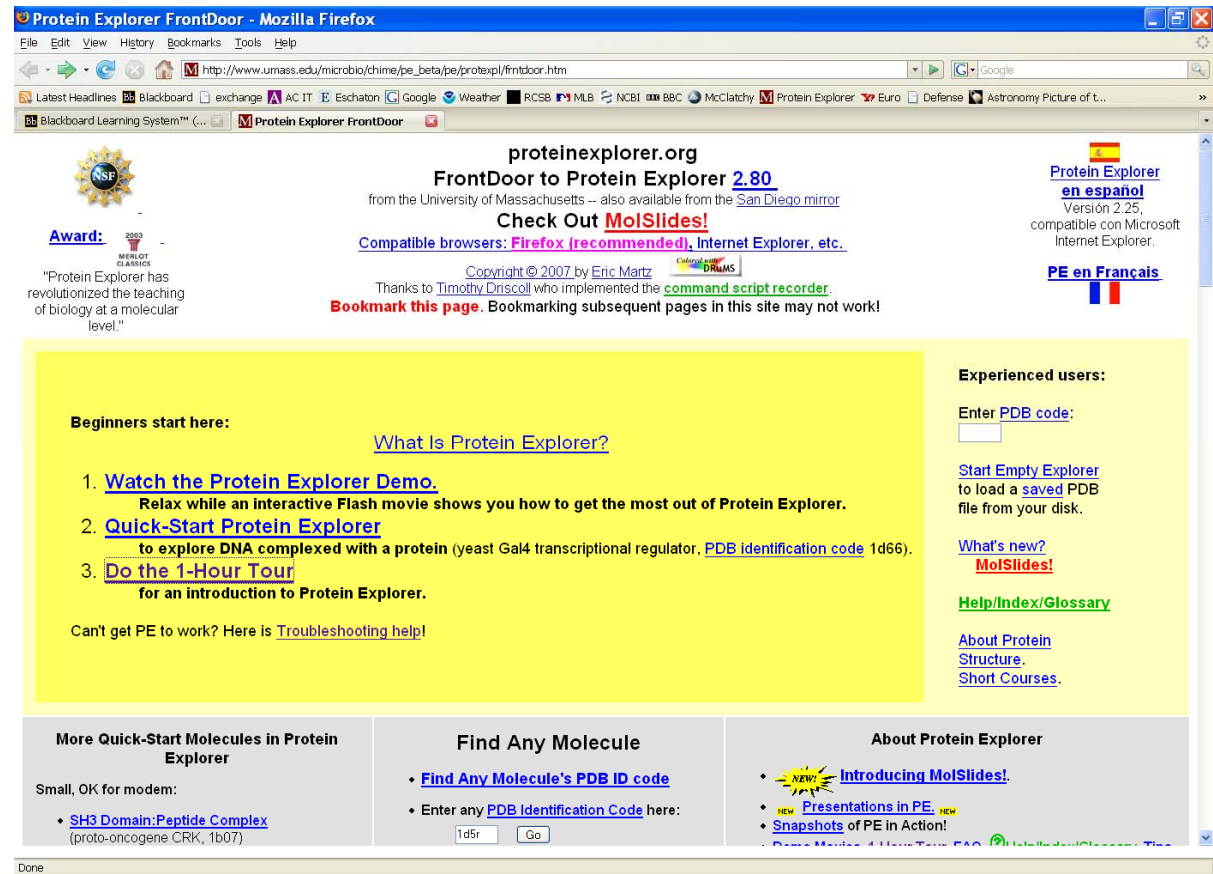
Deposition Summary Hide

Authors: Zeng, L., Li, J., Muller, M., Yan, S., Mujtaba, S., Pan, C., Wang, Z., Zhou, M.M.

Deposition: 2004-12-08

Visualizing pdb files: Protein Explorer

- From Course web site, select “Protein Explorer”
 - Open in new window
 - Requires “Chime”, a free add-in
- Front Door
 - Variety of resources
 - Tutorial (1-hour tour)



NCBI/Cn3D

- Blackboard
- National Center for Biotechnology Information (NCBI)
- www.ncbi.nlm.nih.gov



Databases

- Scroll down on main page
- Select Molecular Databases
- Scroll down again
- Select Structure (MMCB)

Molecular
databases
Sequences,
structures, and
taxonomy

protein function. Click here to find out more about the [Protein Clusters](#) database.

omnibus (GEO)

► Human genome
resources

► Influenza Virus

New dbGaP

NCBI Databases

PubMed Entrez BLAST OMIM Books TaxBrowser Structure

Search Entrez for Go

NCBI

[Site Map](#)
Guide to NCBI resources

[Entrez Help](#)
Help documentation for the Entrez system

[Entrez Tutorial](#)

[Entrez Global Query](#)
Search a subset of Entrez databases

[Entrez Tools](#)
Links to advanced Entrez tools such as Batch Entrez and E-Utilities

[NCBI Handbook](#)
In-depth guide to NCBI resources

[LinkOut](#)
External links to related resources

[Literature](#)
[Databases](#) PubMed, OMIM, Books, PubMed Central

Entrez is the integrated, text-based search and retrieval system used at NCBI for the major databases, including PubMed, Nucleotide and Protein Sequences, Protein Structures, Complete Genomes, Taxonomy, and others. Click on the graphic below for a more detailed view of Entrez integration.

The complete list of Entrez databases can be viewed in the search pull down menu.

Nucleotide Databases

[dbEST](#) [MGC](#)
[dbGSS](#) [PssSet](#)

MMDB database

- Scroll down page
- Select Cn3D v4.1 (you could download from here)

The screenshot displays the NCBI MMDB database interface. On the left is a blue sidebar with navigation links: 'About Entrez's structure database', 'CDD Conserved Domain Database', 'PDBeast Taxonomy in MMDB', 'Cn3D **NEW** 3D-structure viewer', and 'VAST Structure comparisons'. The main content area has two columns. The left column is titled 'New structure viewer' and describes Cn3D as NCBI's 3D structure viewer, available for Windows, MacOS, and Unix, with a 'More...' link. The right column is titled 'About the Database' and describes the Molecular Modeling Database (MMDB) as containing 3D macromolecular structures, including proteins and polynucleotides, with over 40,000 structures linked to other NCBI databases.

About Entrez's structure database

CDD
Conserved Domain Database

PDBeast
Taxonomy in MMDB

Cn3D **NEW**
3D-structure viewer

VAST
Structure comparisons

New structure viewer

Cn3D is NCBI's 3D structure viewer. As a helper application for your Web browser, it allows you to interactively view 3D structures, sequences, and sequence alignments. Cn3D is available for Windows, MacOS, and Unix. [More...](#)

About the Database

The Molecular Modeling Database (MMDB) contains 3D macromolecular structures, including proteins and polynucleotides. MMDB contains over 40,000 structures and is linked to the rest of the NCBI databases, including sequences, bibliographic citations, taxonomic classifications, and sequence and structure neighbors.

Cn3D

- Note tutorial
- Search for 1d5r

Cn3D Tutorial

Cn3D feature highlights

Cn3D FAQ

Frequently Asked Questions

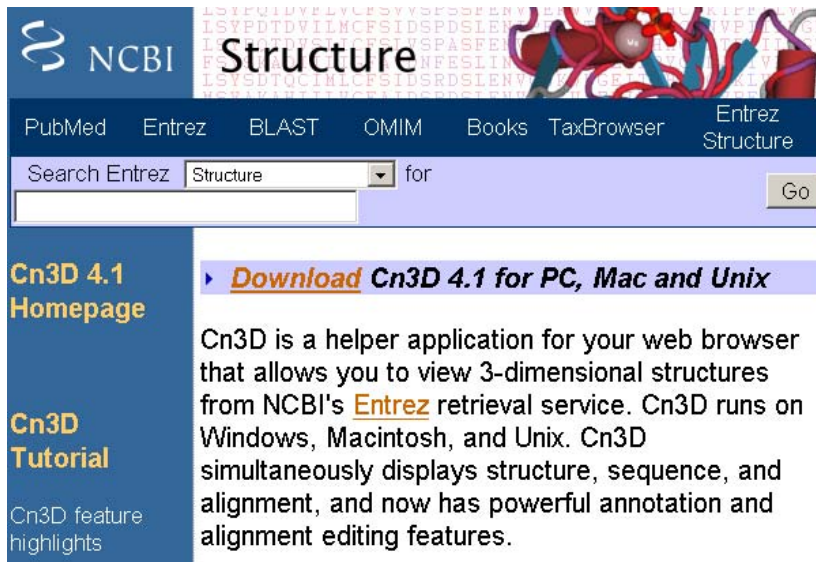
Cn3D Install

Installation and Configuration

MMDB

NCBI's structure database

- [Introduction](#)
 - [What does Cn3D do?](#)
 - [Downloading and installing Cn3D](#)
 - [Document conventions](#)
 - [Literature references](#)
- [Retrieving individual structures \(MMDB\)](#)
 - [From an Entrez literature search](#)
 - [From an Entrez sequence neighbor](#)
 - [From a BLAST search](#)
 - [From a known PDB identifier](#)
- [Viewing individual structures in Cn3D](#)
 - [Basics of Cn3D controls](#)
 - [The structure window main menu](#)
 - [The style panel](#)
 - [Cn3D's sequence viewer](#)
- [Retrieving structure alignments \(VAST\)](#)
- [Viewing structure alignments in Cn3D](#)
 - [Cn3D's alignment viewer](#)
 - [Cn3D's alignment model](#)



NCBI Structure

PubMed Entrez BLAST OMIM Books TaxBrowser Entrez Structure

Search Entrez for

Cn3D 4.1 Homepage

► [Download Cn3D 4.1 for PC, Mac and Unix](#)

Cn3D Tutorial

Cn3D feature highlights

Cn3D is a helper application for your web browser that allows you to view 3-dimensional structures from NCBI's [Entrez](#) retrieval service. Cn3D runs on Windows, Macintosh, and Unix. Cn3D simultaneously displays structure, sequence, and alignment, and now has powerful annotation and alignment editing features.

Seeing what's there...

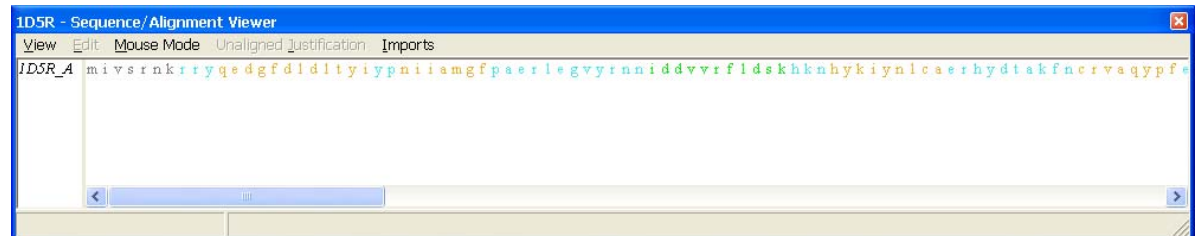
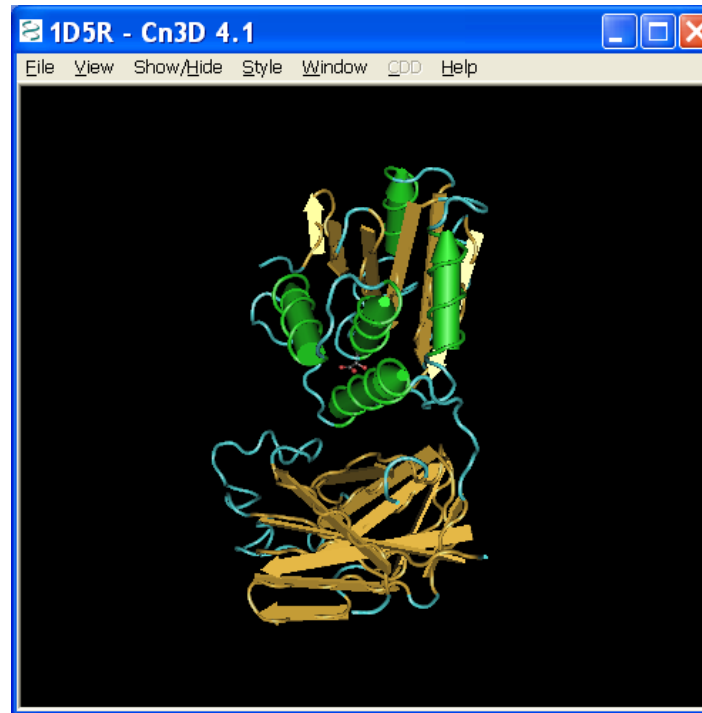
- Note links to other databases (related structures, literature, etc.)
- Click on entry number (1D5R) or thumbnail to get to Structure Summary page

The screenshot shows the NCBI Entrez Structure search results for the query '1d5r'. The top navigation bar includes links to All Databases, PubMed, Nucleotide, Protein, Genome, Structure, PMC, Taxonomy, and Books. The search bar shows '1d5r' with buttons for Go, Clear, and Save Search. Below the search bar, there are tabs for Limits, Preview/Index, History, Clipboard, and Details. The 'Display' section shows 'Summary' selected, with 'Show 20' and 'Send to' options. A list of results is shown with 'All: 1' and 'Bacterial: 0', 'Eukaryotic: 1', 'Ligand: 1', 'NMR: 0', and 'X-ray: 1'. A thumbnail image of the protein structure is displayed, with the entry number '1D5R' highlighted. To the right of the thumbnail, the text reads 'Crystal Structure Of The Pten Tumor Suppressor [mmdblid:11638]'. The left sidebar contains links to About Entrez, Entrez Structure Help | FAQ, Structure Research, The NCBI Structure group, MMDB, About Entrez's structure database, and CDD.

The screenshot shows the NCBI Entrez Structure Summary page for entry 1D5R. The top navigation bar includes links to HOME, SEARCH, SITE MAP, Entrez, Structure, Protein, CDD, PubMed, Taxonomy, PubChem, Help, and Cn3D. The 'Structure Summary' section is highlighted, with 'MMDB' selected. The 'MMDB ID: 11638' and 'PDB ID: 1D5R' are displayed, along with a 'Search' button and a 'PDB or MMDB ID' input field. A large 3D ribbon diagram of the protein structure is shown on the left. To the right of the diagram, the 'Reference' section lists the citation: Lee JO, Yang H, Georgescu MM, Di Cristofano A, Maehama T, Shi Y, Dixon JE, Pandolfi P, Pavletich NP. *Crystal structure of the PTEN tumor suppressor: implications for its phosphoinositide phosphatase activity and membrane association*. Cell 99, p.323-334. Below the reference, a description of the PTEN tumor suppressor is provided, stating that it is mutated in diverse human cancers and in hereditary cancer predisposition syndromes. PTEN is a phosphatase that can act on both polypeptide and phosphoinositide substrates in vitro. The PTEN structure reveals a phosphatase domain that is similar to protein phosphatases but has an enlarged active site important for the accommodation of the phosphoinositide substrate.... A link to 'View full abstract' is provided. The 'Description' section states: 'Crystal Structure Of The Pten Tumor Suppressor. Deposition: 1999/10/11'. The 'Taxonomy' section lists 'Homo sapiens'. Below the taxonomy, a link to 'Related Structure: VAST' is provided. At the bottom, there are buttons for 'Structure View in Cn3D', 'Structure View in RasMol', 'Download Cn3D', and 'View Cn3D Tutorial'. A note at the bottom states: 'Molecular components in the MMDB structure are listed below and may include macromolecular chains, 3D domains, protein classifications (domain families), and ligands, as available. Mouse over each icon for more information on the component.'

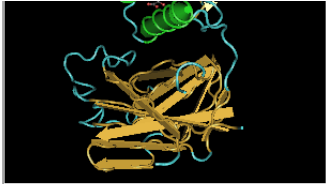
From Structure Summary page...

- Click “View 3D structure” to bring up structure in Cn3D viewer
 - Structure window
 - Style menu to modify views
 - Edit Global style for complete control
 - Sequence window!!
 - Highlight amino acids in structure by highlighting in sequence
 - Alignment tool



VAST

- Click “Structure Neighbors: VAST”
- From Related structures page, select “entire chain”
 - List of structural homologs
 - Sequence homologies diagrammed by red bars
 - Note effect of “mouse-over” on the list of PDB codes
- Select a homolog by checking little left hand box
- Hit “View 3D Alignment button



The PTEN tumor suppressor is mutated in diverse human cancers and in hereditary cancer predisposition syndromes. PTEN is a phosphatase that can act on both polypeptide and phosphoinositide substrates in vitro. The PTEN structure reveals a phosphatase domain that is similar to protein phosphatases but has an enlarged active site important for the accommodation of the phosphoinositide substrate....

» View full abstract

Description: Crystal Structure Of The Pten Tumor Suppressor.
Deposition: 1999/10/11
Taxonomy: Homo sapiens

Structure View in Cn3D Structure View in RasMol

Tasks: Drawing:

VAST related structures have been calculated separately for individual protein chains and 3d domains present in this structure. To see the related structure list for each choose a chain or 3d domain from the table below.

Chain ID	Domains	Residue Range	No. of Neighbors
[A]	entire chain	1 - 324	399
[A]	domain 1	1 - 182	1502
[A]	domain 2	183 - 324	355



Related Structures VAST

PubMed BLAST Structure Taxonomy OMIM Help? Cn3D

VAST related structures for: [MMDB 11638](#), 1D5R sequence A

Overview: There are two main sections to this page. The first section consists of the alignment view controls, the list controls, and the advanced related structure search controls. The second section is the VAST related structure list itself.

of with

using for VAST related structures

subset, sorted by in

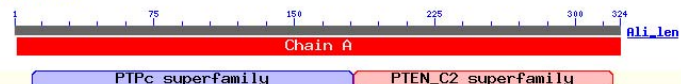
Advanced related structure search

Move the mouse over the red alignment footprints in the graphics below and click, you will obtain a structure-based sequence alignment.

Total related structures: 399; 14 representatives from the [Medium redundancy](#) subset displayed.

Click to: [Check All](#) [Uncheck All](#)

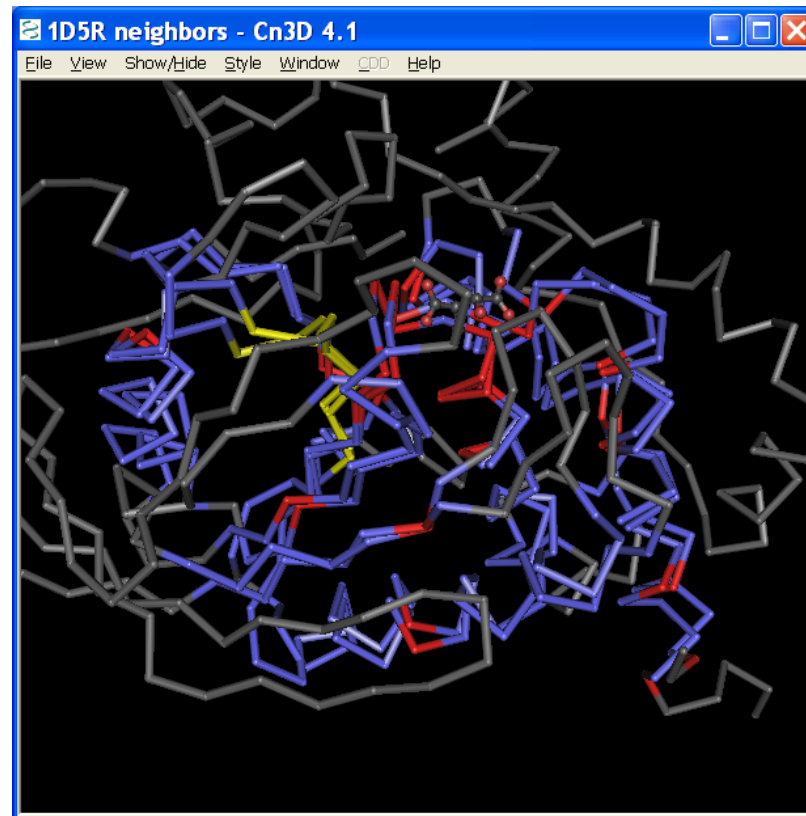
[1D5R A](#)
[3D Domains](#)
[Domain Families](#)
[Super Families](#)



<input type="checkbox"/>	119T A		147
<input type="checkbox"/>	1P89 A		141
<input type="checkbox"/>	10HC A		139

Structure alignments

- Structure Window
 - Superimposed backbones
 - Gray backbones with no corresponding structures
 - Edit global style, turning on helix and strand objects
- Sequence Window
 - Both sequences
 - Try highlighting regions of aligned sequence, vs regions of unaligned sequence
 - Note alignment of dissimilar residues (structure based alignment)



One last thing...

- Course website again/External Links
- Theoretical structures

SWISS-MODEL Repository

[\[Workspace \]](#) [\[Repository \]](#) [\[Modelling \]](#) [\[Tools \]](#)

Welcome to the SWISS-MODEL Repository

The SWISS-MODEL Repository is a database of annotated three-dimensional comparative protein structure models generated by the fully automated homology-modelling pipeline SWISS-MODEL.

Example Queries:
[P24723] [DNAK_PROM6] [IP100518769] [NP_536733] [GI:26454606] [ENTREZ:64401] [Sequence]

SEARCH



The current release of the SWISSMODEL-Repository (8.9) consists of 3454'191 model entries for 2728'637 unique sequences in the UniProt database (Version 13.7.; SwissProt 56.0).

NOTE: The SWISS-MODEL repository contains theoretically calculated models, which may contain significant errors.



BIOZENTRUM
Universität Basel



SIB
Swiss Institute of
Bioinformatics