

Database-driven discovery

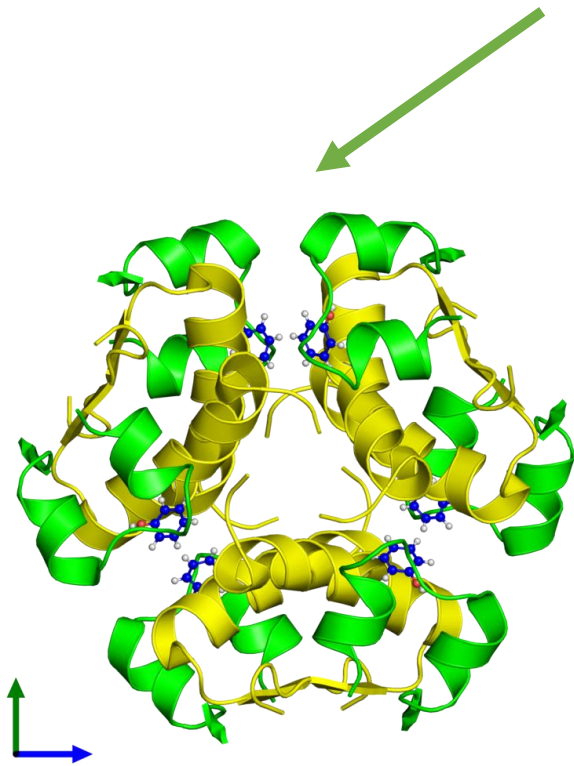
John Berrisford



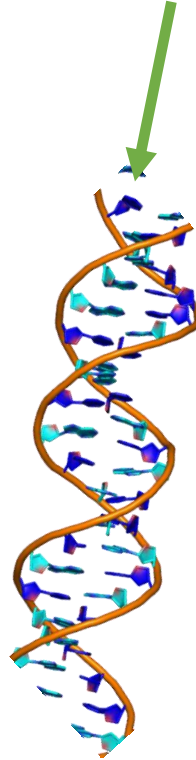
Summary

- Searching the PDB
- Advanced search
- Searching the PDB programmatically

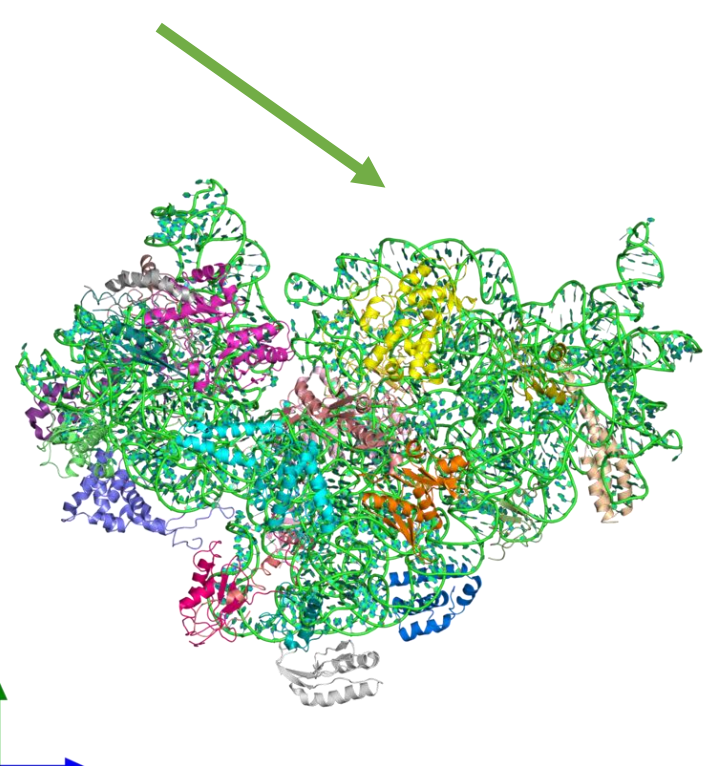
The Protein Data Bank (PDB) is an archive of *experimentally determined* 3-dimensional structures of biological macromolecules



Proteins

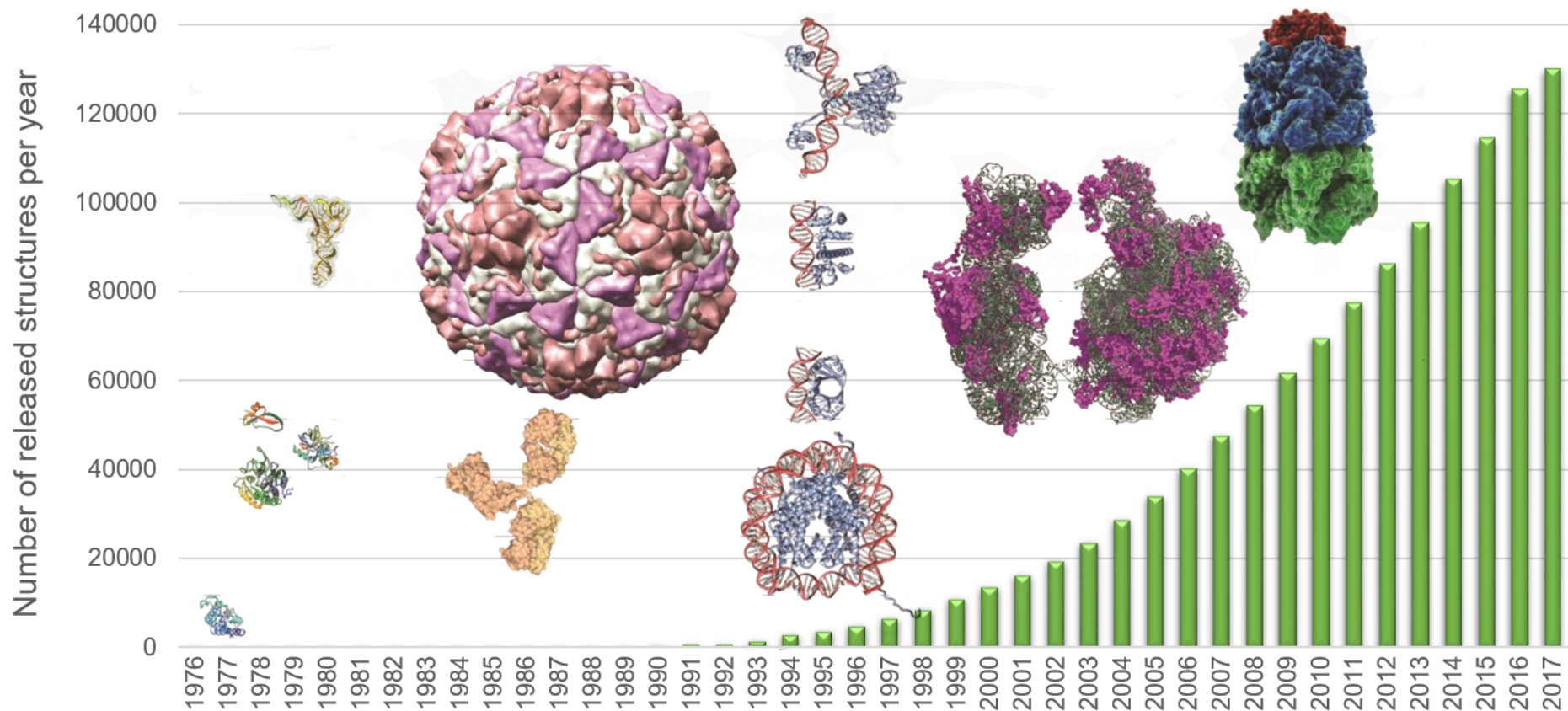


DNA/RNA



Complexes of Protein and NA

PDB over the years



In May 2014, we passed the 100,000 milestone
As of today, ~150,000 structures

At the heart of EMBL-EBI resources

Genes, Genomes & Variation

European Nucleotide Archive
European Variation Archive
Metagenomics Portal

Ensembl
1000 Genomes
RNACentral

European Genome-phenome Archive
Ensembl Genomes

Expression

Array Express

Expression Atlas

PRIDE

Proteins & Protein Families

InterPro

Pfam

UniProt

Molecular & Cellular Structures

Protein Data Bank in Europe
Electron Microscopy Data Bank

Chemical Biology

ChEMBL
MetaboLights

ChEBI

Molecular Systems

BioModels
Reactome

IntAct

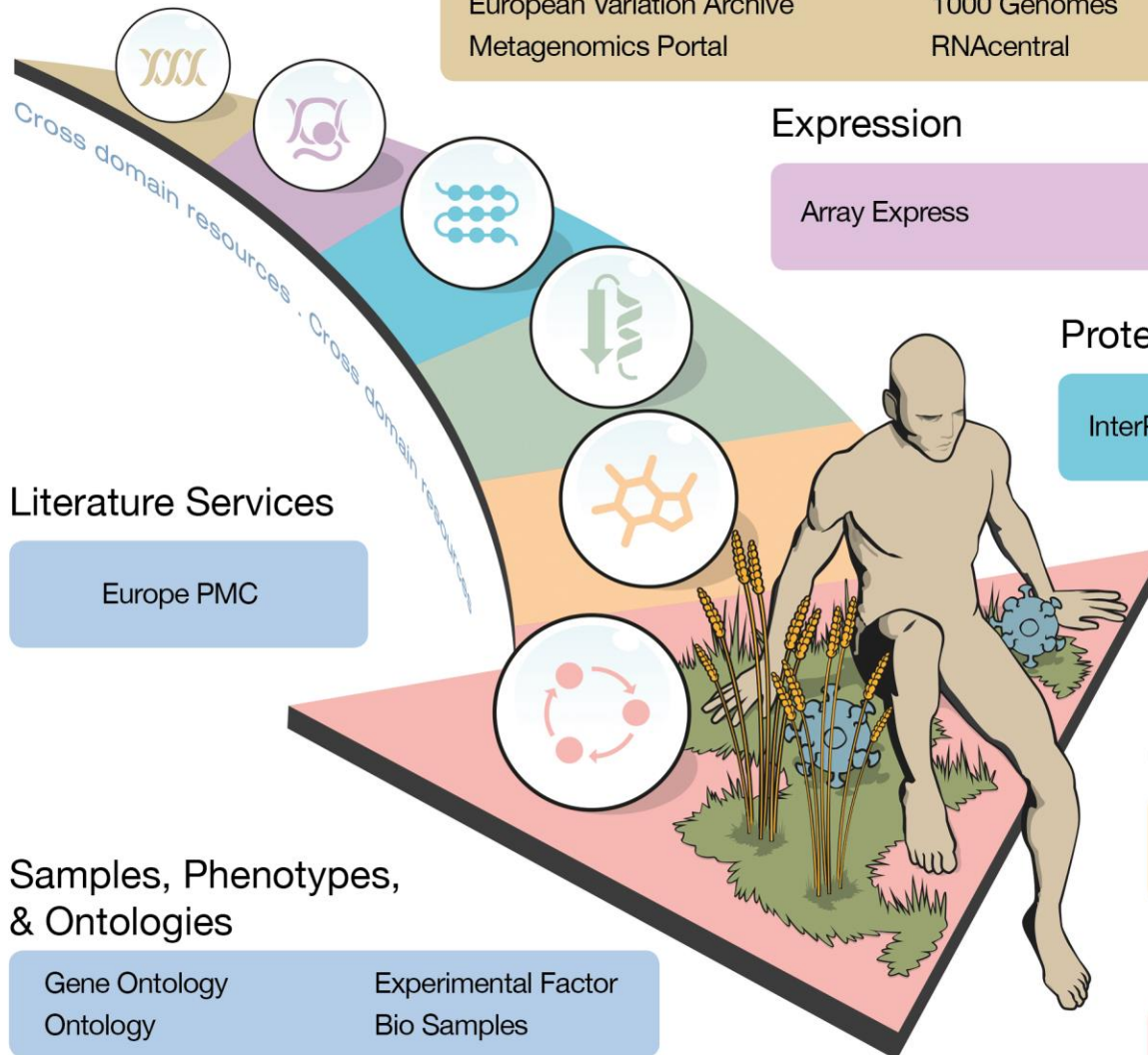
Literature Services

Europe PMC

Samples, Phenotypes, & Ontologies

Gene Ontology
Ontology

Experimental Factor
Bio Samples



Searching the PDB

The problem with the PDB is...



- I can't find what I want
- Too many false hits when I search
 - CaM, CaM-Kinase, CaM binding protein, Cam-like...
- Results are too complicated
 - Which lysozyme to use? 47 species!
 - Which is best?/what is best? >250 ligands
- Redundancy
 - How many unique human protein structures?

Searching the PDB made simple

At PDBe we've implemented:

- Auto-complete suggestions
- Facets to narrow down search results
- Quality presented on search results
- Four views of results
 - Moving away from entry-centricity





Protein Data Bank in Europe

Bringing Structure to Biology

Examples: hemoglobin, BRCA1_HUMAN

Search

EMsearch

[PDBe home](#) [Deposition](#) [PDBe services](#) [PDBe training](#) [Documentation](#) [About PDBe](#)

[Share](#) [Feedback](#)

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

Featured structure

Stop motion: The muscular system



1st May 2018

The image for May in our [2018 calendar](#) captures a molecular snapshot of one of our primary groups of organs – the muscular system. Here we discuss the individual molecules responsible for the large motions of these muscles.

[Read more...](#)

[Previous featured structures](#)

News

David Blow Poster Prize awarded at BCA

13 April, 2018

PDBe Explores Art

29 March, 2018

[Access Updated Validation Reports for](#)

Events

University of Cambridge Protein Structure Analysis course

University of Cambridge, Cambridge, UK

24 May 2018

Three Dimensional Electron Microscopy -

Popular

- [EMsearch](#)
- [PDBeFold](#)
- [PDBePISA](#)
- [PDBeChem](#)
- [Sequence search](#)
- [PDBe REST API](#)
- [EM resources](#)
- [NMR resources](#)
- [EMPIAR](#)
- [Coordinate Server](#)
- [PDB Component Library](#)

- [News](#)
- [Events](#)
- [Training](#)
- [Contact us](#)

Latest archive statistics

As of 23 May 2018 the PDB contains 140591 entries ([latest PDB entries](#), [chemistry](#), [biology](#)) and EMDB contains 6215 entries ([latest map releases](#), [latest header releases](#), [latest updates](#)).

Tweets by @PDBeurope



Protein Data Bank
@PDBeurope

How snail toxins could treat pain. This structure,

Protein Data Bank in Europe

hydro

Search

Enzyme

Hydrolases	(21099)
Glycosidases, i.e. enzymes hydrolyz...	(3634)
Hydro-lyases	(1683)
Phosphoric monoester hydrolases	(1543)
Carboxylic ester hydrolases	(1038)
Carbonic acid hydro-lyase (carbon-...	(845)
Beta-lactam hydrolase	(537)
Phosphoric diester hydrolases	(499)
Hydrolyzing N-glycosyl compounds	(465)
3.4.19.12 : Ubiquitinyl hydrolase 1	(450)

More...

GO mapping

GO:0016787 : hydrolase activity	(16113)
GO:0016798 : hydrolase activity, acti...	(3749)
GO:0004553 : hydrolase activity, hyd...	(2235)
GO:0090305 : nucleic acid phosph...	(1925)
GO:0090502 : RNA phosphodiester...	(775)
GO:0042542 : response to hydroge...	(652)
GO:0090501 : RNA phosphodiester...	(603)
GO:0042744 : hydrogen peroxide c...	(590)
GO:0016788 : hydrolase activity, acti...	(482)
GO:0052689 : carboxylic ester hydr...	(479)

More...

Journal

Int J Hydrogen Energy	(5)
-----------------------	-----

Ligand

NAG : N-[(2R,3R,4R,5S,6R)-6-(hydr...	(6384)
PEG : DI(HYDROXYETHYL)ETHER	(2501)
PEG : 2-(2-hydroxyethyloxy)ethanol	(2501)
MAN : (2S,3S,4S,5S,6R)-6-(hydroxy...	(2087)
BMA : (2R,3S,4S,5S,6R)-6-(hydroxy...	(2012)
FAD : [(2R,3S,4R,5R)-5-(6-aminopu...	(1980)
ADP : [(2R,3S,4R,5R)-5-(6-aminopu...	(1892)
NAD : [(2R,3S,4R,5R)-5-(3-aminoca...	(1239)
NAP : [(2R,3S,4R,5R)-5-(3-aminoca...	(1181)
TRS : 2-AMINO-2-HYDROXYMETHY...	(1155)

More...

Molecule name

Soluble epoxide hydrolase	(108)
Bifunctional epoxide hydrolase 2	(104)
Cytosolic epoxide hydrolase 2	(104)
Pyrophosphate phospho-hydrolase	(96)
4-hydroxy-tetrahydrodipicolinate syn...	(73)

Organism

Hydrozoa	(365)
Arthrobacter Hydrocarboglutamicus	(68)
Aeromonas hydrophila	(42)
Carboxydotherrnus hydrogenoform...	(34)
Aeromonas Hydrophila	(28)

Sequence family

IPR027417 : P-loop containing nucl...	(4780)
IPR017853 : Glycoside hydrolase s...	(2385)
CL0058 : Glyco_hydro_tim	(2139)
IPR029058 : Alpha/Beta hydrolase f...	(1862)
CL0028 : AB_hydrolase	(1763)

Structure domain

Methane Monooxygenase Hydroxyla...	(1278)
P-loop containing nucleoside tripho...	(1196)
alpha/beta-Hydrolases	(524)
Phosphorylase/hydrolase-like	(285)
Glycosyl hydrolase domain	(284)

Enzyme

Hydrolases	(21099)
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Glycosidases, i.e. enzymes hydrolyz...	(3634)
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Hydro-lyases	(1683)
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Phosphoric monoester hydrolases	(1543)
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Carboxylic ester hydrolases	(1038)
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Carbonic acid hydro-lyase (carbon-...	(845)
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Beta-lactam hydrolase	(537)
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Phosphoric diester hydrolases	(499)
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Hydrolyzing N-glycosyl compounds	(465)
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3.4.19.12 : Ubiquitinyl hydrolase 1	(450)
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[More...](#)

Drill down with facets

Latest PDB release

Entries released this week (1)

Entry Information

- Entry status (1)
- Experimental meth
- Authors (3891)
- Homo / hetero ass
- Assembly compos
- Assembly polymer
- Resolution distribut
- Release year distri
- Journal (327)

Macromolecules

- Organism superkingdom (4)
- Organism name (921)

Homo sapiens	(6129)
Bos taurus	(1115)
Escherichia coli	(782)
Gallus gallus	(760)
Escherichia virus T4	(701)
Human immunodeficiency virus 1	(539)

3D Visualisation Download files

complex with a

Released: 24 Jan 2006

X-ray diffraction 2.1Å resolution

Model geometry

Fit model/data

Released: 12 Mar 2014

X-ray diffraction 1.618Å resolution

Model geometry

Fit model/data

Drill down with facets

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PDBe
Protein Data Bank in Europe

Ex - hemoglobin, BRCA1_HUMAN Search
Examples: [hemoglobin](#), [BRCA1_HUMAN](#) [Advanced search](#)

Feedback

PDBE / SEARCH

Enzyme name : Hydrolases 

AND Organism name : Homo sapiens 

[remove all filters](#)

Advanced search

Download

10 /page

Filter by :

Latest PDB release

- Entries released this week (1)
- revised

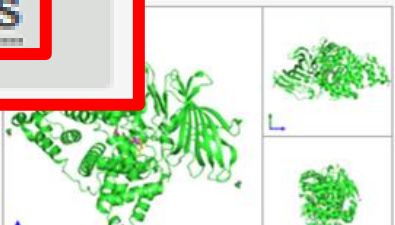
Entry Information

- Entry status (1)
- Experimental methods (6)
- Authors (15974)
- Homo / hetero assembly (2)
- Assembly composition (6)

Bound ligands: [1V6](#) [28T](#) [YB](#) [ACY](#) [ZN](#)

[3D Visualisation](#) [Download files](#)

on
tion
Mar 2014



Advanced search and sequence search

- Search for queries by typing or scrolling
- Select a query to add it to your search form

The screenshot displays the PDBE (Protein Data Bank in Europe) website. The top navigation bar includes links for EMBL-EBI, Services, Research, Training, and About us. The PDBE logo is prominently displayed on the left. A search bar on the right contains the example query "Ex. - hemoglobin, BRCA1_HUMAN" and a "Search" button. Below the search bar, there are links for "Examples: hemoglobin, BRCA1_HUMAN" and "Advanced search". A "Feedback" link is also visible. In the foreground, an "Advanced search form" modal is open. It features a "Select to add a search field :" dropdown menu with the following options: "molecule", "Macromolecules", "Molecule name" (highlighted), "Molecule type", "Molecule expression method", and "Macromolecule molecular weight". The EMBL-EBI logo is visible in the bottom right corner of the page.

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PDBe
Protein Data Bank in Europe

Ex. - hemoglobin, BRCA1_HUMAN Search

Examples: [hemoglobin](#), [BRCA1_HUMAN](#) [Advanced search](#)

Feedback

PDBE / SEARCH

Advanced search form ✕

Select to add a search field :

molecule ✕ ▲

Macromolecules

Molecule name

Molecule type

Molecule expression method

Macromolecule molecular weight

EMBL-EBI

Advanced search and sequence search

- Begin typing to get autocomplete suggestions for that query

The screenshot shows the PDB (Protein Data Bank) website interface. At the top, there is a navigation bar with links for EMBL-EBI, Services, Research, Training, and About us. The PDB logo is prominently displayed on the left. On the right, there is a search bar with the text "Ex. - hemoglobin, BRCA1_HUMAN" and a "Search" button. Below the search bar, there are examples: "hemoglobin" and "BRCA1_HUMAN".

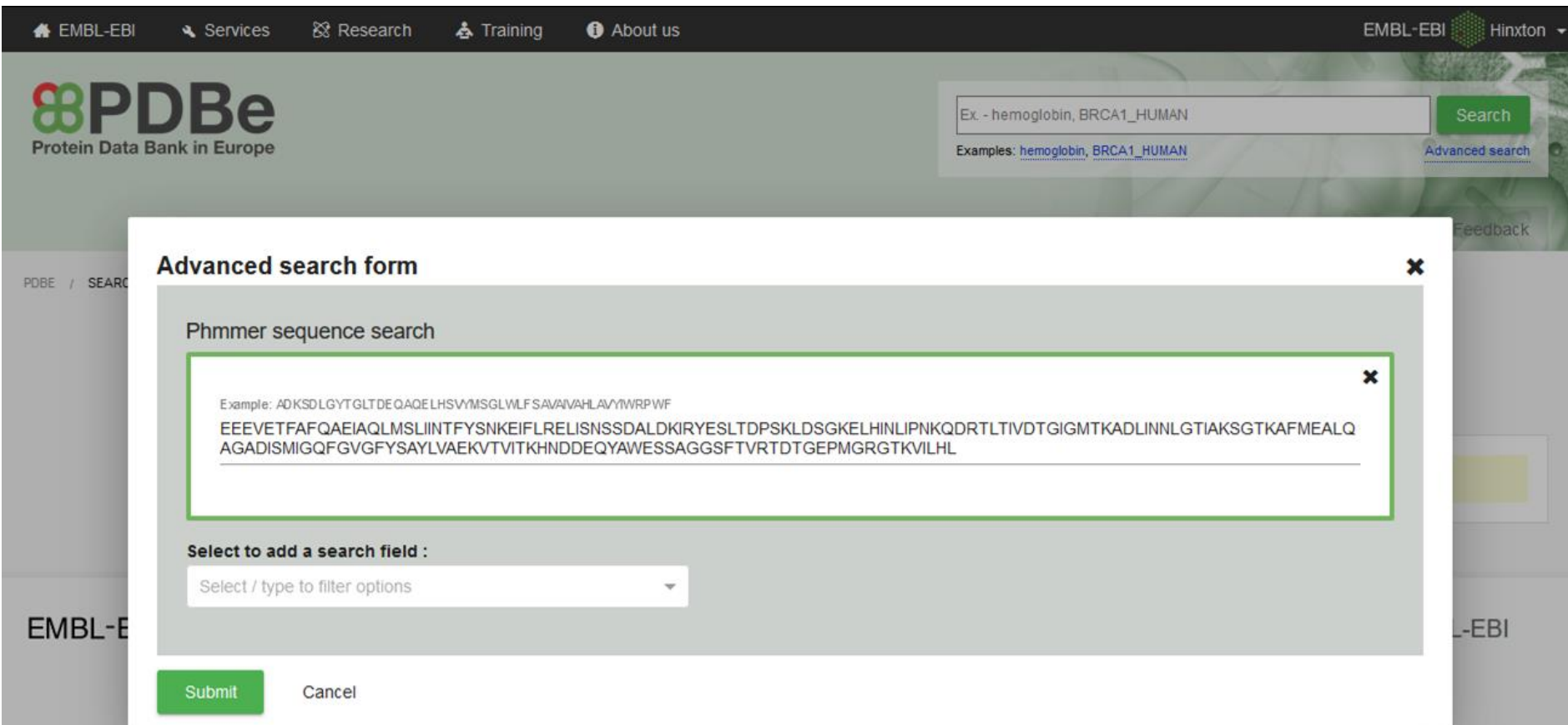
An "Advanced search form" modal is open in the center. It has a title bar with a close button (X). The form is titled "Advanced search form" and contains a section for "Molecule name" with an information icon (i). Below this, there is a dropdown menu labeled "condition" with "Contains" selected. An example text "Example: Carbonic anhydrase 2" is shown. The input field contains the text "hemoglobin". A dropdown menu is open below the input field, showing the following suggestions:

- hemoglobin beta chain (330)
- hemoglobin subunit alpha (326)
- hemoglobin subunit beta (325)
- hemoglobin alpha chain (322)

At the bottom of the modal, there are two buttons: "Submit" and "Cancel".

Advanced search and sequence search

- Can also search using a protein sequence via Phmmer



The screenshot displays the PDBE (Protein Data Bank in Europe) website interface. At the top, there is a navigation bar with links for EMBL-EBI, Services, Research, Training, and About us. The PDBE logo is prominently displayed on the left. On the right, there is a search bar with the example text 'Ex - hemoglobin, BRCA1_HUMAN' and a 'Search' button. Below the search bar, there are links for 'Examples: hemoglobin, BRCA1_HUMAN' and 'Advanced search'. The main focus is the 'Advanced search form' modal window, which is titled 'Advanced search form' and has a close button (X) in the top right corner. Inside the modal, there is a section for 'Phmmer sequence search'. This section contains a text input field with a green border, which is highlighted by a green rectangle. The input field contains the following text: 'Example: ADKSDLGYTGLTDEQAQELHSVYMSGLVLFSAVAVAHLAVYWRPWF' followed by a protein sequence: 'EEEVETFAFQAEIAQLMSLIINTFYSNKEIFLRELISNSSDALDKIRYESLTDPSKLD SGKELHINLIPNKQDRTLTI VDTGIGMTKADLINNLGTIAKSGTKAFMEALQAGADISMIGQFGVGFYSAYLVAEKVTITKHNDDEQYAWESSAGGSFTVRTDTGEP MGRGTKVILHL'. Below the input field, there is a dropdown menu labeled 'Select to add a search field :'. The dropdown menu is currently open, showing the text 'Select / type to filter options'. At the bottom of the modal, there are two buttons: 'Submit' and 'Cancel'.

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PDBe
Protein Data Bank in Europe

Ex - hemoglobin, BRCA1_HUMAN

Search

Examples: [hemoglobin](#), [BRCA1_HUMAN](#)

[Advanced search](#)

Feedback

PDBE / SEARCH

Advanced search form

Phmmer sequence search

Example: ADKSDLGYTGLTDEQAQELHSVYMSGLVLFSAVAVAHLAVYWRPWF

EEEVETFAFQAEIAQLMSLIINTFYSNKEIFLRELISNSSDALDKIRYESLTDPSKLD SGKELHINLIPNKQDRTLTI VDTGIGMTKADLINNLGTIAKSGTKAFMEALQAGADISMIGQFGVGFYSAYLVAEKVTITKHNDDEQYAWESSAGGSFTVRTDTGEP MGRGTKVILHL

Select to add a search field :

Select / type to filter options

Submit Cancel

Advanced search and sequence search



Structure of TRAP1 fragment

Sung N, Chang C, Lee S, Tsai FTF

Acta Crystallogr D Struct Biol (2016) [PMID: [27487821](#)]

Source organism: [Homo sapiens](#)

Assembly composition: protein only structure

Bound ligands: [ANP](#) [SO4](#) [MG](#) [PO4](#) [GOL](#)

3D Visualisation

Download files

Accuracy: 0.9

Bit score: 145.11

E-value: 1.6e-41

Identity count: 82

Chain ID: A

Sequence Alignment:

Query : FAFQAEIAQLMSLIINTFYSNKEIFLRELISNSSDALDKIRYESLTDPSKLD SGKELHINLIPNKQDRTLTIIVDTGIGMTKADLINNL

Match : FQAE +L+ ++ ++YS KE+F+RELISN+SDAL+K+R++ ++D L E++I+L N + T+TI DTGIGMT+ +L++NL

Target : HEFQAETKLLDIVARSLYSEKEVFIRELISNASDALEKLRHKLVS DGQALP---EMEIHLQTNAEKGTITIQTDTGIGMTQEELVSNL



[Click here to check for other PDB entries with identical sequence](#)

X-ray diffraction

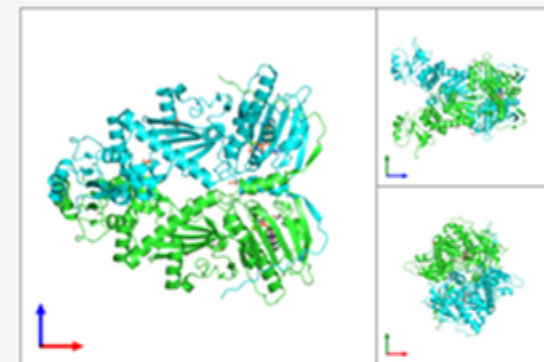
2.429Å resolution

Released: 10 Aug 2016

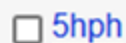
Model geometry



Fit model/data



LiteMol and Downloads on search



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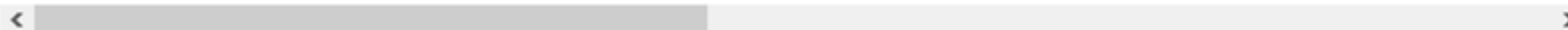
Chain ID: A

Sequence Alignment:

Query : FAFQAEIAQLMSLIINTFYSNKEIFLRELISNSSDALDKIRYESLTDPSKLD SGKELHINLIPNKQDRTLTIVDTGIGMTKADLINNL

Match : FQAE +L+ ++ ++YS KE+F+RELISN+SDAL+K+R++ ++D L E++I+L N + T+TI DTGIGMT+ +L++NL

Target : HEFQAETKLLDIVARSLYSEKEVFIRELISNASDALEKLRHKLVS DGQALP---EMEIHLQTNAEKGTITIQTDTGIGMTQEELVSNL



[Click here to check for other PDB entries with identical sequence](#)

X-ray diffraction

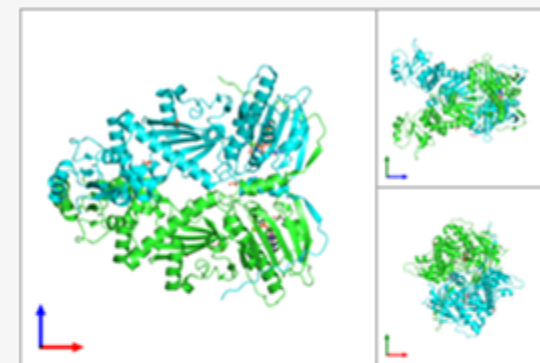
2.429Å resolution

Released: 10 Aug 2016

Model geometry



Fit model/data

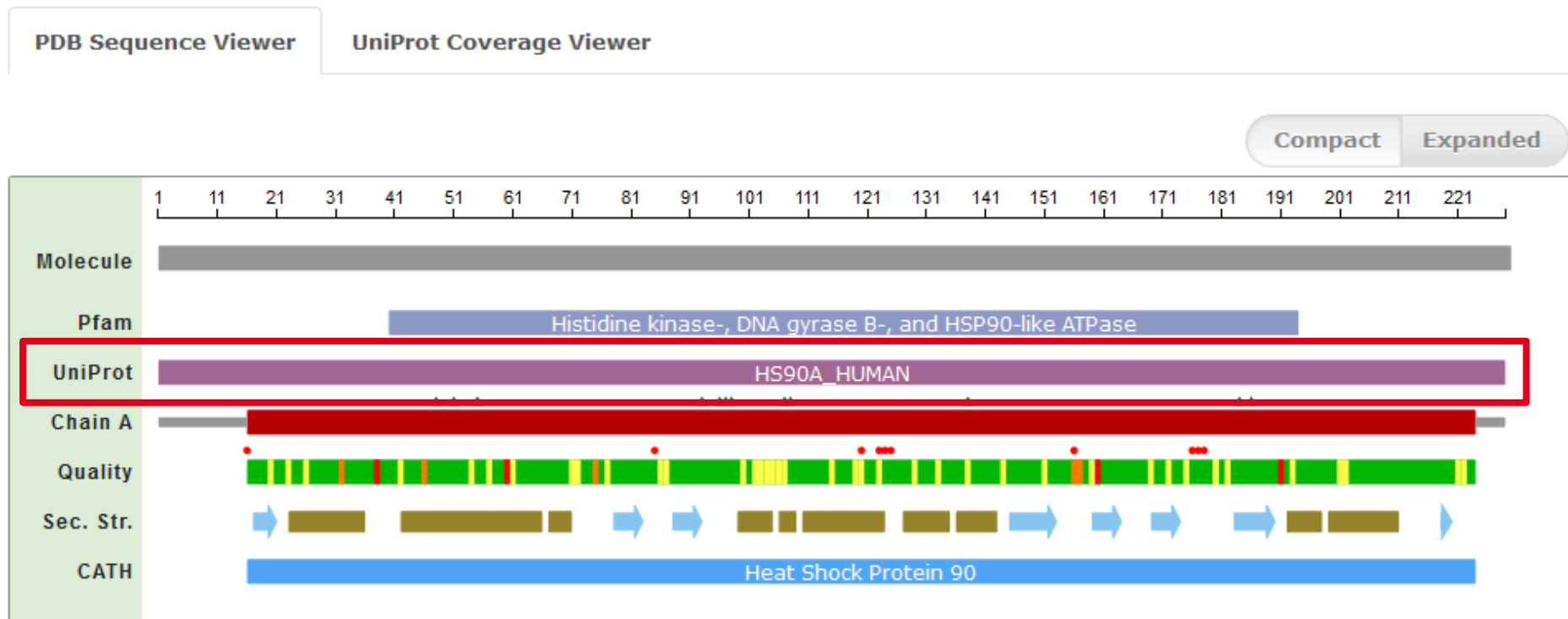


Programmatic access to the PDB

- What information can you get?

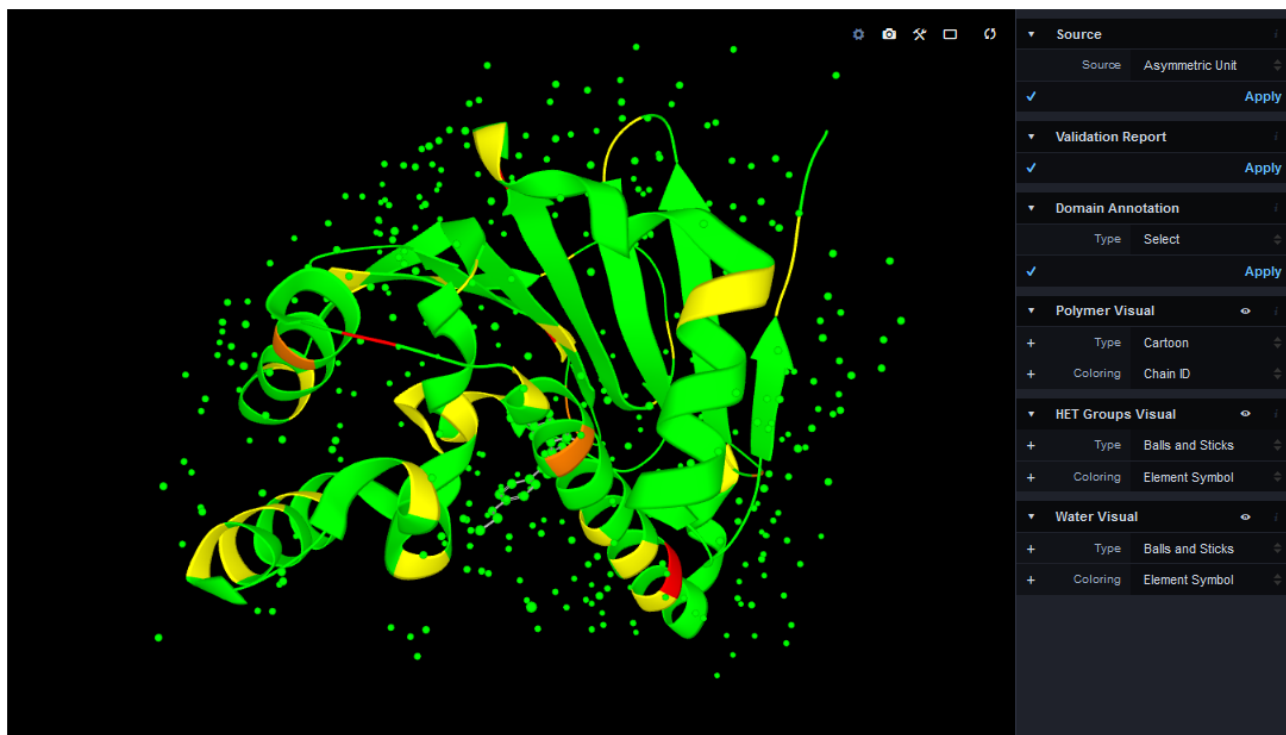
Showing sequence annotation at PDBe.org

- Component for displaying sequence annotation
- Uses API to get this information



LiteMol – powered by PDBe REST API

- New, lightweight structure viewer at PDBe
- Uses API to get structure and annotation data
 - Including residue-level validation information



```
"author_insertion_code": "",  
"author_residue_number": 120,  
"alt_code": "",  
"outlier_types": [  
  "clashes"
```

```
"author_insertion_code": "",  
"author_residue_number": 156,  
"alt_code": "",  
"outlier_types": [  
  "bond_lengths",  
  "planes"
```

```
"author_insertion_code": "",  
"author_residue_number": 191,  
"alt_code": "",  
"outlier_types": [  
  "clashes",  
  "bond_lengths",  
  "bond_angles",  
  "sidechain_outliers"
```


Searching the PDB programmatically

- It is possible to search the PDB programmatically and get access to the data in the PDB archive

RESTful API for PDBe data

- Allows access to vast amounts of PDBe data
- Powers the PDBe search and web pages
 - Will always be well maintained!

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 text "Protein Data Bank in Europe Bringing Structure to Biology". A search bar is located on the right side of the header, with a "Search" button and examples of search terms: hemoglobin, BRCA1_HUMAN. Below the header is a secondary navigation bar with links for PDBe home, Deposition, PDBe services, PDBe training, Documentation, and About PDBe. The main content area features a "Featured structure" section titled "Focusing on Crystallin" with a date of "1st June 2017". The featured structure is a 3D model of a protein complex. To the right of the featured structure is a "Popular" section with a list of links: EMsearch, PDBeFold, PDBePISA, Sequence search (highlighted with a red box), PDBe REST API (highlighted with a red box), EM resources, NMR resources, EMPIAR, Coordinate Server, and PDB Component Library. Other links in the "Popular" section include News, Events, Training, and Contact us.

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Services Research Training About us

Protein Data Bank in Europe
Bringing Structure to Biology

Search

Examples: hemoglobin, BRCA1_HUMAN

EMsearch

PDBe home Deposition PDBe services PDBe training Documentation About PDBe

Share Feedback

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

Featured structure

Focusing on Crystallin

1st June 2017

As you read the words on this page, the light enters your eyes and the eye lens focuses it on the retina. From here the image is sent to your brain for processing. The major protein from the eye lens is shown here in June's featured structure from our 2017 calendar.

Popular

- EMsearch
- PDBeFold
- PDBePISA
- Sequence search
- PDBe REST API**
- EM resources
- NMR resources
- EMPIAR
- Coordinate Server
- PDB Component Library


- News
- Events
- Training
- Contact us

RESTful API for PDBe data

- Allows access to vast amounts of PDBe data
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EMBL-EBI

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 Protein Data Bank in Europe
Bringing Structure to Biology

Search

Examples: hemoglobin, BRCA1_HUMAN

EMsearch

PDBe home Deposition PDBe services PDBe training Documentation About PDBe

Share Feedback

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Popular

EMsearch News

Sequence search

PDBe REST API


EM resources

Coordinate Server

PDB Component Library

Featured structure

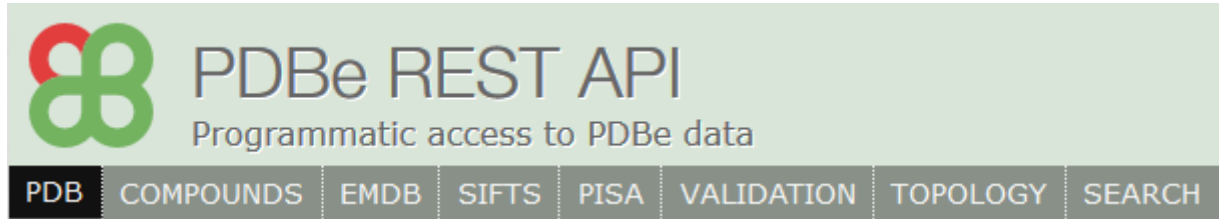
Focusing on Crystallin



As you read the words on this page, the light enters your eyes and the image is sent to your brain for processing. The major protein from the eye lens is shown here in June's featured structure from our 2017 calendar.

What can the REST API give you?

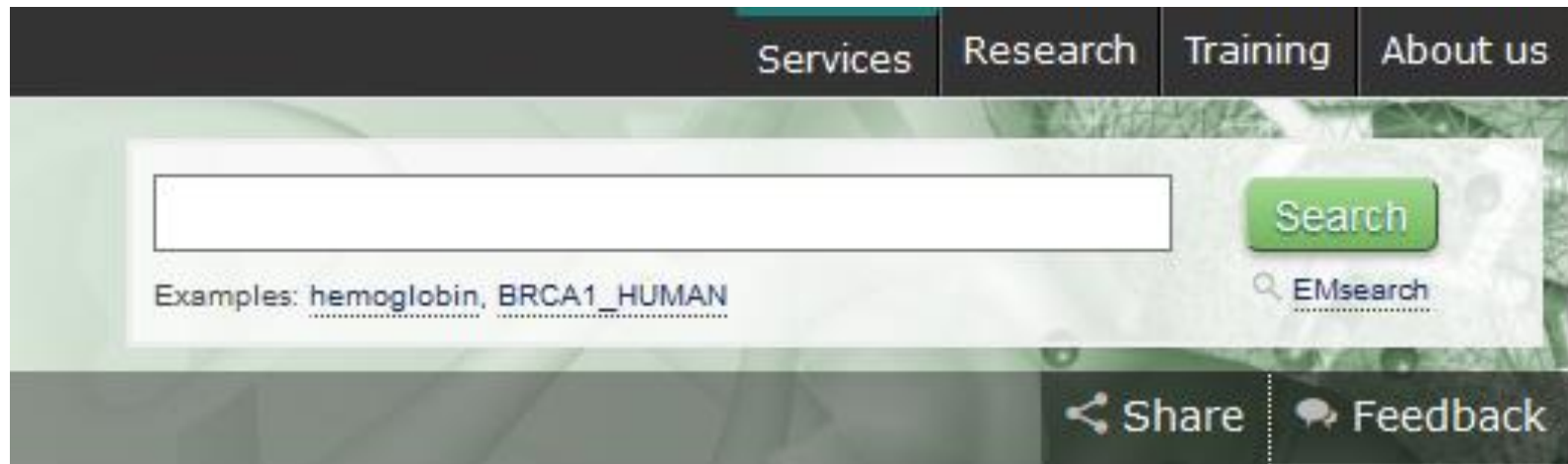
- Split into 8 groups



- These REST calls are based on different subsets of data
 - These are grouped for ease of use
- These are available on the documentation page
 - Thorough set of example calls
 - Give URL and output JSON on the page

PDBe web search is based on the API

- Initial queries typed into autocomplete search bar
- Can then refine search by additional queries
 - These are the facets on the left-hand side
- URL contains the queries involved in the search
 - Directly corresponding to API calls



Search in the documentation page



PDBe REST API
Programmatic access to PDBe data

PDB COMPOUNDS EMDB SIFTS PISA VALIDATION TOPOLOGY **SEARCH**

Share Feedback

Version 1.5

REST calls related to PDBe search service

Show/Hide All Calls

Search on Solr instance based on polymeric entities in the PDB.

<http://www.ebi.ac.uk/pdbe/search/pdb/select?:query>

A document in this Solr instance represents a polymeric entity of type protein, DNA, RNA or sugar.

Output from the call depends on the query sent to Solr. Query parameters are well documented in Solr documentation.

Each document has a wide range of properties, grouped as follows:

- Basic information about the entry
 - `pdb_id` : PDB entry id code.
 - `number_of_polymer_entities` : Number of unique polymers in the entry.
 - `number_of_bound_entities` : Number of unique bound molecules (excluding water) in the entry.
 - `number_of_polymers` : Number of polymer chains in the entry.
 - `number_of_bound_molecules` : Number of bound molecules in the entry.
 - `number_of_polymer_residues` : Number of polymer residues in all polymers.
 - `entry_authors` : List of depositors who deposited this entry.
 - `all_authors` : Combined list of depositors and authors of primary citation.
 - `title` : Title of the entry as provided by the depositor.
 - `revision_date` : Date of latest revision of the entry - this is a timestamp in format YYYY-MM-DDThh:mm:ssZ.
 - `revision_year` : Year of latest revision of the entry.
 - `deposition_date` : Date when entry was deposited - this is a timestamp in format YYYY-MM-DDThh:mm:ssZ.
 - `deposition_year` : Year of deposition of the entry.
 - `status` : Release state of the entry, e.g. REL, OBS etc.
 - `release_date` : Date of release of the entry - this is a timestamp in format YYYY-MM-DDThh:mm:ssZ.
 - `release_year` : Year of release of the entry.

Search queries in the documentation

— Search on Solr instance based on polymeric entities in the PDB.

<http://www.ebi.ac.uk/pdbe/search/pdb/select?:query>

A document in this Solr instance represents a polymeric entity of type protein, DNA, RNA or sugar.

Output from the call depends on the query sent to Solr. Query parameters are well documented in Solr documentation.

Each document has a wide range of properties, grouped as follows:

- **pdb_id** : PDB entry id code.

entry.

- number_of_bound_entities : Number of unique bound molecules (excluding water) in the entry.

- number_of_polymers : Number of polymer chains in the entry.

- number_of_bound_molecules : Number of bound molecules in the entry.

- number_of_polymer_residues : Number of polymer residues in all polymers.

- entry_authors : List of depositors who deposited this entry.

- all_authors : Combined list of depositors and authors of primary citation.

- title : Title of the entry as provided by the depositor.

- revision_date : Date of latest revision of the entry - this is a timestamp in format YYYY-MM-DDThh:mm:ssZ.

- revision_year : Year of latest revision of the entry.

- **deposition_year** : Year of deposition of the entry.

- release_date : Date of release of the entry - this is a timestamp in format YYYY-MM-DDThh:mm:ssZ.

- release_year : Year of release of the entry.

- number_of_protein_chains : Number of protein chains in the entry.

- number_of_DNA_chains : Number of DNA chains in the entry.

- number_of_RNA_chains : Number of RNA chains in the entry.

Search in the documentation page

String Options string allowed by Solr syntax. Details about constructing Solr queries can be found from webpages such as [this](#).

postdata String Send one or more query options in post data instead of appending to URL.

☒ Quotes

RunCall

Select

Expand

Collapse

2+

3+

GET : [http://www.ebi.ac.uk/pdbe/search/pdb/select?q=molecule_name:"Dihydrofolate reductase" AND organism_scientific_name:"Homo sapiens"&wt=json](http://www.ebi.ac.uk/pdbe/search/pdb/select?q=molecule_name:)

HTTP status : 200 : OK (Hover to find undocumented bits in the output.)

```
{
  "responseHeader": {
    "status": 0,
    "QTime": 0,
    "params": {
      "q": "molecule_name:'Dihydrofolate reductase' AND organism_scientific_name:'Homo sapiens'",
      "wt": "json"
    }
  },
  "response": {
    "numFound": 75,
    "start": 0,
    "docs": [
      {
        "all_authors": [
          "Borhani DW",
          "Campbell SR",
          "Dixon RW",
          "Fairchild RG",
          "Kisliuk RL",
          "Leung AK",
```

Practical example of how to get data from the PDB

- For this tutorial we will use Jupyter notebooks to use the PDBe search API
- <https://github.com/PDBeurope/pdbe-api-training>