

Exploring the PDB

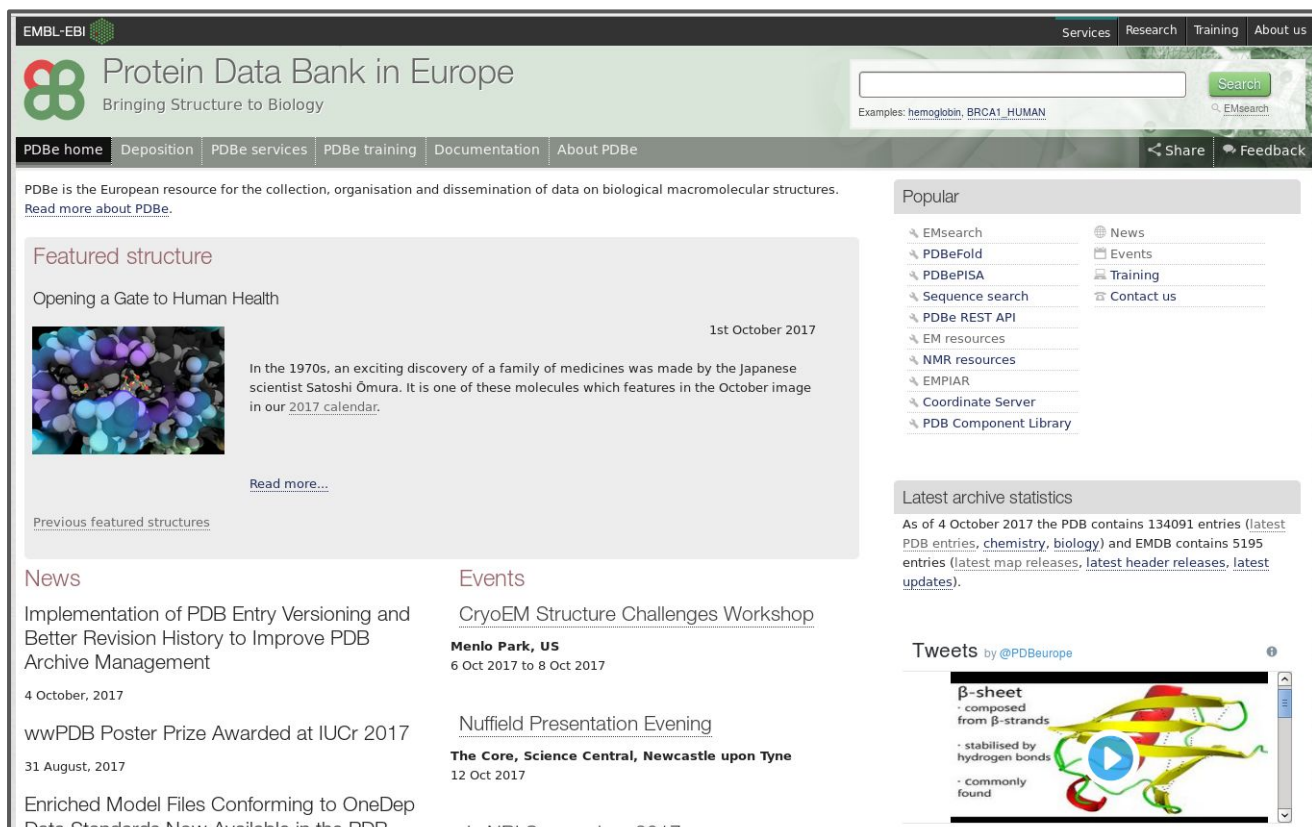
The Protein Data Bank in Europe (PDBe) provides access to three dimensional structures of proteins, DNA and RNA.

The PDBe website offers a simple and informative way to explore and visualise these molecules in 3D allowing you learn about their function within nature. In textbooks, proteins are often shown as 2D images, and while this can be a good way to understand the basic principles, proteins truly come alive when seen in 3D. Seeing how they are arranged and interact in 3D gives a fascinating insight into protein biochemistry.

Using the PDBe website you can search for a known protein to explore, such as insulin or haemoglobin, you can take a look at the featured structure or search for entries that were only just released this week. You can even travel back into history, and view structures solved in the 1970s. The hard part is narrowing down your options and choosing just one of the interesting structures to investigate from the thousands available!

In this activity follow the numbered steps for a guided tour of the PDB archive.

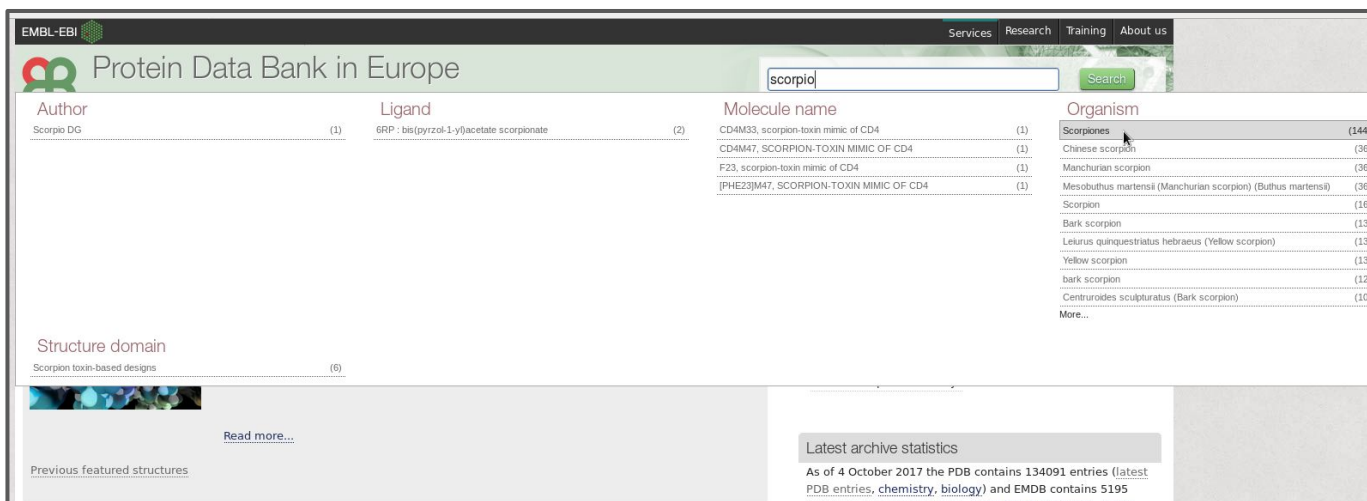
1. Finding the PDB online. All these 3D structures can be accessed at pdbe.org



The screenshot shows the PDBe website homepage. At the top, there is a navigation bar with links for Services, Research, Training, and About us. Below this is the PDBe logo and the tagline "Bringing Structure to Biology". A search bar is located on the right side of the header. The main content area is divided into several sections: "Featured structure" with a 3D molecular model and text about a discovery in the 1970s; "News" with a list of recent updates; "Events" with information about workshops and presentations; "Popular" with a list of frequently used tools and services; and "Latest archive statistics" showing the number of entries in the database. A "Tweets by @PDBEurope" section is also visible at the bottom right.

Exploring the PDB

2. Searching the PDB. The search bar is on the top right of the page. Start typing and the search will try and suggest what you're looking for. Maybe it's the molecule name, a species, or person who did the experiment.

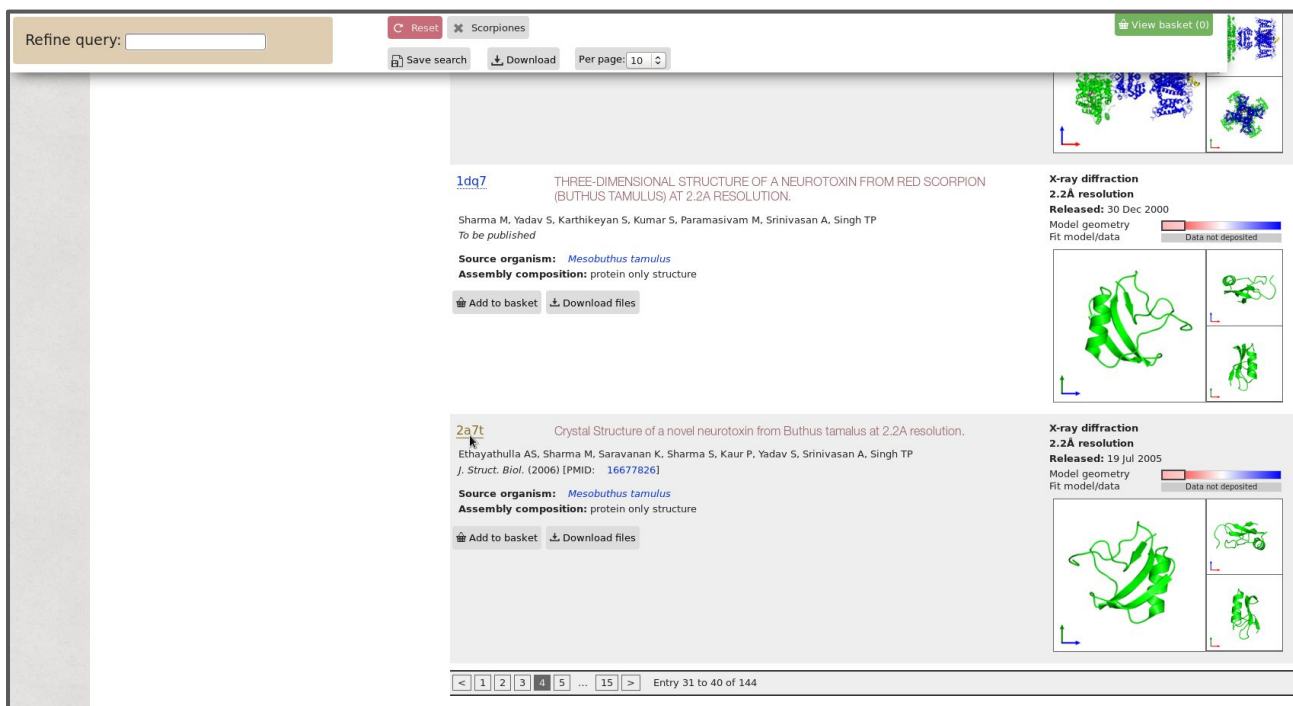


The screenshot shows the PDB search results for the query 'scorpio'. The results are organized into several columns:

- Author:** Scorpio DG (1)
- Ligand:** GRP : bti(pyrzok-1-y)acetate scorpionate (2)
- Molecule name:**
 - CD4M33, scorpion-toxin mimic of CD4 (1)
 - CD4M47, SCORPION-TOXIN MIMIC OF CD4 (1)
 - F23, scorpion-toxin mimic of CD4 (1)
 - [PHE23]M47, SCORPION-TOXIN MIMIC OF CD4 (1)
- Organism:**
 - Scorpiones (144)
 - Chinese scorpion (36)
 - Manchurian scorpion (36)
 - Mesobuthus martensii (Manchurian scorpion) (Buthus martensii) (36)
 - Scorpion (16)
 - Bark scorpion (13)
 - Leiurus quinquestriatus hebraeus (Yellow scorpion) (13)
 - Yellow scorpion (13)
 - bark scorpion (12)
 - Centruroides sculpturatus (Bark scorpion) (10)
 - More...
- Structure domain:** Scorpion toxin-based designs (6)

Additional features include a 'Read more...' link, 'Previous featured structures', and 'Latest archive statistics' showing 134091 entries as of 4 October 2017.

3. Results of a search. Results are presented as a list which you can scroll through. Each structure is given a unique four letter ID code.



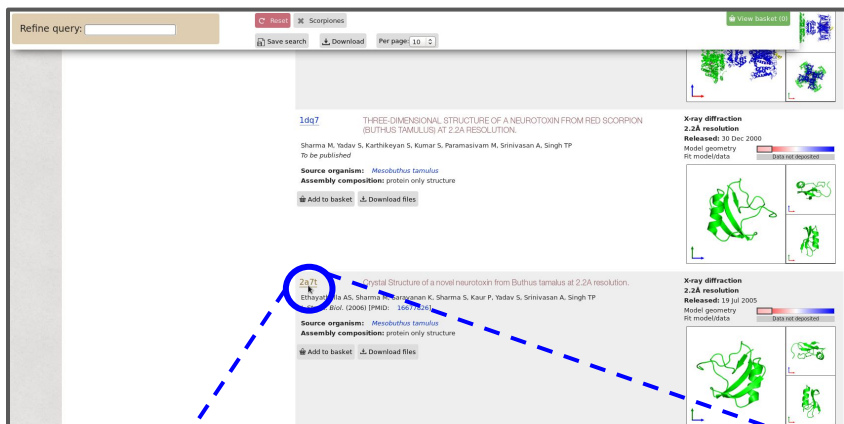
The screenshot shows the detailed view of search results for 'Scorpiones'. The interface includes a 'Refine query' box, 'Reset', 'Save search', 'Download', and 'Per page: 10' options. The results are displayed as a list of entries, each with a unique ID code and associated information:

- 1dq7:** THREE-DIMENSIONAL STRUCTURE OF A NEUROTOXIN FROM RED SCORPION (BUTHUS TAMULUS) AT 2.2Å RESOLUTION. Released: 30 Dec 2000. Source organism: *Mesobuthus tamulus*. Assembly composition: protein only structure.
- 2a7t:** Crystal Structure of a novel neurotoxin from Buthus tamalus at 2.2Å resolution. Released: 19 Jul 2005. Source organism: *Mesobuthus tamulus*. Assembly composition: protein only structure.

Each entry includes a 3D ribbon diagram of the protein structure and a 'View basket (0)' button. The page also features a pagination bar at the bottom showing 'Entry 31 to 40 of 144'.

Exploring the PDB

4. Selecting results from search. Click the four letter PDB code (blue circle) to investigate an 3D structure on its own entry page.



The entry page is a summary of information about the whole structure.

EMBL-EBI

Protein Data Bank in Europe
Bringing Structure to Biology

Services Research Training About us

Examples: hemoglobin, BRCA1_HUMAN

PDBe > 2a7t

Crystal Structure of a novel neurotoxin from *Buthus tamalus* at 2.2Å resolution.

Source organism: *Mesobuthus tamalus*

Primary publication:
 [Crystal structure of a highly acidic neurotoxin from scorpion *Buthus tamalus* at 2.2Å resolution reveals novel structural features.](#)
 Sharma M, Ethayathulla AS, Jabeen T, Singh N, Sarvanan K, Yadav S, Sharma S, Srinivasan A, Singh TP
J. Struct. Biol. **155** 52-62 (2006)
 PMID: 16677826

X-ray diffraction
2.2Å resolution

Released: 19 Jul 2005

Model geometry
Fit model/data Data not deposited

Quick links

2a7t overview

- Citations
- Structure analysis
- Function and Biology
- Ligands and Environments
- Experiments and Validation

• View

• Downloads

• 3D Visualisation

Function and Biology Details

Biochemical function: • toxin activity

Biological process: • defense response

Cellular component: • extracellular region

Sequence domains:

- Scorpion long chain toxin
- Knottin, scorpion toxin-like superfamily
- Scorpion long chain toxin/defensin
- Knottin, scorpion toxin-like

Structure domain:

- Long-chain scorpion toxins

Ligands and Environments

No bound ligands

No modified residues

Experiments and Validation Details

Structure analysis Details

Assembly composition: monomeric (preferred)

Entry contents: 1 distinct polypeptide molecule

Macromolecule:

Neurotoxin BTN

Chains: A, B Molecule details >

Length: 64 amino acids

Theoretical weight: 7.05 KDa

Source organism: *Mesobuthus tamalus*

UniProt:

- Canonical: P60277 (Residues: 1-64; Coverage: 100%)

Sequence domains: Scorpion toxin-like domain

Structure domains: Defensin A-like

X-ray source: RIGAKU RU200

Spacegroup: P2₁

Unit cell:

a: 50.871Å	b: 21.001Å	c: 52.451Å
α: 90°	β: 94.45°	γ: 90°

R-values:

R	R _{work}	R _{free}
0.206	0.205	0.225

Citations

5 citation in other articles

Purification, characterization, and bioactivity of a new analgesic-antitumor peptide from Chinese scorpion *Buthus martensii* Karsch. Shao et al. (2014)

[4 more](#)

Exploring the PDB

5. Molecule Page. Can be found by clicking on the Molecule details text (yellow circle).

Protein Data Bank in Europe
Bringing Structure to Biology

Example hemoglobin_BRC1_HUMAN

Services Research Training About us

Feedback

PDBe · 2a7t

Crystal Structure of a novel neurotoxin from *Buthus tamulus* at 2.2Å resolution

Source organism: *Mesobuthus tamulus*

Primary publication: Crystal structure of a highly acidic neurotoxin from scorpion *Buthus tamulus* at 2.2Å resolution reveals novel structural features.

Sharma M, Ethayathulla AS, Jabeen T, Singh N, Sarvanan K, Yadav S, Sharma S, Srinivasan A, Singh TP
J. Struct. Biol. 155 52-62 (2006)
PMID: 16677826

Function and Biology

Biochemical function: toxin activity, defense response, extracellular region

Biological process: toxin activity, defense response, extracellular region

Cellular component: extracellular region

Sequence domains: Scorpion long chain toxin, Knottin, scorpion toxin-like superfamily, Scorpion long chain toxin/defensin, Knottin, scorpion toxin-like

Structure domain: Long-chain scorpion toxins

Structure analysis

Assembly composition: monomeric (preferred)

Entry contents: 1 distinct polypeptide molecule

Macromolecule: Neurotoxin BTN

Chains: A, B

Length: 64 amino acids

Theoretical weight: 7.05 KDa

Source organism: *Mesobuthus tamulus*

UniProt: Canonical: P60277 (Residues: 1-64; Coverage: 100%)

Sequence domains: Scorpion toxin-like domain

Structure domains: Defensin A-like

X-ray diffraction

2.2Å resolution

Released: 19 Jul 2005

Model geometry

Fit model/data

Quick links

2a7t overview

Citations

Structure analysis

Function and Biology

Ligands and Environments

Experiments and Validation

Downloads

3D Visualisation

Citations

5 citation in other articles

Purification, characterization, and bioactivity of a new analgesic-antitumor peptide from Chinese scorpion *Buthus martensii* Karsch. Shao et al. (2014)

X-ray source: RIGAKU RU200

Spacegroup: P2₁

Unit cell: a: 50.871Å b: 21.003Å c: 52.451Å

Angles: α: 90° β: 94.45° γ: 90°

R-values: R: 0.206 R_{work}: 0.205 R_{free}: 0.225

As a PDB entry might contain several different molecules, this page contains details of each one.

Protein Data Bank in Europe
Bringing Structure to Biology

Example hemoglobin_BRC1_HUMAN

Services Research Training About us

Feedback

PDBe · 2a7t Neurotoxin BTN

Chains: A, B

Length: 64 amino acids

Theoretical weight: 7.05 KDa

Source organism: *Mesobuthus tamulus*

UniProt: Canonical: P60277 (Residues: 1-64; Coverage: 100%)

FASTA Sequence: >>>2a7t|A B
GQDQTAADKDKTCTCTFRTNFCVLCRDKGKSGACMAMPYGVKDELPTFVPSKSGACR

Visualisation

PDB Sequence Viewer UniProt Coverage Viewer

Search similar proteins

Similar 3D structures (RMSD)

Similar sequences (BLAST)

BLAST P60277 (UniProt)

1D primary structure (amino acid sequence) of the protein.

2D visualisation window shows secondary structure.

Visualisation

PDB Sequence Viewer UniProt Coverage Viewer

Compact Expanded

Molecule

Pfam Scorpion toxin-like domain

UniProt SCXI_MEST1

Chain A

Quality

Sec. Str.

CATH Defensin A-like strand in a sheet in chain A

SCOP Long-chain scorpion toxins

load more charts

2a7t:A Annotation

Zoom view of molecule page

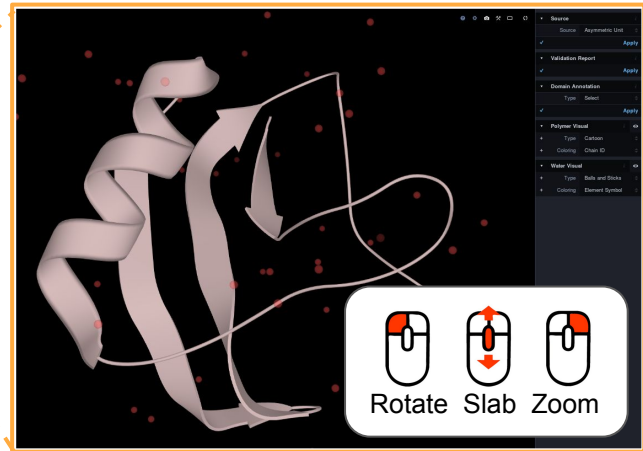
Hovering the mouse over an amino acid or feature will highlight it in all three panels.

Interactive 3D visualisation window.

Exploring the PDB

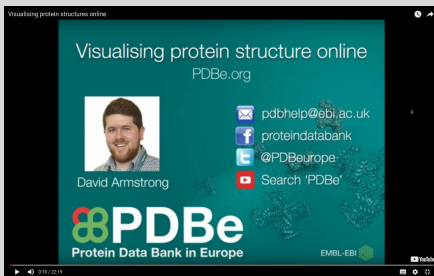
6. Open Structure in 3D. Go back to the entry page, then select **3D Visualisation** (yellow circle).

7. Viewing in 3D



The protein or DNA can be manipulated by clicking and dragging your mouse across the screen.

Further Details on 3D Visualisation



A guide to using LiteMol can be found in PDBe's webinar https://youtu.be/mMS6ZZVeB_8

The protein can be viewed in different ways using this tab.

Activities

- What different representations or colours can you display the molecule in?
- Search and explore proteins (or DNA or RNA) that interest you
- Look for new 3D structures just released this week
- Find a structure with DNA in it
- Find structure from a woolly mammoth