



The Structure Database from NCBI

Macromolecular structure resources

<https://www.ncbi.nlm.nih.gov/structure/>

National Center for Biotechnology Information • National Library of Medicine • National Institutes of Health • Department of Health and Human Services

Scope and Access

The Structure database, also known as Molecular Modeling Database (MMDB), contains experimentally determined structures imported from the Protein Databank (PDB). The records have been curated to add information on explicit chemical bonding data, uniform secondary structure and domain features, as well as links to other Entrez databases such as Taxonomy, PubMed, Protein, and Conserved Domains. In addition, if multiple conformations of a structure are present in the PDB file, two coordinate subsets are added to each record: a set containing only backbone atoms of all structures, and a set representing a single-conformer model. The Entrez search/retrieval system provides access to the content through a web browser (<https://www.ncbi.nlm.nih.gov/structure/>). Content download by FTP is also available (<ftp://ftp.ncbi.nlm.nih.gov/mmdb/>). Detailed records along with their sequences can be viewed and manipulated using the freely available Cn3D molecular visualization program (<ftp://ftp.ncbi.nlm.nih.gov/cn3d/>). NCBI performs extensive analyses to identify related structures using the Vector Alignment Search Tool (VAST). A VAST-powered service for researchers to analyze newly determined structures is at <https://www.ncbi.nlm.nih.gov/Structure/VAST/vastsearch.html>.



Structure Homepage

The Structure homepage (right) provides links to help documents (A), tools (B) and relevant resources (C). A search can be done by entering a set of terms in the box and clicking the "Search" button (D).

Searching for Structures

The system displays search results as a list of summaries (E) with their titles and image thumbnails (F) linking to more detailed descriptions. Links under each summary provide additional functionality or information (G): "View in iCn3D" launches Cn3D to allow interactive examination, manipulation and annotation of the structure record; "Similar Structure" retrieves a list of structures similar to the entry; "PubMed" links to abstract describing that structure; "Protein" links to the sequences for these protein chains; "Conserved Domain" links to domains contained within the protein chains; and "PubChem Compound" lists PubChem compounds co-crystallized with the structure. The list can be further refined using functions in the right-hand column, by methodology filters (H), or by properties of the structure records given in "Refine your results" section (I).

Displaying the Structure Record

Clicking the title or the thumbnail image (A) of a structure record opens the detailed description of the record. This display contains a summary of the structure (B) with links to the corresponding record at PDB and relevant publication in PubMed (C). A list of similar structures determined by Vector Alignment Search Tool can be retrieved by clicking the "VAST+" button (D). A larger image (E) below provides more details of the structure. The two links (F) within the image allows the interactive examination of the structure in iCn3D, or the full-featured standalone program Cn3D, respectively. The Download button (G) saves the structure in selected formats.

The "Molecules Components in ..." table (H) further below contains detailed annotation of the structure. The colored bars (I) link to a list of similar structures as determined by VAST. The domains (J) link to conserved domain records with additional information on sequence conservation and functional assignment. Compounds present in the structure, the substrate analog 5-adenosylhomocysteine (K) in this case, will be listed and linked to entries in the PubChem Compound database.

A [Structure And Mechanism Of Mrna Cap \(Guanine N-7\) Methyltransferase\[Transferase\]](#)

Taxonomy: Encephalitozoon cuniculi
 Proteins: 1 Chemicals: 1 modified: 2012-10-09
 MMDb ID: 26188 PDB ID: 1R14
[View in iCn3D](#) [Similar Structures](#) [PubMed](#) [Proteins](#) [Conserved Domains](#) [PubChem Compound](#)

1R14: Structure And Mechanism Of Mrna Cap (Guanine N-7) Methyltransferase

B PDB ID: 1R14 [Download](#)
 MMDb ID: 26188
 PDB Deposition Date: 2003/11/16
 Updated in MMDb: 2012/10
 Experimental Method: x-ray diffraction
 Resolution: 2.4 Å
 Source Organism: Encephalitoz...
 Similar Structures: [VAST+](#)
[Download sequence data](#)

C Citation: [Structure and mechanism of mRNA cap \(guanine-N7\) methyltransferase](#)
 Fabrega C, Hausmann S, Shen V, Shuman S, Lima CD
 Mol. Cell (2004) 13 p.77-89

D [Abstract](#)
 A suite of crystal structures is reported for a cellular mRNA cap (guanine-N7) methyltransferase in complex with AdoMet, AdoHcy, and the cap guanylate. Superposition of ligand complexes suggests an in-line mechanism of methyl transfer, albeit without direct contacts between the enzyme and either the N7 atom of guanine (the attacking nucleophile), the methyl carbon of AdoMet, ...
[read more](#) <https://www.ncbi.nlm.nih.gov/Structure/pdb/1R14>

Biological Unit Asymmetric Unit

Biological Unit for 1R14: monomeric; determined by author

E Molecular Graphic Interactions

A

Drag symbols to move
 Double click symbols to explore

G [Download Structure](#)
 ASN.1 (Cn3D)
 PDB
 XML
 JSON
 PNG (image)

Format: ASN.1 (Cn3D)
 Data Set: Single 3D structure
[Download Cn3D](#)

F [3D view](#) [full-featured 3D viewer](#)

VAST Similar Structures

PubMed BLAST Structure Taxonomy OMIM Help?

VAST related structures for: MMDb 26188, 1R14 sequence A domain 1.

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

View 3D Alignment of All Atoms with Cn3D Display [Download Cn3D!](#)

View Sequence Alignment using Hypertext for: Selected VAST related structures

List Medium redundancy subset, sorted by Aligned Length in Graphics

Select related structures with PDB IDs

Mouse over the red alignment footprints in the graphics below and click, you will obtain a structure

Total related structures 18825; 1 - 60 of 1523 representatives from the Medium redundancy set

Click to: [Check All](#)

1R14 A
 3D Domains
 Domain Families

1R15 A
 1R15 A_1
 2VDW A
 3BGV B_1

H Molecular Components in 1R14

Label	Count	Molecule
Protein (1 molecule)		
A	1	mRNA Capping Enzyme (Gene symbol: ECU10_0380)
Chemical and Non-standard biopolymers (1 molecule)		
K	1	S-Adenosylmethionine

I [1 Protein](#)
 3D Domains
 Domain Families
 Super Families

J [AdoMet_MTases superFamily](#)

K [S-Adenosylmethionine](#)

* Click molecule labels to explore molecules

Conserved Protein Domain Family
AdoMet_MTases

cd02440: AdoMet_MTases

S-adenosylmethionine-dependent methyltransferases (SAM or AdoMet-MTase), class I; AdoMet-S-adenosyl-L-methionine (SAM or AdoMet) as a substrate for methyltransfer, creating the product (AdoHcy). There are at least five structurally distinct families of AdoMet-MTases, class I being within this class enzymes can be classified by different substrate specificities (small molecules different target atoms for methylation (nitrogen, oxygen, carbon, sulfur, etc.).

Links
 Source: Cdd
 Taxonomy: cellular organisms
 PubMed: 2 links
 Book: 1 link
 Protein: Representatives
 Specific Protein
 Related Protein
 Related Structure
 Architectures
 Superfamily: cd17173

Conserved Features/Sites
 S-adenosylmet...
Feature 1: S-adenosylmethionine binding site [chemical binding site]
Evidence:
 Structure: 2DPM, Streptococcus pneumoniae Dpn II DNA methylase with bound S-adenosylmethionine
 View structure with Cn3D
 Citation: PMID 9862809
[Download Cn3D for Viewing 3D Structure](#) [Scroll to Sequence Alignment Display](#)

cd02440 is part of a hierarchy of related CD models. Use the graphical representation to navigate this hierarchy. cd02440 is a member of the superfamily

cd02440 Sequence Cluster [Zoom In](#) [Interactive Display with CDTree](#)

Sub-family Hierarchy
 cd02440 AdoMet_MTases

Statistics
 PSSM-Id: 100107
 View PSSM: cd02440
 Aligned: 102 rows
 ThresholdBitScore: 29.3203
 ThresholdSettingG: 15988002
 Created: 29-May-2008
 Updated: 17-Jan-2013

Structure

Display is for the curated cd02440 from the superfamily.

PubChem About Blog Submit Contact

COMPOUND SUMMARY

S-Adenosyl-L-methionine

PubChem CID: 34756

Structure:

Chemical Safety: Irritant
 DATASHEET AVAILABLE: Laboratory Chemical Safety Summary (LCSS)

InChI Key: MEFKPWEQBLKI-AIRLKBTKGSA-O

Molecular Formula: C₁₅H₂₃N₆O₅⁺

Viewing the Structure Using iCn3D

Structure And Mechanism Of Mrna Cap (Guanine N-7) Methyltransferase
 Taxonomy: Euceleutherozoa cuniculi
 Proteins: 1 Chemicals: 1 modified: 2012-10-09
 MMDB ID: 26188 PDB ID: 1RI4
[View in iCn3D](#) [Similar Structures](#) [PubMed](#) [Proteins](#) [Conserved Domains](#) [PubC](#)

Structure visualization and manipulation are now integrated into the browser through a JavaScript-based program called iCn3D. Clicking “View in iCn3D” link (A) or the arrow icon (p. 2, E) launches the program in the current browser window.

The screenshot shows the iCn3D interface with a 3D ribbon structure of the protein. A red box highlights a specific region of the structure. To the right, two panels show 1D sequences. The top panel is titled "Select residues in sequences" and contains instructions for selecting residues. The bottom panel is also titled "Select residues in sequences" and shows a sequence with some residues highlighted in yellow and red. A red box in the 3D structure highlights a region, and a red box in the bottom sequence panel highlights the corresponding residues. Labels A, B, C, and E point to various UI elements: A points to the "View in iCn3D" link, B points to the 3D structure, C points to the "Select residues in sequences" panels, and E points to the "View in iCn3D" link in the top panel.

File Select Style Color Surface Analysis Other ?

Advanced
 by Distance
 Complement
 Defined Sets
 All
 Sequence
 Interactions
 Picking with "Alt" + Click
 Display
 Highlight Color
 Highlight Style

The iCn3D display (B) shows the 3D structure and the 1D sequences in side-by-side panels, with basic instruction and selection control buttons given at the top of the sequence panel (C). The two panels use the same color scheme and communicate with each other. The example highlights residues within 3 Angstroms away from the substrate, where corresponding residues are highlighted in both panels (E). This display is manipulated through the following steps:

- 1) Click the substrate to highlight it first (i.e., S in the sequence panel or its counterpart in the structure panel)
- 2) Click the “Select” menu option and check the “By Distance” option
- 3) In the dialog box, set the distance to 3 Angstroms, and click “Display”

Select a sphere around current sel...

1. Sphere with a radius: 3 Å
2. Display sphere around currently selected atoms

The menu at the top (F) provides access to additional functions through cascading options or dialog boxes. Specifically, a) “File” allows structure access (retrieve, open) and saving, b) “Select” picks and highlights residues based on various user-defined criteria, c) “Style” and “Color” determine the render style and color scheme, d) “Surface” determines how the surface is presented, e) “Analysis” provides access to functions, such as distance measure, and f) “Other” lists a set of general controls, such as reset to default, as well as the online help document, which is also accessible through the “?” symbol to the right.

Viewing a Structure Record with Functional Annotation

The links to the structure view show only a single record and its sequences, which does not provide functional annotations. However, a significant number of structure records are linked to the Conserved Domains database (CDD), which may contain groups of structures along with multiple sequence alignments to provide information on functional annotation.

The screenshot displays the NCBI Conserved Protein Domain Family page for **AdoMet_MTases** (cd02440). The page is divided into several sections:

- Top Navigation:** Includes links for Entrez, CDD, Structure, Protein, and Help.
- Domain Summary:** Shows the domain name **AdoMet_MTases** and its superfamily. A yellow arrow (A) points to the domain graphic, and another (B) points to the "Structure View" button.
- Links Panel:** Provides source, taxonomy, PubMed links, and protein-specific information. A yellow arrow (C) points to the "Structure View" button.
- Conserved Features/Sites:** Lists features like the S-adenosylmethionine binding site with supporting evidence. A yellow arrow (D) points to the "View structure with Cn3D" link.
- Statistics:** Displays PSSM-ID, View PSSM, Aligned rows, ThresholdBitScore, ThresholdSettingGi, Created, and Updated dates.
- Structure Panel:** Shows options for Structure View, Program (Cn3D), Drawing (All Atoms), and Aligned Rows (up to 10). A yellow arrow (E) points to the "Download Cn3D" button.
- Sequence Cluster and Sub-family Hierarchy:** Provides a sequence cluster and a sub-family hierarchy. A yellow arrow (F) points to the "Interactive Display with CDTree" button.
- CDD Annotations:** Shows annotations and evidence for the S-adenosylmethionine binding site. A yellow arrow (G) points to the "Highlight" button.
- CDD Descriptive Items:** Provides a detailed description of the domain. A yellow arrow (H) points to the "Show Annotations Panel" button.
- Sequence/Alignment Viewer:** Displays a sequence alignment with highlighted residues. A yellow arrow (I) points to the highlighted residues, and another (J) points to the "Highlight" button in the CDD Annotations panel.

Additional text on the page includes:

- mRNA Capping Enzyme (Gene symbol: ECU10_0380):** A graphical representation of the protein structure with a yellow arrow (A) pointing to it.
- Feature 1: S-adenosylmethionine binding site [chemical binding site]:** Evidence includes a structure from *Streptococcus pneumoniae* Dpn II DNA methylase with bound S-adenosylmethionine (PMID 9862809).
- cd02440 Sequence Cluster:** A tree diagram showing the relationship between different CD models.
- Sub-family Hierarchy:** A diagram showing the hierarchy of related CD models.
- AdoMet_MTases - Cn3D 4.2:** A 3D structure viewer showing the protein structure with highlighted residues (yellow) and a yellow arrow (G) pointing to a specific residue.