

Globalization of the Protein Data Bank



熊茜茜，胡翠云，匡瑶，王天祎

2012.6.4



Outline

- Development of the PDB
- Worldwide PDB
- Other PDBs

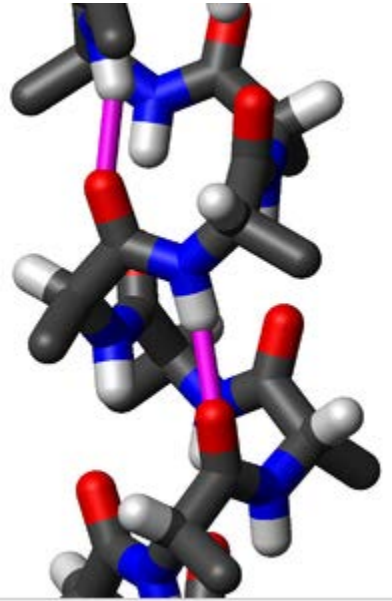


Development of the PDB

Chemistry

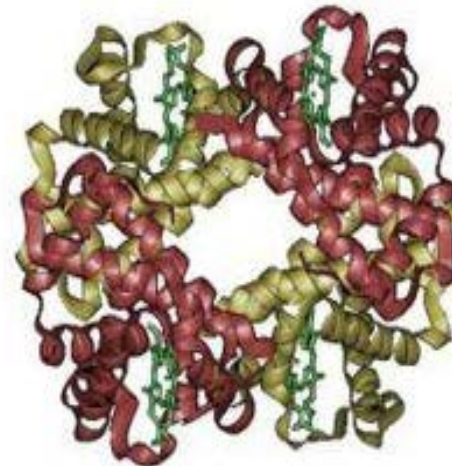
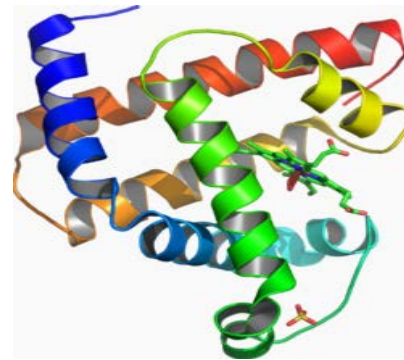


Biological structure



Pauling and Corey (1951)

Myoglobin (1958)



Hemoglobin (1959)

PDB is Born in 1971

- Protein Data Bank was found at Brookhaven National Laboratory with only 7 structures
- Founding Director: Walter C. Hamilton
- Announced in *Nature New Biology* with the following caveat:
“The success of the proposed system will depend on the response of protein crystallographers supplying data.”

CRYSTALLOGRAPHY

Protein Data Bank

A repository system for protein crystallographic data will be operated jointly by the Crystallographic Data Centre, Cambridge, and the Brookhaven National Laboratory. The system will be responsible for storing atomic coordinates, structure factors, and electron density maps and will make these data available on request. Distribution will be on magnetic tape in machine-readable form whenever possible. There will be no charge for the service other than handling costs. Files will be updated as new material is received. The total holding will be announced annually in the organic bibliographic volumes of the reference series "Molecular Structures and Dimensions" published for the Crystallographic Data Centre and the International Union of Crystallography by Oosthoek's, Utrecht.

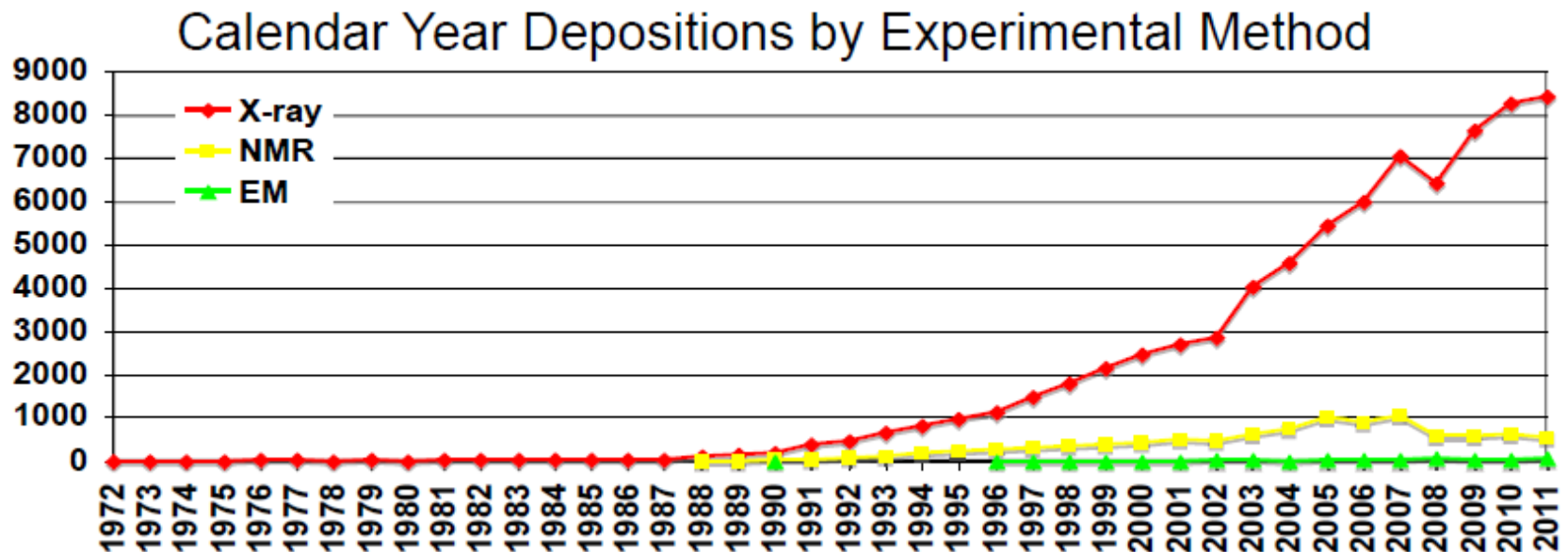
The success of the proposed system will depend on the response of the protein crystallographers supplying data. These will be accepted either "raw" or refined, in machine-readable form or as manuscripts. Laboratories intending to join the scheme should communicate with Mrs Olga Kennard or Dr D. G. Watson at the University Chemical Laboratories, Lensfield Road, Cambridge, who are responsible for the organization of the system. Data can be submitted to Cambridge or to Dr W. C. Hamilton at the Brookhaven National Laboratory, Upton, New York 11973, where the data will be computer processed.

The two centres will maintain identical files and both will provide data services. The new data bank is intended to supplement existing publication media so that depositing material in this form is not a substitute for the publication of the results of structural investigations in a scientific journal.

Growth of the PDB

10,000-Fold Growth in Four Decades

- 7 → 81,957 entries
- Electron Microscopy is beginning to hit its stride



Globalization of the PDB



wwpdb.org

wwPDB Established in 2003

Membership

-  (Research Collaboratory for Structural Bioinformatics - Rutgers University/UC San Diego)
-  (Osaka University)
-  (EMBL EBI)
-  (University of Wisconsin)*

RCSB PDB



Features

- The single worldwide repository for macromolecular structures;
- A controllable and user-friendly interface;
- Multiple structural information and related cross links ;
- Diverse software for online structural analysis;
- PDB-101: an educational resource ;

[All Categories](#) [Author](#) [Macromolecule](#) [Sequence](#) [Ligand](#) [?](#)

Search | All Categories:

[Browse](#) [Advanced](#)

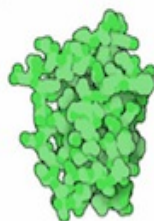
Biological Macromolecular Resource

Full Description

Featured Molecules Hide

Structural View of Biology

List View of Archive By: [Title](#) | [Date](#) | [Category](#)



Molecule of the Month **Leptin**

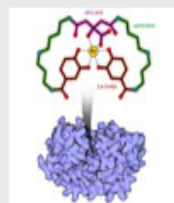
The delivery of nutrients to cells throughout the body is controlled by a complex network of signaling molecules. Some of these signals happen without us really noticing, for instance, when insulin and glucagon control the level of glucose that is delivered through the blood after we eat. The signaling protein leptin, however, has a more apparent effect, acting within the system that makes us hungry when we need food.

[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.

[Full Article](#) | [Archive](#) | [PSI Structural Biology Knowledgebase](#)



Structure Comparison Tool Hide

[Customize This Page](#)

[MyPDB](#) Show

[Home](#) Show

[Deposition](#) Show

[Tools](#) Hide

[Download Files](#)
[Compare Structures](#)
[File Formats](#)
[Services: RESTful | SOAP](#)
[Widgets](#)

[PDB-101](#) Hide

[Structural View of Biology](#)
[Understanding PDB Data](#)
[Molecule of the Month](#)
[Educational Resources](#)

[Help](#) Hide

[Launch Help System](#)
[Display Settings](#)
[Video Tutorials](#)
[Glossary of Terms](#)
[PDBMobile FAQ](#)

[New Structures](#) Hide

[Latest Release](#)
[New Structure Papers](#)
[Search Unreleased Entries](#)

[New Features](#) Hide

[SMILES String Search From Top Bar](#)
Latest features released:

Website Release Archive:

[RCSB PDB News](#) Hide

[Weekly](#) | [Quarterly](#) | [Yearly](#)

2012-05-29
[Tour the PDB with Drill-down Pie Charts](#)



Feature 1: controllable and user-friendly interface

The image displays a user interface for customizing a web page. On the left is a 'Customize This Page' sidebar with sections for Main Panels, Side Panels, and Presets. The main area contains several widgets, each with a title bar and a 'Hide' button. The 'MyPDB' widget shows a welcome message and user-specific links. The 'Home' widget lists general site information and policies. The 'Tools' widget provides links to download files and compare structures. The 'PDB-101' widget offers educational resources. The 'Help' widget provides links to the help system and glossary. The 'Deposition' widget lists services related to protein deposition.

Customize This Page

Main Panels

- Featured Molecules
- Download Files
- Structure Comparison
- Sequence Search
- Latest Structures
- Explore Archive

Side Panels

- New Structures
- New Features
- RCSB PDB News
- wwPDB News
- FTP Archives
- ADIT Deposition

Presets

- Default

MyPDB Hide

Welcome xiong!

- Saved Query Manager
- Query Results (208)
- Query History (1)
- Personal Annotations
- User Account
- Logout

Home Hide

- News & Publications
- Usage/Reference Policies
- Deposition Policies
- Website FAQ
- Deposition FAQ
- Contact Us
- About Us
- Careers
- External Links
- Sitemap
- New Website Features

Tools Hide

- Download Files
- Compare Structures
- File Formats
- Services: RESTful | SOAP
- Widgets

PDB-101 Hide

- Structural View of Biology
- Understanding PDB Data
- Molecule of the Month
- Educational Resources

Help Hide

- Launch Help System
- Display Settings
- Video Tutorials
- Glossary of Terms
- PDBMobile FAQ

Deposition Hide

- All Deposit Services
- Electron Microscopy
- X-ray | NMR
- Validation Server
- BioSync Beamlines/Facilities
- Related Tools

Auto-guided search interface

The screenshot displays the RCSB PDB search interface. At the top, navigation tabs include 'All Categories', 'Author', 'Macromolecule', 'Sequence', and 'Ligand'. A search bar contains the query 'arsenate reductase'. To the right of the search bar, the 'Advanced' search option is circled in red. Below the search bar, a red dashed box highlights a pop-up window with four panels: 'Molecule Name', 'Enzyme Classification', 'Structural Domains', and 'Ontology Terms'. The 'Molecule Name' panel lists 'Arsenate reductase (16)', 'Putative arsenate reductase (2)', and 'Arsenate reductase (ArsC) (1)'. The 'Enzyme Classification' panel lists '1.20.4.1: Arsenate reductase (glutaredoxin) (27)' and '1.20.9.1: Arsenate reductase (azurin) (2)'. The 'Structural Domains' panel lists 'Arsenate reductase ArsC ... (3)' and 'Arsenate reductase ArsC ... (12)'. The 'Ontology Terms' panel lists 'arsenate reductase (glutaredoxin ... (11)', 'SSP6 : ARSENATE REDUCTASE [Genome ... (3)', 'D08.811.682.113: Arsenate Reductases [MeSH ... (12)', 'arsenate reductase (thioredoxin ... (13)', 'SA : ARSENATE REDUCTASE [Genome ... (9)', and 'arsenate reductase (azurin ... (2)'. A 'Find all' link is present below the 'Molecule Name' panel. On the left side of the interface, there are sections for 'Customize This Page', 'MyPDB' (with a 'Hide' button), and 'Home' (with a 'Hide' button). The 'MyPDB' section includes 'Welcome xiong!', 'Saved Query Manager', 'Query Results (38)', 'Query History (3)', 'Personal Annotations', 'User Account', and 'Logout'. The 'Home' section includes 'News & Publications', 'Usage/Reference Policies', 'Deposition Policies', 'Website FAQ', 'Deposition FAQ', 'Contact Us', and 'About Us'. On the right side, there are sections for 'New Structures' (with a 'Hide' button), 'New Features' (with a 'Hide' button), and 'RCSB PDB News' (with a 'Hide' button). The 'New Structures' section includes 'New Structures', 'Test Release', 'New Structure Papers', and 'Search Unreleased Entries'. The 'New Features' section includes 'MILES String Search From Top Bar', 'Latest features released:', and 'Website Release Archive:'. The 'RCSB PDB News' section includes 'Weekly | Quarterly | Yearly'. At the bottom of the search results, there is a 'Full Article' link and a 'close' button.

Search | All Categories: arsenate reductase

All Categories Author Macromolecule Sequence Ligand

Browse Advanced

Customize This Page

MyPDB Hide

Welcome xiong!

Saved Query Manager
Query Results (38)
Query History (3)
Personal Annotations
User Account
Logout

Home Hide

News & Publications
Usage/Reference Policies
Deposition Policies
Website FAQ
Deposition FAQ
Contact Us
About Us

Molecule Name

- Arsenate reductase (16)
- Putative arsenate reductase (2)
- Arsenate reductase (ArsC) (1)

Find all

Enzyme Classification

- 1.20.4.1: Arsenate reductase (glutaredoxin) (27)
- 1.20.9.1: Arsenate reductase (azurin) (2)

Structural Domains

- Arsenate reductase ArsC ... (3)
- Arsenate reductase ArsC ... (12)

Ontology Terms

- arsenate reductase (glutaredoxin ... (11)
- SSP6 : ARSENATE REDUCTASE [Genome ... (3)
- D08.811.682.113: Arsenate Reductases [MeSH ... (12)
- arsenate reductase (thioredoxin ... (13)
- SA : ARSENATE REDUCTASE [Genome ... (9)
- arsenate reductase (azurin ... (2)

More

close 012-05-29

Full Article

our the PDB with Drill-down Bio Charts

Convenient query refinement

38 Structure Hits 14 Citations 23 Ligand Hits 45 Web Page Hits

Query Parameters:

Text Search for: arsenate reductase

Query Details

Save Query to MyPDB

Query Refinements: *Select an item or pie chart* ?

Hide



Organism

- Escherichia coli (11)
- Staphylococcus aureus (9)
- Bacillus subtilis (6)
- Synechocystis sp. PCC 6803 (4)
- Corynebacterium glutamicum (2)
- Brucella abortus (1)
- Vibrio cholerae (1)
- Other (4)



Taxonomy

- Bacteria (36)
- Archaea (1)
- Eukaryota (1)



Experimental Method

- X-ray (29)
- Solution NMR (9)



X-ray Resolution

- less than 1.5 Å (5)
- 1.5 - 2.0 Å (18)
- 2.0 - 2.5 Å (5)
- 2.5 - 3.0 Å (1)
- more choices...



Release Date

- 2000 - 2005 (12)
- 2005 - 2010 (19)
- 2010 - today (7)
- this year (1)
- more choices...



Polymer Type

- Protein (38)



Enzyme Classification

- 1: Oxidoreductases (29)
- 3: Hydrolases (13)



SCOP Classification

- Alpha and beta proteins (a/b) (15)

Refine Query with Advanced Search

Remove Similar: Select Percent Similarity

My PDB

Located on the top left panel of Home page

- Query Results and Query History are synchronized updated when searching the target
- History and Results can be saved , refined and removed

↑ MyPDB Hide

Welcome xiong!

Saved Query Manager
Query Results (38)
Query History (2)
Personal Annotations
User Account
Logout

All queries performed during the current web session are shown.

Session Queries

Text Search for: **arsenate reductase**
and
TAXONOMY is just Escherichia coli

View 11 Results

Refine / Modify

Save Query to MyPDB

- Personal Annotation adds structure a personal description

1. **1SK0**

Personal Annotation:
Arsenate reductase 1

↑ MyPDB Personal Annotations Hide

Tag this structure? No ▾

Add your annotation:

arsenate reductase 1|

Save Annotation Cancel

Feature 2: Multiple structural information and related cross links

Summary Sequence Annotations Seq. Similarity 3D Similarity Literature Biol. & Chem. Methods Geometry Links

ARSENATE REDUCTASE FROM E. COLI

DOI:10.2210/pdb1i9d/pdb

1I9D [Display Files](#) [Download Files](#) [Share this Page](#)

Primary Citation

Insights into the structure, solvation, and mechanism of ArsC arsenate reductase, a novel arsenic detoxification enzyme.

Martin, P., DeMel, S., Shi, J., Gladysheva, T., Gatti, D.L., Rosen, B.P., Edwards, B.F.

Journal: (2001) Structure 9: 1071-1081

PubMed: 11709171 [Search Related Articles in PubMed](#)

PubMed Abstract:

In Escherichia coli bearing the plasmid R773, resistance to arsenite, arsenate, antimonite, and tellurite is conferred by the arsRDABC plasmid operon that codes for an ATP-dependent anion pump. The product of the arsC gene, arsenate reductase (ArsC), is required to... [\[Read More & Search PubMed Abstracts \]](#)

† Molecular Description Hide

Classification: Oxidoreductase [?](#)

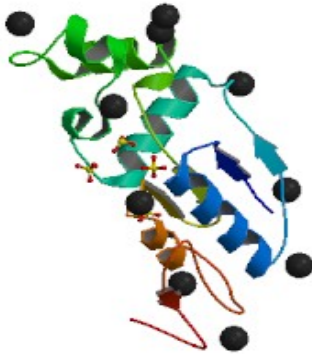
Structure Weight: 17546.68

Molecule: ARSENATE REDUCTASE

Polymer: 1 **Type:** protein **Length:** 141

Chains: A

Biological Assembly 1 [?](#)



[More Images...](#)

[View in Jmol](#)

Simple Viewer Kiosk

Protein Workshop

Biological assembly 1 assigned by authors

Information categories

Summary:

Sequence:

Annotations:

Seq. Similarity:

3D similarity:

Literature:

Biol. & Chem. :

Methods:

Geometry:

Links:

Information categories — Summary

It contains molecular description; primary citation; source; ligand chemical component; external domain annotations and structural biology knowledgebase Data

Source Hide

Polymer: 1

Scientific Name:	Escherichia coli	 Taxonomy	Expression System:	Escherichia coli
------------------	----------------------------------	--	--------------------	----------------------------------

Deposition Summary Hide

Authors: [Martin, P.](#), [Edwards, B.F.](#),

Deposition: 2001-03-19

Release: 2001-12-05

Last Modified (REVDAT): 2011-07-13




MyPDB Personal Annotations Hide

[Click here](#) to add your annotation.

Information categories — Summary

ARSENATE REDUCTASE FROM E. COLI

DOI:10.2210/pdb1i9d/pdb

-  Display Files ▾
-  Download Files ▾
-  Share this Page ▾

Primary Citation


Insights into the structure, solvation, and mechanism of ArsC arsenate reductase, a novel arsenic detoxification enzyme.



Literature

↑ Molecular Description

Hide

Classification: Oxidoreductase 
Structure Weight: 17546.68



Sequence

↓ External Domain Annotations

Show

↓ Structural Biology Knowledgebase Data


Show

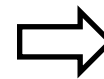


Annotation

↑ Ligand Chemical Component

Hide


Identifier	Formula	Name	Interactions
CS Search Download	<input type="text" value="Cs+"/> Cs	CESIUM ION	



Biol. & chem.
Methods

↓ Experimental Details

Hide

Method: X-RAY DIFFRACTION
Exp. Data:
[Structure Factors](#)
[EDS](#) 



Information categories — Sequence

Annotations Add Annotations

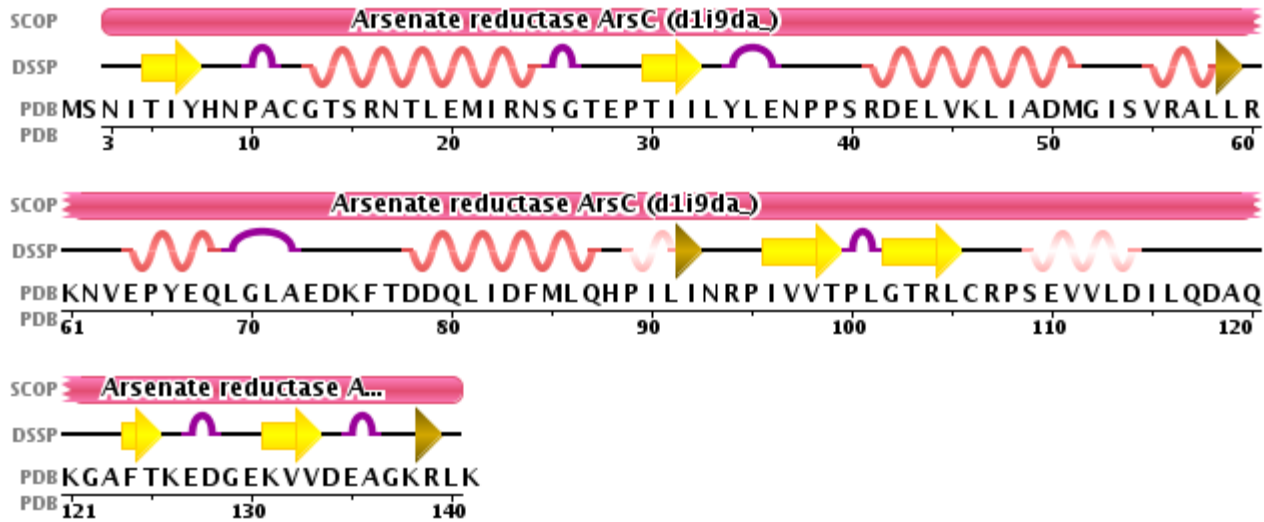
Select

Domain Assignment: **SCOP** **d1i9da** Arsenate reductase ArsC: 138 residues [\[hide\]](#) [\[reference\]](#)

Secondary Structure: **DSSP** 36% helical (7 helices; 51 residues)
15% beta sheet (9 strands; 22 residues)
[\[hide\]](#) [\[reference\]](#)

Select

- Select
- Domain Assignment
 - CATH
 - Domain Parser
 - Protein Domain Parser
- Domain Assignment from Sequence
 - PFAM
 - Interpro
- Secondary Structure
 - STRIDE
 - Author Sec. Struc.



Information categories — — Methods

X-ray diffraction:

Crystal experiments: methods, pH, temperature, buffer condition;

Crystal Data: unit cell, space group

Diffraction: diffraction experiments and equipment

Refinement

Software and computing

Methods offers details of the structural calculation and is the standard of the quality of the structure.

Information categories — Links

STRUCTURE SUMMARY

- [Protein Databank in Europe \(PDBe\)](#)
- [Protein Data Bank Japan \(wwPDB Partner\) \(PDBj\)](#)
- [PSI Structural Biology Knowledgebase \(PSI/KB\)](#)
- [Protein Interfaces, Surfaces and Assemblies \(PISA\)](#)
- [Molecular Modeling DataBase \(NCBI/Entrez\) \(MMDB\)](#)
- [PDBsum](#)
- [Jena Library](#)
- [PDBWiki](#)
- [Proteopedia](#)
- [OCA Browser \(OCA\)](#)
- [PDB_REDO](#)

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](#)

STEREOCHEMICAL QUALITY

- [WHAT_CHECK \(WHAT IF\)](#)
- [PROCHECK](#)

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 \(DSSP\)](#)

EXPERIMENTAL DATA

- [Electron Density Server \(EDS\)](#)

BIOLOGICAL DETAILS

- [CSA](#) : *No external link available*
- [IEDB](#) : *No external link available*

PATHWAYS

- [METACYC](#) : *No external link available*

PROTEIN MOTIONS

- [Molecular Movements Database \(MMD\)](#)

Feature 3: Diverse software for online structural analysis

- **For structure display**

Jmol

Simple Viewer

Kiosk

Protein Workshop

RCSB PDB ligand explorer 3.9

- **For structure comparison**

RCSB PDB Protein Comparison Tool

Software for structure display

Biological Assembly 1 ?




More Images...

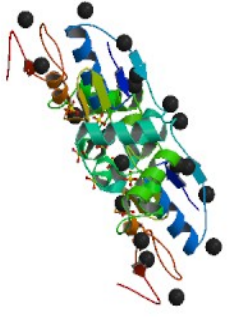
 **View in Jmol**

Simple Viewer Kiosk
Protein Workshop

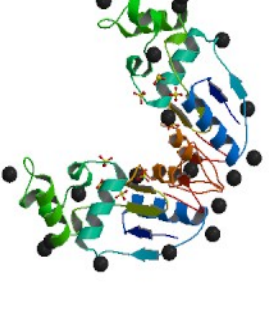
Biological assembly 1 assigned by authors



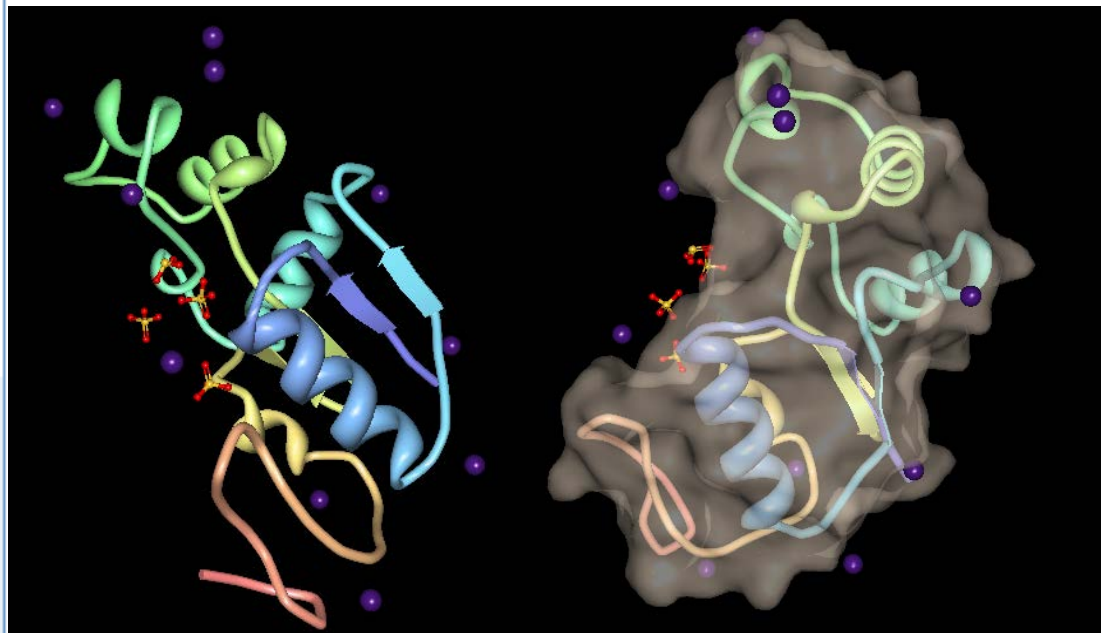
Assumed Biological Molecule
Biological Assembly 1 (250 pixels)



Assumed Biological Molecule
Biological Assembly 2 (250 pixels)

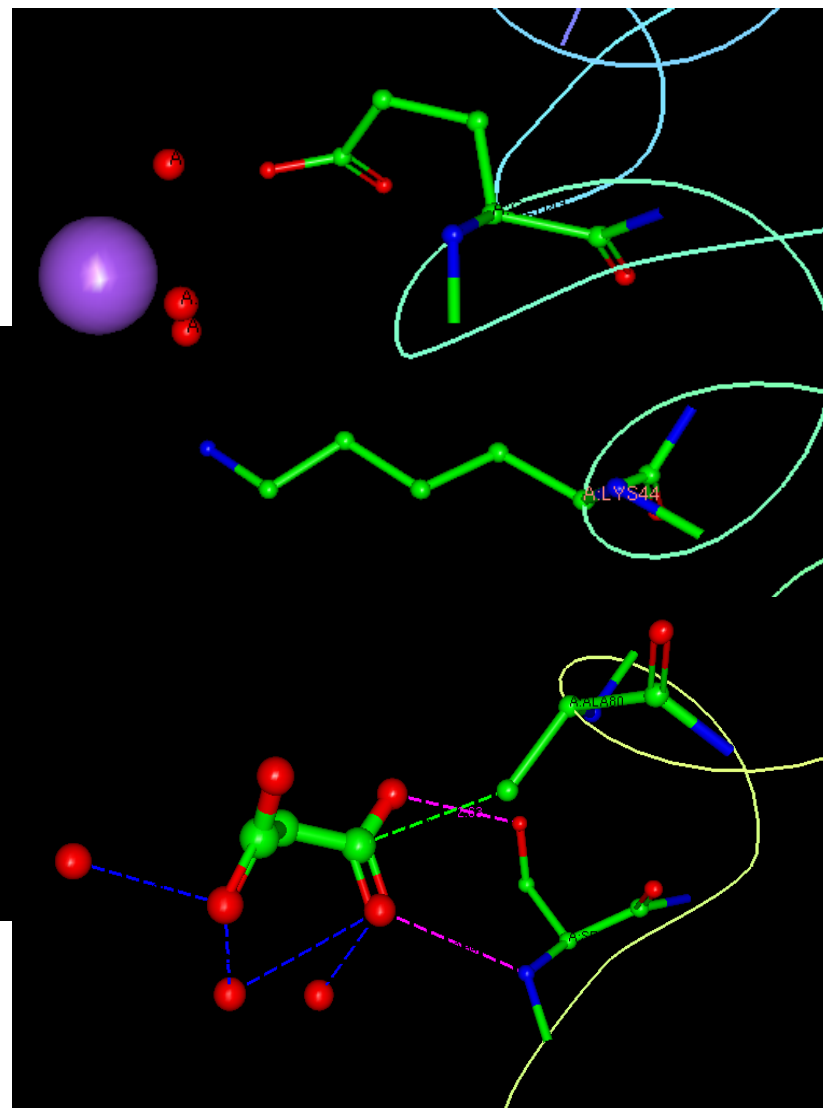


Assumed Biological Molecule
Biological Assembly 3 (250 pixels)



RCSB PDB Ligand explorer 3.9

Software for ligand interaction



Software for structure comparison

In the 3D similarity category, picking the structure based on 40% sequence identity clustering and selecting the comparison method.



Structure Alignment View

Pre-calculated jFATCAT_rigid results for 2L17.A vs. d1jf8a_.

■ **Query:** (orange/dark grey)
Arsenate reductase



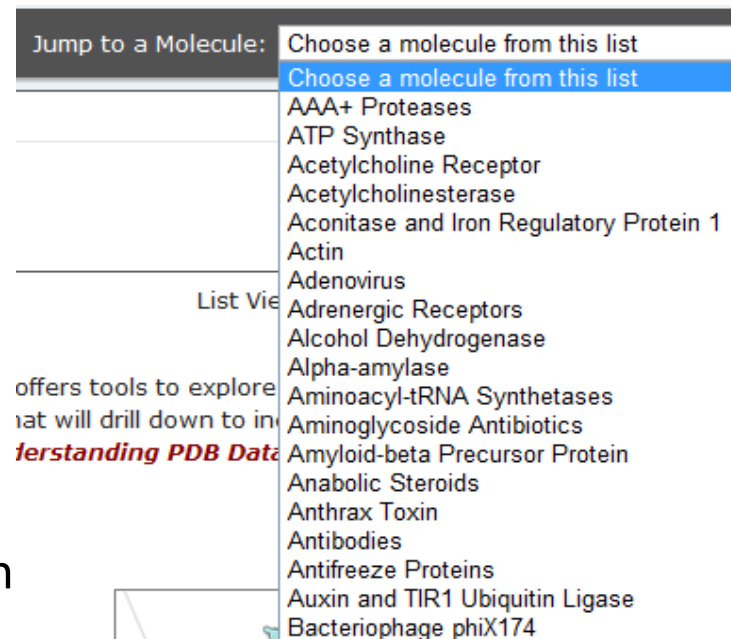
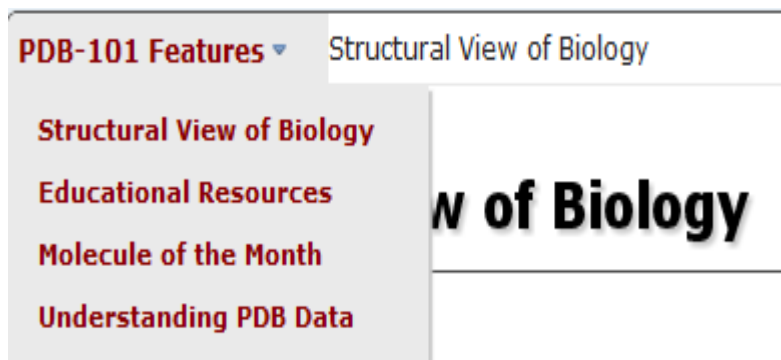
PDB ID: **2L17**
Chain ID: A
Length: 131
Similarity: 98%
EC number: **1.20.4.1**

■ **Subject:** (cyan/light grey)
arsenate reductase1jf8 A: c.44.1.1 Phosphotyrosine protein phosphatases I



PDB ID: **1JF8**
SCOP domain: d1jf8a_
Length: 130
Similarity: 98%
EC number(s): **1.20.43.1.3.48**

Feature 4: PDB-101



Structural View of Biology: starts with key topic categories and subcategories that will drill down to individual molecules. It is built around the *Molecule of the Month* series.

List View of Archive By: **Title** | **Date** | **Category**



Educational Resources:

help researchers and educators interested in how to understand PDB data, visualize structures, read coordinate files, and interpret potential challenges.

Posters/Exhibits

Website Tutorials

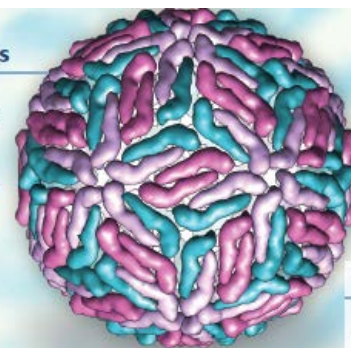
Animations

Activities/Lessons

Events

Dengue fever virus

Dengue fever virus usually causes flu-like symptoms, but the infection can be deadly in some cases.
PDB ID: 1k4r

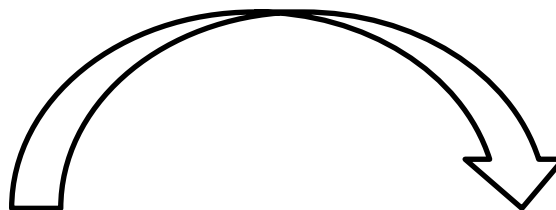


Understanding PDB Data: Looking at Structures

Looking at Structures

- **Introduction**
- **Biological Assemblies**
- **Dealing with Coordinates**
- **Methods for Determining Structure**
- **Missing Coordinates and Biological Assemblies**
- **Molecular Graphics Programs**
- **Resolution**
- **R-value and R-free**
- **Structure Factors and Electron Density**
- **Primary Sequences and the PDB Format**

Designed for



- **Find the information from PDB Data**
- **Transform PDB files to visible structures**
- **Make good use of the coordinate files**
- **Establish a good connection between the structure and biological function**



Other Protein Data Bank

Summary

Name	Website	Content	Usage
PDBSum	http://www.ebi.ac.uk/pdbsum/	PDB information assembly	Provides an at-a- glance overview of the contents of each 3D structure in PDB
SCOP	http://scop.mrc-lmb.cam.ac.uk/scop/	Protein structure classification	Establishes the relationship of structural and evolutionary based on known protein structure
CATH	http://www.biochem.ucl.ac.uk/bsm/cath/	Protein structure classification	Protein domain structure classification

PDBsum

The PDBsum is a pictorial database that provides an at-a-glance overview of the contents of each 3D structure deposited in the Protein Data Bank

The screenshot shows the PDBsum website interface. On the left is a navigation menu with categories like Highlights, List of PDB codes, Het Groups, Ligands, Drugs, Enzymes, ProSite, Pfam, Species, Generate, Gallery, and Figure stats. The main content area features a breadcrumb trail (EBI > Databases > Structure Databases > PDBsum), a search bar for PDB codes (4 chars) with a 'Find' button and an example '1kfv', and a text search bar with a 'Search' button. Below the search bars is a description of PDBsum as a pictorial database and a 'Read more ...' link. On the right, there are sections for 'Contents' (84,975 entries, 1,734 superseded, last update: 2 June, 2012) and 'In-house version' (proprietary, for companies to process own structures). A 'Contact us' link is visible in the top right corner.

EBI > Databases > Structure Databases > PDBsum Contact us

PDBsum

PDBsum is a pictorial database that provides an at-a-glance overview of the contents of each 3D structure deposited in the Protein Data Bank (PDB).

It shows the molecule(s) that make up the structure (ie protein chains, DNA, ligands and metal ions) and schematic diagrams of the interactions between them. [Read more ...](#)

PDB code (4 chars) **Find** Example: "1kfv"

Text search **Search**
Scans all TITLE, HEADER, COMPND, SOURCE and AUTHOR records in the PDB (eg to find a given protein by name).

Contents

PDBsum contains **84,975** entries, including **1,734** superseded
Last update: 2 June, 2012

In-house version

PDBsum Proprietary
In-house version for companies to process own structures (see below left)



PDB id: 2117

Name: Oxidoreductase

Title: An arsenate reductase in the reduced state

Structure: Arsenate reductase. Chain: a. Synonym: synarsc. Engine

Source: Synechocystis. Organism_taxid: 1148. Strain: pcc 6803. Expressed in: escherichia coli. Expression_system_taxid:

NMR struc: 20 models

Authors: C.Yu,B.Xia,C.Jin

Key ref: C.Yu et al. (2011). 1H, 13C and 15N resonance assignment of arsenate reductase from Synechocystis sp. strain PCC 6803. *Biomol NMR* 35:85-87. PubMed id: [20960080](#) DOI: [10.1007/s12104-010-9100-4](#)

Date: 26-Jul-10 **Release date:** 13-Apr-11

Protein chain A



P74313 (P74313_SYNY3) - Arsenate reductase

Seq: LWVFC 131 a.a.

Struc: 131 a.a.

Key: Family PfamA domain Secondary structure

[Links](#)

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[OCA](#)

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[CATH](#)

[SCOP](#)

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[HSSP](#)

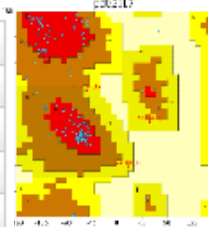
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- University College London.
- **A manually curated classification of protein domain structures.**
- **4 levels:** Class, Architecture, Topology (fold family) and Homologous superfamily.
- **4 classes:** mainly-alpha, mainly-beta and alpha-beta, low secondary structure content (Base on protein domain).

CATH Version 3.4

Based on PDB release: Nov 13, 2010

Changes since v3.3:

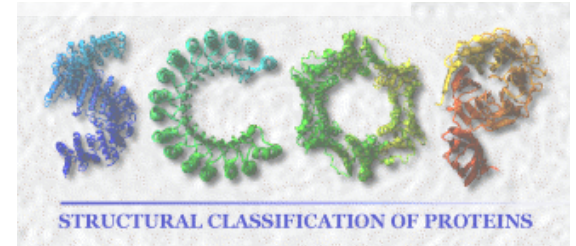
- 24,232 newly assigned domains
- 163 new homologous superfamilies
- 49 new folds (topologies)

Level	Sequence Identity	Overlap
S	35%	80%
O	60%	80%
L	95%	80%
I	100%	80%

The table below summarises the number of clusters within each of the four classes in CATH.

Class	Architecture	Topology	Homologous Superfamily	S35 Family	S60 Family	S95 Family	S100 Family	Domains
1	5	376	839	2763	3571	4679	9217	32396
2	20	228	514	2514	3573	5668	9824	39140
3	14	577	1082	5849	8381	10626	21900	79038
4	1	101	114	204	253	352	547	2346
Total	40	1282	2549	11330	15778	21325	41488	152920

Structural Classification Of Proteins



- Medical Research Council Laboratory of Molecular Biology and Centre for Protein Engineering.
- **Aim to provide a detailed and comprehensive description of the structural and evolutionary relationships between all proteins whose structure is known, including all entries in the PDB.**

Scop Classification Statistics

SCOP: Structural Classification of Proteins. **1.75** release
38221 PDB Entries (23 Feb 2009). 110800 Domains. 1 Literature Reference
(excluding nucleic acids and theoretical models)

Class	Number of folds	Number of superfamilies	Number of families
All alpha proteins	284	507	871
All beta proteins	174	354	742
Alpha and beta proteins (a/b)	147	244	803
Alpha and beta proteins (a+b)	376	552	1055
Multi-domain proteins	66	66	89
Membrane and cell surface proteins	58	110	123
Small proteins	90	129	219
Total	1195	1962	3902

Thanks