

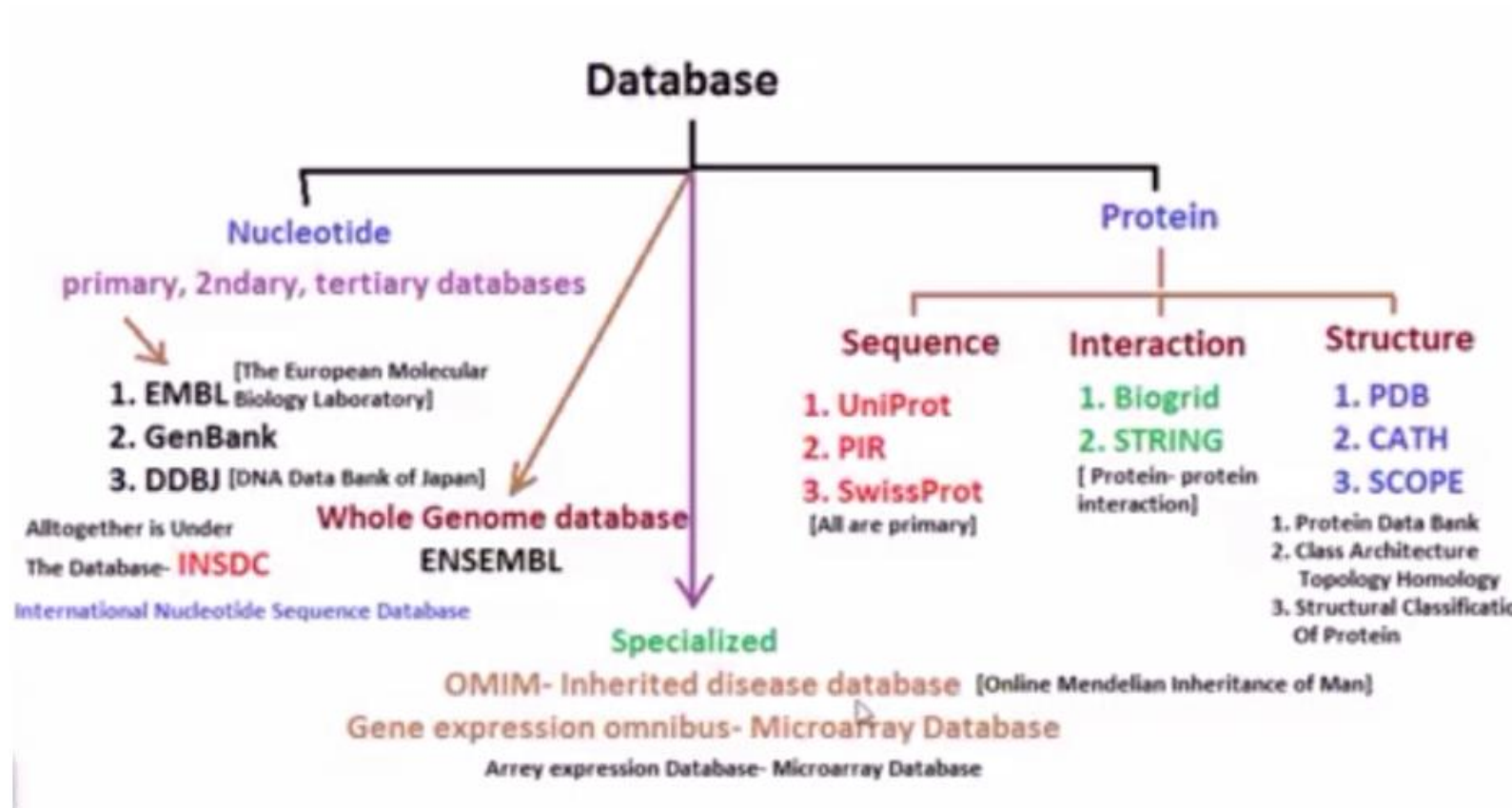
Structural Databases I

MIC 405c | Microbial Genomics & Proteomics

Dr Shilpa Kaistha

Department of Microbiology

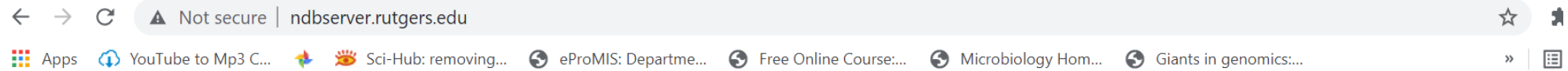
IBSBT, CSJMU, Kanpur



Structure Databases

- NDB: Nucleic Acid Structure Database
- MSD:The Macromolecular Structure Database –
A relational database representation of clean Protein Data Bank (PDB)
- 3DSeq: 3D sequence alignment server- Annotation of the alignments between sequence database and the PDB
- FSSP: Based on exhaustive all-against-all 3D structure comparison of protein structures currently in the Protein Data Bank (PDB)
- DALI: Fold Classification based on Structure-Structure Assignments
- 3Dee: Database of protein domain definitions wherein the domains have been clustered on sequence and structural similarity

Nucleic Acid Database



About NDB

Standards

Education

Tools

Software

Download



A Portal for Three-dimensional Structural Information about Nucleic Acids
As of 26-May-2021 number of released structures: 11337

Search DNA

Search RNA

Advanced Search

Enter an NDB ID or PDB ID



Search for released structures

Welcome to the NDB

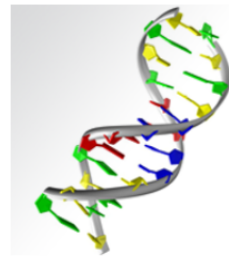
The NDB contains information about experimentally-determined nucleic acids and complex assemblies. Use the NDB to perform searches based on annotations relating to sequence, structure and function, and to download, analyze, and learn about nucleic acids.

Search Structures

[Search DNA](#)
Search DNA and its complexes

[Search RNA](#)
Search for RNA structures in the NDB archive or in the Non-Redundant list

[Advanced Search](#)
Search for structures based on structural features, chemical features, binding modes, citation and experimental information



Featured Tools

[RNA 3D Motif Atlas](#), a representative collection of RNA 3D internal and hairpin loop motifs

[Non-redundant Lists](#) of RNA-containing 3D structures

[RNA Base Triple Atlas](#), a collection of motifs consisting of two RNA basepairs

[WebFR3D](#), a webserver for symbolic and geometric searching of RNA 3D structures

[R3D Align](#), an application for detailed nucleotide to nucleotide alignments of RNA 3D structures



NDB ID: 6X1J **PDB ID: 6X1J** [🔗](#)

Title:

THE HOMING ENDONUCLEASE I-WCAI BOUND TO ITS DNA RECOGNITION SEQUENCE

Molecular Description:

Probable intron-encoded endonuclease 1/DNA Complex

Deposited:

2020-05-19

Released:

2021-05-26

Structural Keywords:

B DOUBLE HELIX

Nucleic Acid Sequence:

[Click to show/hide 2 nucleic acid sequences](#)

Protein Sequence:

[Click to show/hide 1 protein sequences](#)

Primary Citation:

Nawimanager, R., Yuan, Z., Schultz, M., Joshi, R., Lohman, J.R., Gimble, F.S.
The homing endonuclease I-WcaI bound to its DNA recognition sequence
To Be Published, , pp. - , 0.

Experimental Information:

X-RAY DIFFRACTION

Space Group:

P 1 2 1

Cell Constants:

a = 67.601 b = 37.281 c = 94.064 (Ångstroms)

α = 90.0 β = 100.44 γ = 90.0 (degrees)

Refinement:

the REFMAC program. The R value is 0.229 for 31986 reflections

as/xray/structures/6/6x1j/6X1J-biol1.jpg

Structural Features

[RNAML](#)

[Base Pair Hydrogen Bonding Classification](#)

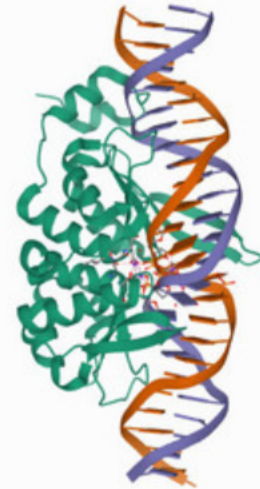
[Nucleic Acid Backbone Torsions](#)

[Base Pair Morphology Parameters](#)

[Base Pair Morphology Step Parameters](#)

[Conformer Analysis \(DNATCO\)](#)

Biological Assembly 1



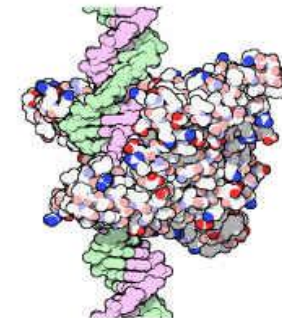
RNA View



Protein DataBank (PDB)

- Important in solving real problems in molecular biology
- Protein Databank
 - PDB Established in 1972 at Brookhaven National Laboratory (BNL)
 - Sole international repository of macromolecular structure data
 - Moved to Research Collaboratory for Structural Bioinformatics

<http://www.rcsb.org/>



PDB

Repository of

- 3D structural data of protein/protein-NA complexes (atomic coordinated, chemical data)
- Data from X ray crystallography, XRD, NMR, eM etc
- Submit Data: PDB AutoDep Input Tool
- Visualise
- Analyse

NDB ID: 6X1J **PDB ID: 6X1J** [🔗](#)

Title:

THE HOMING ENDONUCLEASE I-WCAI BOUND TO ITS DNA RECOGNITION SEQUENCE

Molecular Description:

Probable intron-encoded endonuclease 1/DNA Complex

Deposited:

2020-05-19

Released:

2021-05-26

Structural Keywords:

B DOUBLE HELIX

Nucleic Acid Sequence:

[Click to show/hide 2 nucleic acid sequences](#)

Protein Sequence:

[Click to show/hide 1 protein sequences](#)

Primary Citation:

Nawimanager, R., Yuan, Z., Schultz, M., Joshi, R., Lohman, J.R., Gimble, F.S.
The homing endonuclease I-WcaI bound to its DNA recognition sequence
To Be Published, , pp. - , 0.

Experimental Information:

X-RAY DIFFRACTION

Space Group:

P 1 2 1

Cell Constants:

a = 67.601 b = 37.281 c = 94.064 (Ångstroms)

α = 90.0 β = 100.44 γ = 90.0 (degrees)

Refinement:

the REFMAC program. The R value is 0.229 for 31986 reflections

as/xray/structures/6/6x1j/6X1J-biol1.jpg

Structural Features

[RNAML](#)

[Base Pair Hydrogen Bonding Classification](#)

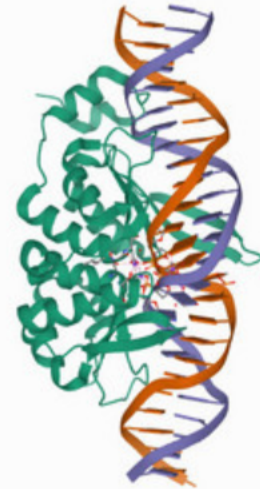
[Nucleic Acid Backbone Torsions](#)

[Base Pair Morphology Parameters](#)

[Base Pair Morphology Step Parameters](#)

[Conformer Analysis \(DNATCO\)](#)

Biological Assembly 1



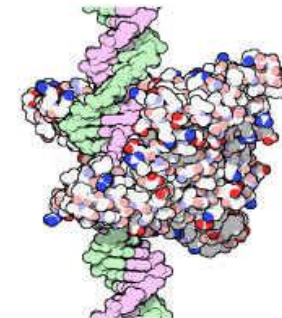
RNA View



Protein DataBank (PDB)

- Important in solving real problems in molecular biology
- Protein Databank
 - PDB Established in 1972 at Brookhaven National Laboratory (BNL)
 - Sole international repository of macromolecular structure data
 - Moved to Research Collaboratory for Structural Bioinformatics

<http://www.rcsb.org/>



PDB

Repository of

- 3D structural data of protein/protein-NA complexes (atomic coordinated, chemical data)
- Data from X ray crystallography, XRD, NMR, eM etc
- Submit Data: PDB AutoDep Input Tool
- Visualise
- Analyse



- Welcome
- Deposit
- Search
- Visualize
- Analyze
- Download
- Learn

A Structural View of Biology

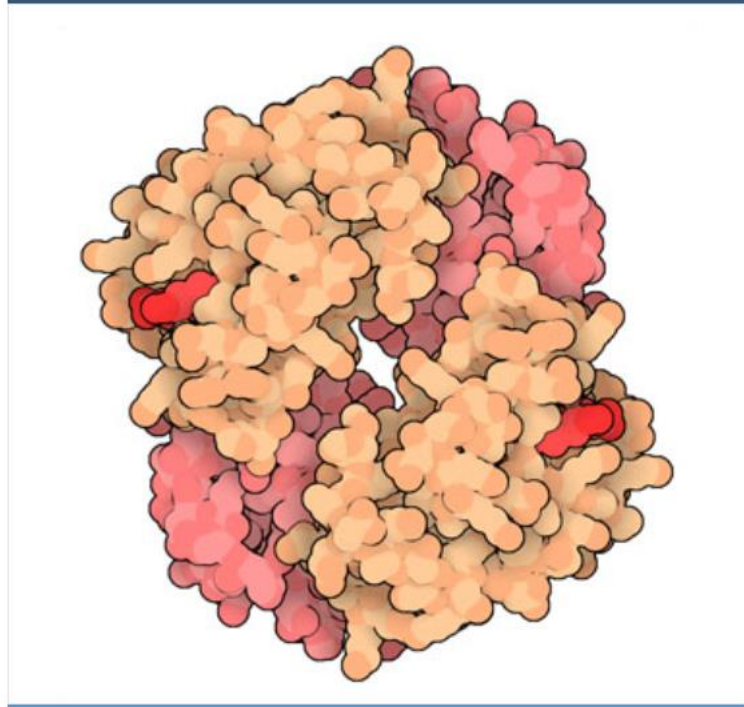
This resource is powered by the Protein Data Bank archive-information about the 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease.

As a member of the wwPDB, the RCSB PDB curates and annotates PDB data.

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.



May Molecule of the Month



Fetal Hemoglobin

178229

PDB entries from
2021-05-26



PDBj
Protein Data Bank Japan

English 日本語 简体中文 繁體中文 한국어

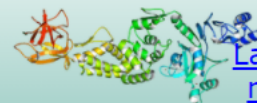
Search



[wwPDB](#) [RCSB PDB](#) [PDBe](#) [BMRB](#) [Adv. Search](#) [Search help](#)

Worldwide
Protein Data Bank
Foundation

7MSW



[Latest new entries](#)

Home

- Top Page
- Statistics
- Help
- FAQ
- Contact Us
- Cite Us / Terms and Conditions
- Links
- Settings

Data deposition (OneDep)

- Help
- Deposition to PDB, EMDB or BMRB

Download

PDBj (Protein Data Bank Japan) is a project team operating under the Joint Usage and Research activities of the [Institute for Protein Research](#), Osaka University. We maintain the single global PDB/BMRB/EMDB archives of macromolecular structures and provide integrated tools, in collaboration with [RCSB PDB](#) and [BMRB](#) in the USA, and [PDBe](#) in the EU. PDBj is supported by [JST-NBDC](#) and [AMED-BINDS](#). [PDBj's new logo](#) design incorporates cytochrome c (PDBID: [1cyc](#)), which was the first structure determined in Japan.

Guide for first time visitors

The material of this site is aimed mainly for researchers. For general people, please refer [PDBj numon](#) ("numon" means introduction or beginner) site. When accessed with old web browser, the web pages may be displayed under limited function mode. In order to use the full function mode, refer [prerequisite](#) page. For details about this site, see [interactive tutorials](#).

Find the service you need

Choose a keyword listed below or input keywords into the textbox at the right of the keyword list. The brief explanation of the matched services will be displayed.

- Click the 'Show all services' button to display the explanation for all services.
- Input some keywords into the 'Word Search Box' to narrow down the search results.

Molecule of the Month

[Fetal Hemoglobin](#)



[Article List](#)

PROTEIN DATA BANK



Hot Structural News on COVID-19



New PDBe-KB COVID-19 Data Portal



Our new PDBe-KB [COVID-19 data portal](#) brings together all available PDB data from SARS-CoV-2 structures, to help researchers easily identify important structural features to support the development of treatments and vaccines.

[Visit the PDBe-KB COVID-19 data portal](#)

PDBe is the European resource for the collection, organisation and dissemination of data on biological macromolecular structures. [Read more about PDBe.](#)

Featured structure

The unzipping enzyme



01 May 2021

There is an enzyme that plays a role in all cellular DNA transactions, including DNA replication and repair, transcription, translation, ribosome synthesis, RNA maturation and splicing, and nuclear export processes.

[Unwind and read more...](#)

Popular

- PDBe-KB
- EMsearch
- PDBeFold
- PDBePISA
- PDBeChem
- PDBe REST API
- EM resources
- NMR resources
- EMPIAR
- Coordinate Server
- PDB Component Library
- News
- Events
- Training
- Contact us

Latest archive statistics

As of 26 May 2021 the PDB contains 178229 entries ([latest PDB entries](#), [chemistry](#), [biology](#)) and EMDB contains 15243 entries ([latest map releases](#), [latest updates](#)).



Welcome

Deposit

Search

Visualize

Analyze

Download

Learn

Deposit Options

- Prepare Data
- Validate Data
- Deposit Data
- Deposition Help

Documentation

- PDBx/mmCIF Dictionary Resources
- Chemical Component Dictionary
- Biologically Interesting Molecule Reference Dictionary (BIRD)
- PDB Format Guide

Deposition Preparation Tools

Data Extraction

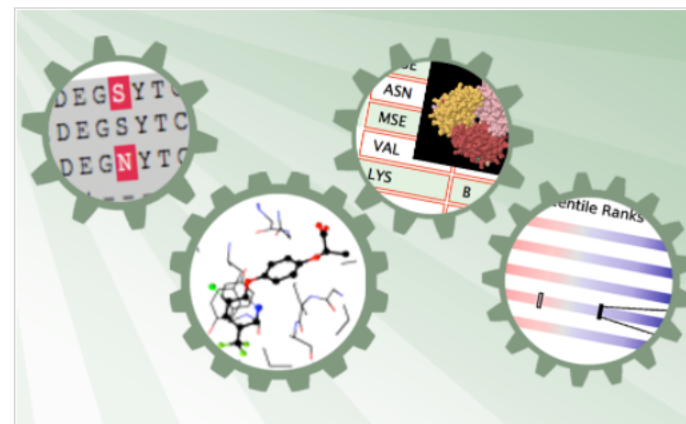
- [pdb_extract](#): Extract and harvest data in PDBx/mmCIF format from structure determination programs
- [SF-Tool](#): Convert structure factor files among various formats

Small Molecules

- [Ligand Expo](#): Search the Chemical Component Dictionary for the IDs of released ligands

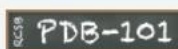
Data Format Conversion

- [PDBML2CIF](#): Convert PDBML-format data into PDBx/mmCIF-format
- [PointSuite](#): Generate symmetry records for macromolecular assemblies with point and helical symmetries
- [MAXIT](#): Translate data between file formats and more



Effective use of PDB

- Queries are of three types
 - PDBid - As quoted in paper
 - Search Lite - one or more keywords
 - Search Fields - A detailed query form
- Query results
 - Structure Explorer - details of the structure
 - Query Result Browser - for multiple structures
- PDB Viewer



Welcome

Deposit

Search

Visualize

Analyze

Download

Learn

Viewers

3D Structure Viewers

Sequence

Protein Feature View

Genome View

Mol* 3D Viewer

Launch Mol* from the Structure Summary page for any entry.

A [standalone version of Mol*](#) is available. Users can upload their custom files into this tool.

A [detailed Mol* User Guide](#) is available.



PDB ID: 4HHB

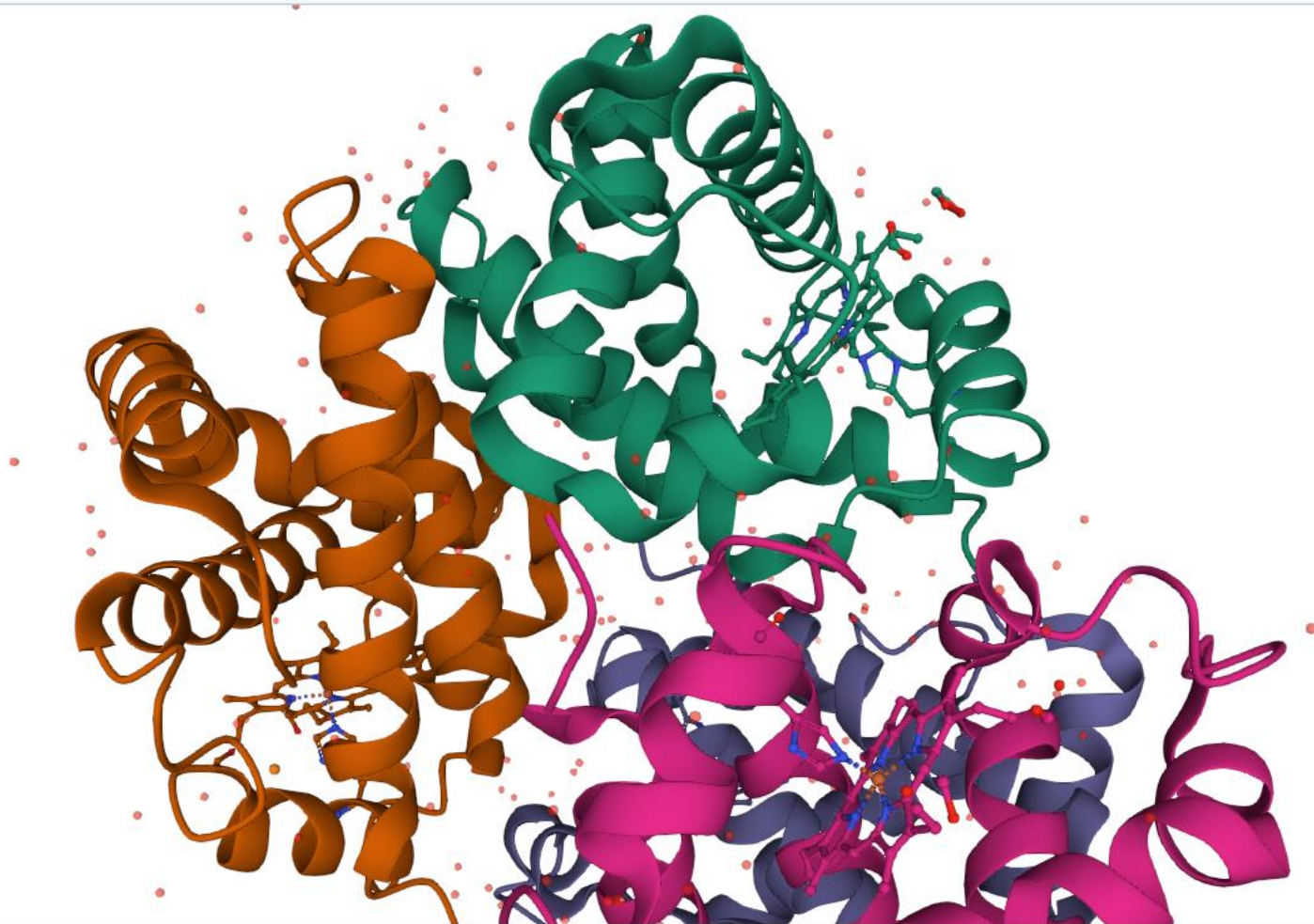


PDB ID: 3J3Q



PDB ID: 1BTN

1 11 21 31 41 51 61 71 81 91 101 111
VLSPADKTNVKAANGKVGHAHAGEYGAEALERMFLSFPTTKTYFPHFDLSHGSAQVKGHGKKVADALTNAVAHVDDMPNALSALS
DLHAHKLRVDPVFNKLLSHCLLVTLAAHLF
121 131 141
AEFTPAVHASLDKFLASVSTVLTSKYR



4HHB | THE CRYSTAL STRUCTURE OF...

| | |
|--------|----------------------------|
| Type | Assembly |
| Asm Id | 1: Author And Software ... |

Nothing Focused

Measurements

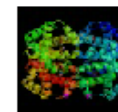
Structural Motif Search

Submit Search (3 selections required)
Add one or more selections (toggle mode)

Components 4HHB

| Preset | + Add | | | |
|---------|--------------|---|---|---|
| Polymer | Cartoon | 👁 | 🗑 | ⋮ |
| Ligand | Ball & Stick | 👁 | 🗑 | ⋮ |
| Water | Ball & Stick | 👁 | 🗑 | ⋮ |
| Ion | Ball & Stick | 👁 | 🗑 | ⋮ |

Unit Cell P 1 21 1



Summary Information



Summary Information

[View Structure](#)

[Download/Display File](#)

[Structural Neighbors](#)

[Geometry](#)

[Other Sources](#)

[Sequence Details](#)

[Crystallization Info](#)

[Previous version\(s\):
1HHB](#)

Explore

[SearchLite](#) [SearchFields](#)

Compound: **Hemoglobin (Deoxy)**

Authors: **G. Fermi, M. F. Perutz**

Exp. Method: **X-ray Diffraction**

Classification: **Oxygen Transport**

Source: **Homo Sapiens**

Primary Citation: **Fermi, G., Perutz, M. F., Shaanan, B., Fourme, R.: The crystal structure of human deoxyhaemoglobin at 1.74 Å resolution. *J Mol Biol* 175 pp. 159 (1984)**

[[Medline](#)]

Deposition Date: **07-Mar-1984**

Release Date: **17-Jul-1984**

Resolution [Å]: **1.74**

R-Value: **0.135**

Space Group: **P 21**

Unit Cell: dim [Å]: a 63.15 b 83.59 c 53.80

angles [°]: alpha 90.00 beta 99.34 gamma 90.00

Polymer Chains: **A, B, C, D**

Residues: **574**

Atoms: **4779**

HET groups:

| <i>ID</i> | <i>Name</i> | <i>Formula</i> |
|----------------------------|--|---|
| HEM | PROTOPORPHYRIN IX CONTAINING FE | C₃₄H₃₂N₄O₄FE₁ |
| PO4 | PHOSPHATE ION | O₄P₁ |

Other Versions: **[2HHB](#), [3HHB](#)**

Cn-3D- structure viewers

ncbi.nlm.nih.gov/Structure/CN3D/cn3d.shtml

Apps YouTube to Mp3 C... Sci-Hub: removing... eProMIS: Departme... Free Online Course:... Microbiology Hom... Giants in genomics:...

NCBI

Structure

Structure

Limits Advanced search

Search

Help

Structure Group 3D Macromolecular Structures Conserved Domains

Cn3D macromolecular structure viewer

ABOUT TUTORIAL FAQ INSTALL PUBLICATIONS NEWS RESOURCES DISCOVER

About Cn3D

Cn3D ("see in 3D") is a helper application for your web browser that allows you to view 3-dimensional structures from NCBI's [Entrez Structure](#) database. Cn3D is provided for [Windows](#) and [Macintosh](#), and can be compiled on [Unix](#). Cn3D simultaneously displays structure, sequence, and alignment, and now has powerful annotation and alignment editing features. *(For those who prefer to view 3D structures on the web, without the need to install a separate application, [iCn3D](#) ("I see in 3D") is available as of April 2016.)*

Below is a relatively simple sample of what **Cn3D** can do. There are many more examples in the [Tutorial](#), along with instructions to help new users get started!

Highlights

Web-based Structure Viewer

- [iCn3D](#) ("I see in 3D"), released in April 2016, provides interactive views of three-dimensional macromolecular structures on the web.
- There is no need to install a separate application in order to use [iCn3D](#); you just need to use a web browser that supports [WebGL](#).
- [iCn3D](#) also allows you to customize the display of a structure and generate a URL that allows you to share the link and to

A comprehensive help document

Cn3D FAQ

Frequently Asked Questions

Cn3D Install

Installation and Configuration

MMDB

NCBI's structure database

PDBeast

Taxonomy in MMDB

VAST

Structure comparisons

VAST Search

The screenshot shows the Cn3D 3.0 software interface. The main window displays a 3D ribbon model of a protein structure. Two cysteine residues are highlighted in green and labeled "Cys-63" and "Cys-68". Other residues are shown in red, yellow, and purple. The interface includes a menu bar with "File", "View", "Style", "Color", "Option", and "Help".

Below the main window is a secondary window titled "DDV" (Distance-Derived Data Viewer). It features a menu bar with "File", "Alignment", "Options", and "Help". The window contains a "Go to:" field with "row:" and "col:" input boxes, both set to "0". Below this is a sequence alignment view showing two sequences: "1DOI" and "1AWD". The sequence "1DOI" is highlighted in yellow, and the sequence "1AWD" is shown in red. The alignment is displayed with a scale from 0 to 30. The status bar at the bottom of the DDV window shows "Ready !".

Rasmol/RasTop

RasMol is a molecular graphics program intended for the visualisation of proteins, nucleic acids and small molecules.

The program reads in a molecule coordinate file and interactively displays the molecule on the screen in a variety of colour schemes and molecule representations.

Currently available representations include depth-cued wireframes, 'Dreiding' sticks, spacefilling (CPK) spheres, ball and stick, solid and strand biomolecular ribbons, atom labels and dot surfaces.


RasTop 2.2
Molecular Graphics Visualization Tool

Content:
[About RasTop](#)
[What's new?](#)
[Building RasTop](#)
[Translating RasTop](#)
[Comments & Bugs](#)
[About this site](#)

Authors

Source:
Herbert J. Bernstein,
Christian Duque,
Gary Grossman,
Marco Molinaro,
Arne Mueller,
Naoum Salame,
Roger Sayle,
Philippe Valadon.

Help and Translations:
Frances C. Bernstein,
Herbert J. Bernstein,
William McClure,
Eric Martz,
Naoum Salame,
Philippe Valadon,
Margaret Wong.

Open RasMol Site:


Welcome to RasTop molecular visualization software, Version 2.2. RasTop is a graphical interface to the program RasMol. RasTop allows the viewing and the direct manipulation of macromolecules and small molecules on screen. RasMol was developed initially by Roger Sayle at the University of Edinburgh's Biocomputing Research Unit and the BioMolecular Structure Department, Glaxo Research and Development, Greenford, U.K. Many people since contributed to its code. In 1999, Herbert J. Berstein released a compiled version named Rasmol 2.7.1 of different source variants under a GPL-like license (see [NOTICE](#)). Many thanks to these people for giving RasMol freely to the community. Many thanks also to Herbert Berstein, Frances Bernstein, William McClure, Eric Marz, Margaret Wong, and Roger Sayle for their contributions to the Help and giving the permission to re-use their work. See the complete list of contributors to this version in the file [copyright](#).

NEW USERS

Expert Protein Analysis System (Original): ExPASy-integrated genomics, proteomics resource of SIB

The screenshot shows the ExPASy website interface. At the top, there is a browser address bar with the URL `expasy.org` and several open tabs. Below the browser is the ExPASy logo and the text "Swiss Bioinformatics Resource Portal". A search bar with a red magnifying glass icon is present, with a hint "e.g. BLAST, UniProt, MSH6, Albumin...". On the left side, there is a navigation menu with categories: "Genes & Genomes" (with sub-items: Genomics, Metagenomics, Transcriptomics), "Proteins & Proteomes" (checked), "Evolution & Phylogeny" (with sub-items: Evolution biology, Population genetics), and "Structural Biology". The main content area is titled "SIB Resources" and contains five resource cards: "STRING" (Protein-protein interaction networks and enrichment analysis), "SWISS-MODEL" (Protein structure homology-modelling), "UniProtKB/Swiss-Prot" (Protein knowledgebase), "neXtProt" (Human protein knowledgebase), and "SwissLipids" (Knowledge resource for lipids). At the bottom left, a URL bar shows `https://www.expasy.org/resources/nextprot`.