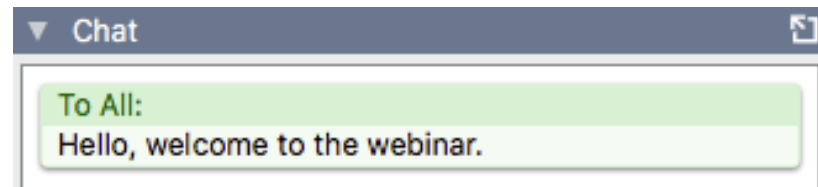


## Welcome - webinar instructions

- GoToTraining works best in **Chrome** or on Linux, **Firefox**
- All **microphones will be muted** while the trainer is speaking
- If you have a question please use the **chat box** at the bottom of the GoToTraining box



- Please complete the **feedback survey** which will launch at the end of the webinar

# PDBe API webinar series: Using the PDBe graph API

[PDBe.org/aggregated-api](https://pdbe.org/aggregated-api)



Sreenath Nair



[pdhelp@ebi.ac.uk](mailto:pdhelp@ebi.ac.uk)



[proteindatabank](https://www.facebook.com/proteindatabank)



[@PDBEurope](https://twitter.com/PDBEurope)



[proteindatabank](https://www.youtube.com/proteindatabank)



[pdbeurope](https://www.instagram.com/pdbeurope)



[pdbart](https://www.pinterest.com/pdbart)



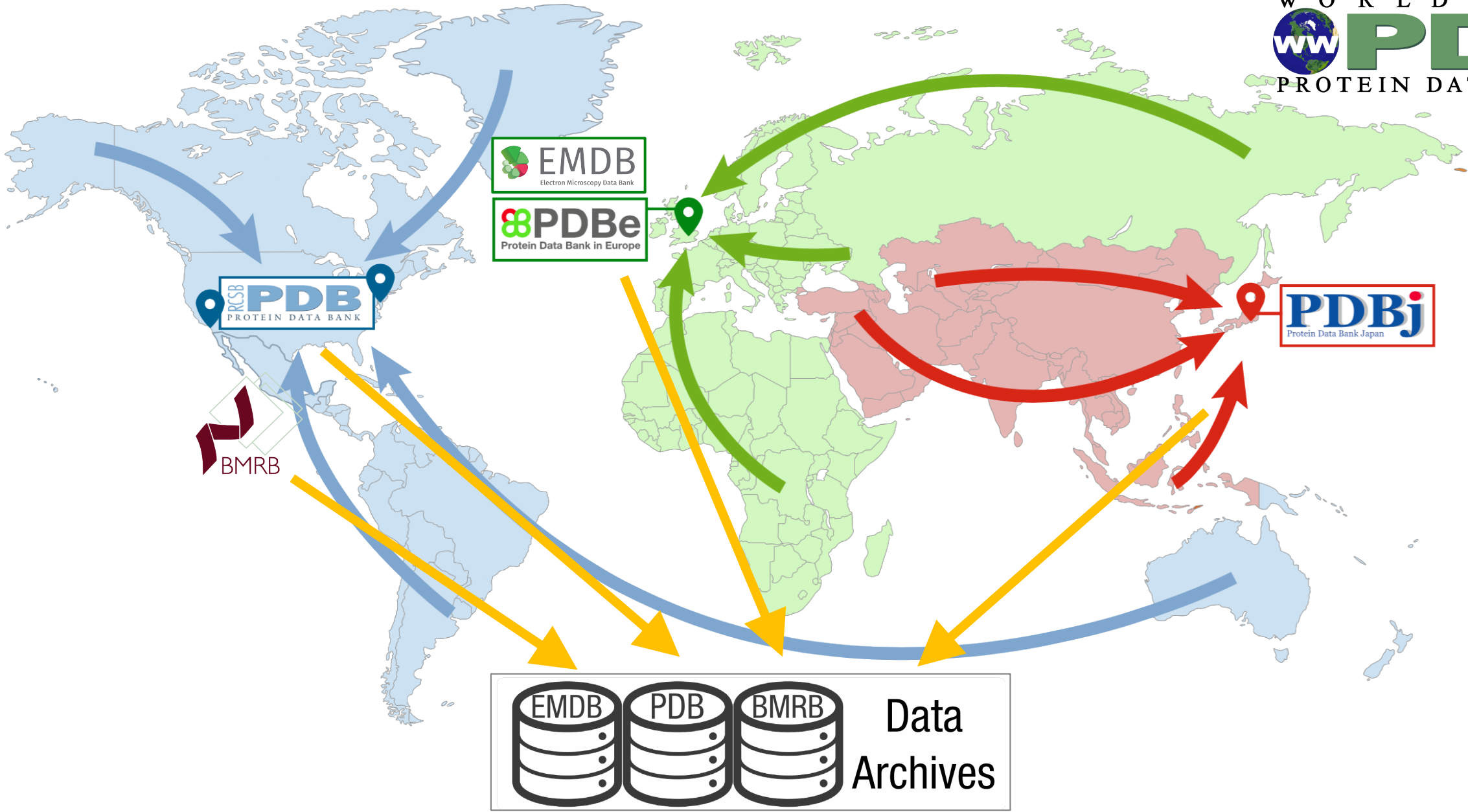
# PDBe API webinar series

- Sep 15th Introduction to PDBe programmatic access
- Sep 22nd Searching with the PDBe API
- Sep 29th Creating complex PDBe API queries
- Oct 6th Using the PDBe graph API**
- Oct 13th PDBe tools in github
- Oct 20th Data visualisation at PDBe

# Summary of the webinar

- Data in PDBe
- PDBe Graph DB
- PDBe Graph API
- Where do we use it?
- Use cases





**EMDB**  
Electron Microscopy Data Bank

**PDBe**  
Protein Data Bank in Europe

**RCSB PDB**  
PROTEIN DATA BANK

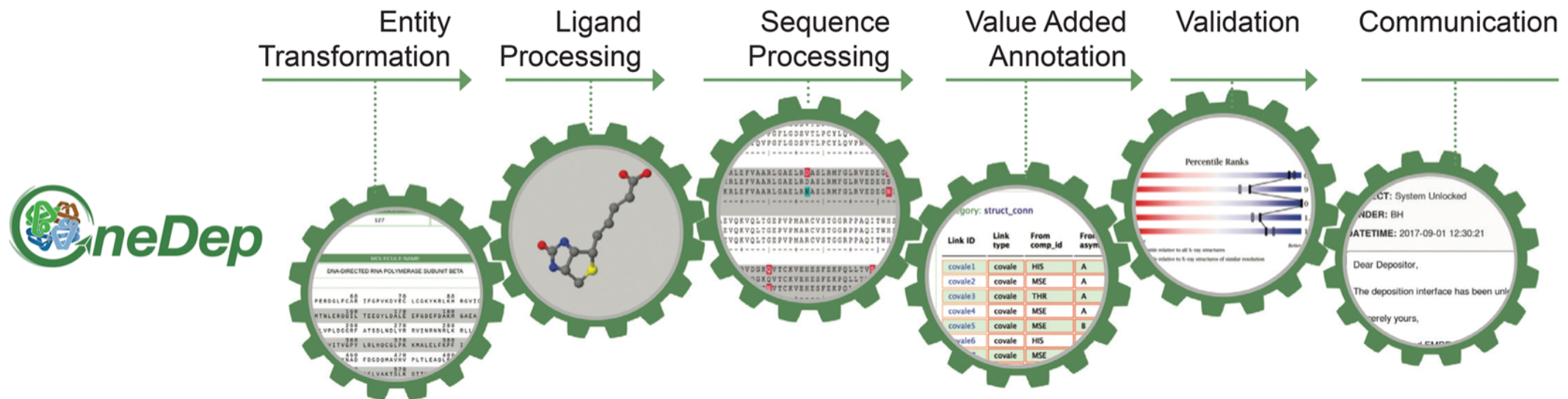
**PDBj**  
Protein Data Bank Japan

**BMRB**

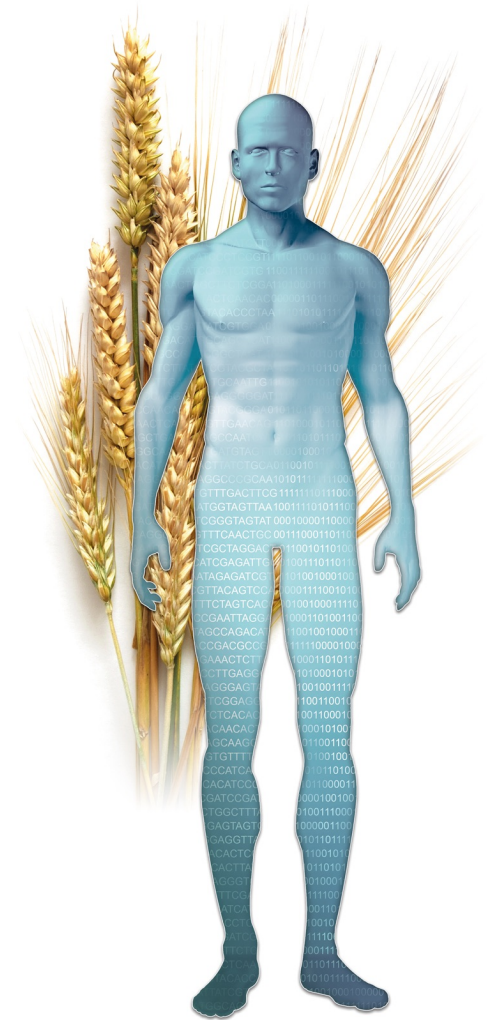
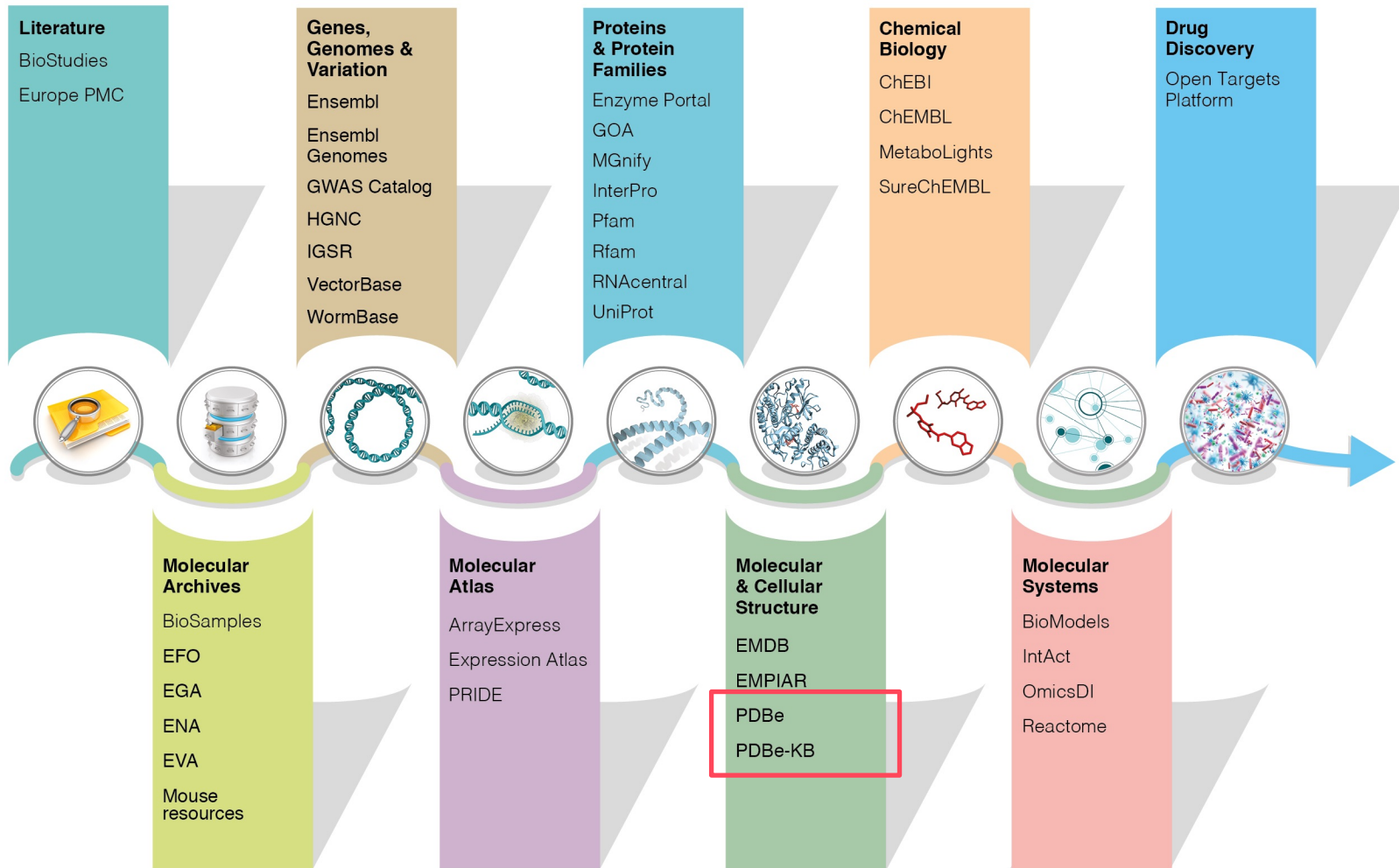
**EMDB** **PDB** **BMRB** **Data Archives**

# Data added through deposition

- Provided by depositor or added during curation
- Data added to define experimental methods, sequence information, connectivity, validation and more...
- Added to the archive mmCIF file or validation XML



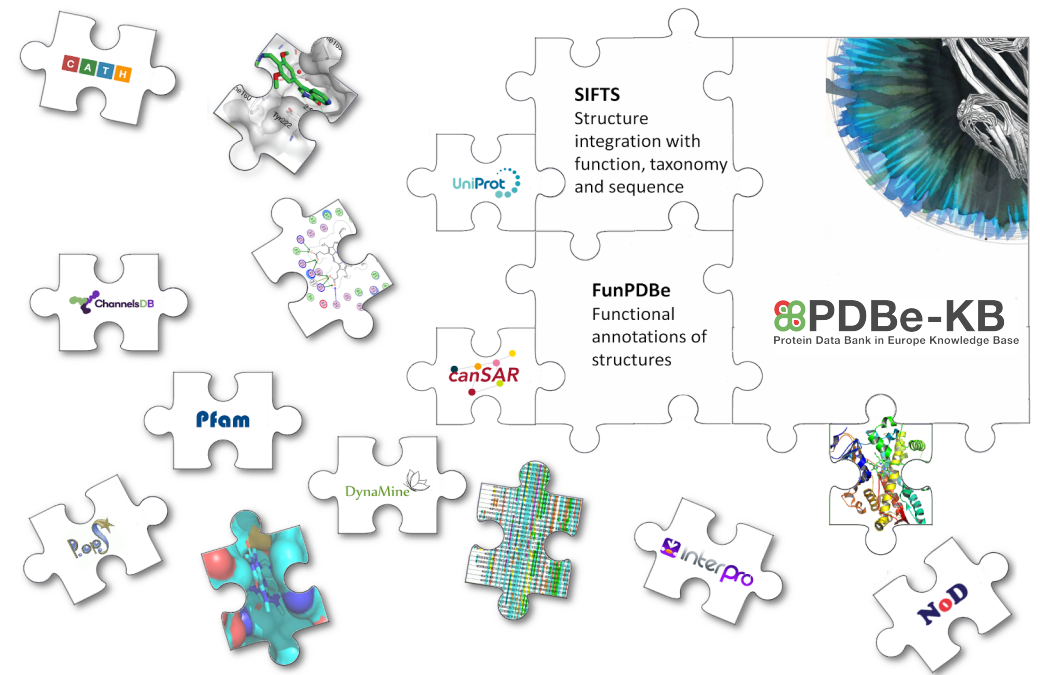
# At the heart of EMBL-EBI resources



# Protein Data Bank in Europe - Knowledge Base (PDBe-KB)

Placing macromolecular structure data in their **biological context** by establishing a **community-driven, integrated resource** for structural annotations to promote basic and applied research

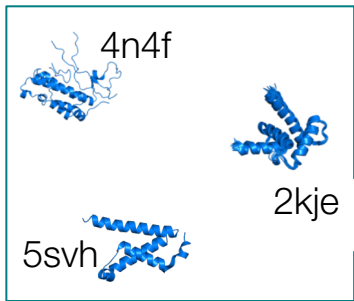
- Data standards
- Data access mechanisms
- Reduce fragmentation



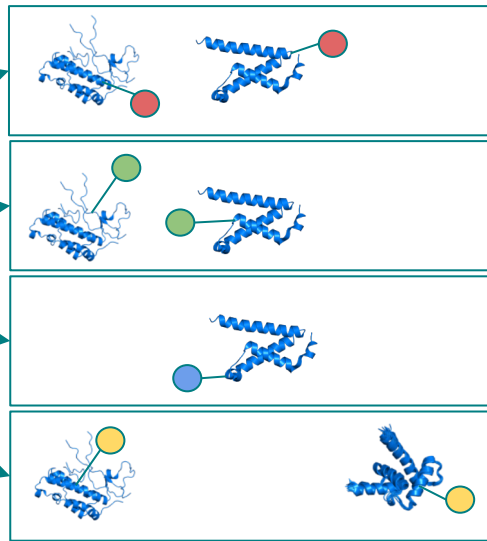
# Data enrichment and integration in PDBe-KB

PDBe-KB integrates structural and functional annotations at residue level to help answer some specific scientific questions

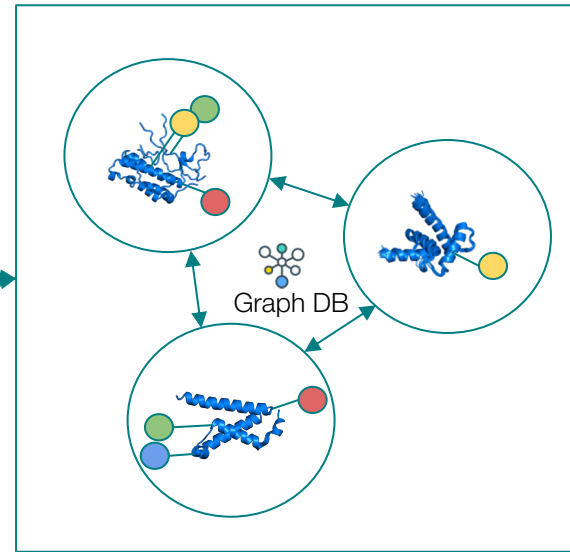
PDB entries



Specialist databases  
annotating PDB entries



Interconnected,  
annotated PDB entries



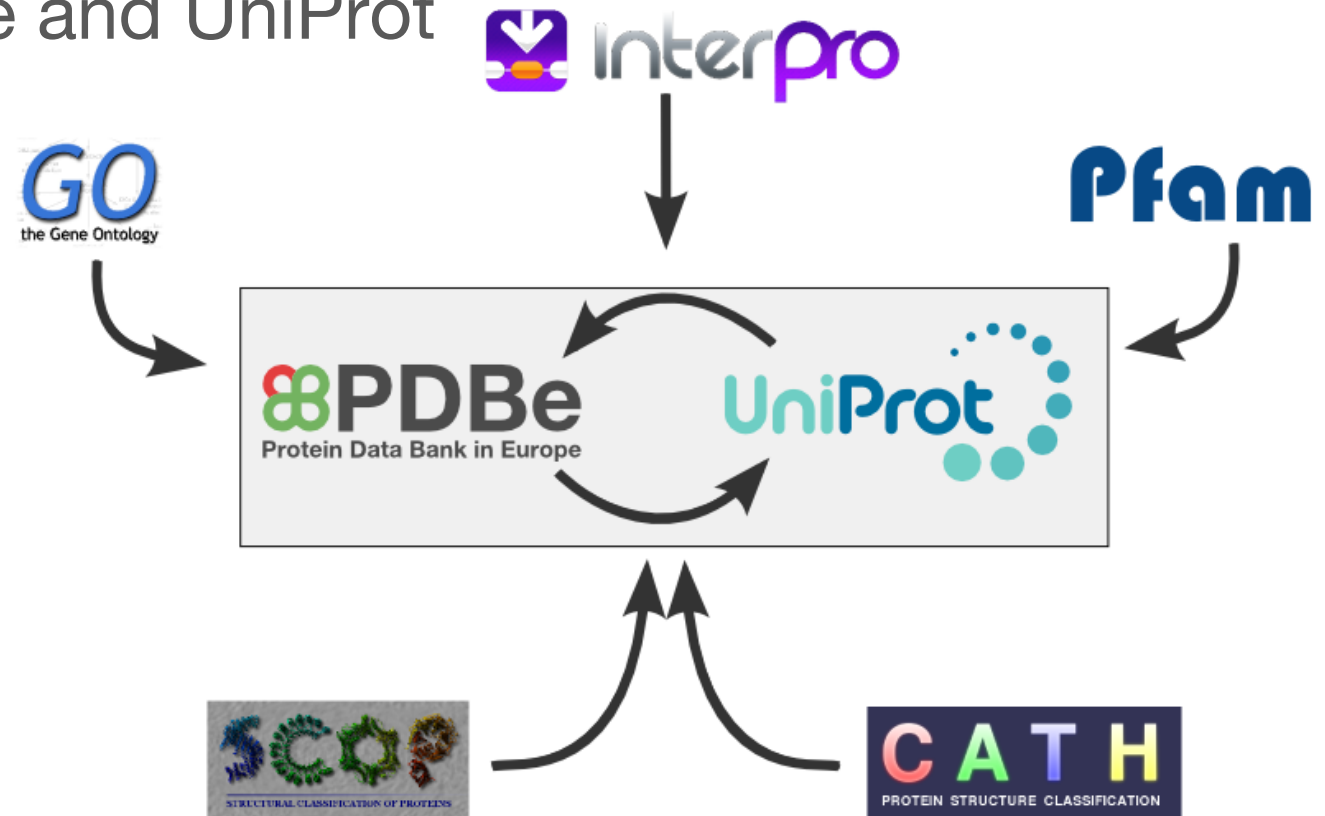
Data is exposed using  
novel, aggregated views

- Domains
- Rfam classification
- Functional sites (e.g. ligand binding)
- Post-translational modifications
- Physico-chemical parameters (residue depth, flexibility, etc.)
- Interacting residues/interfaces

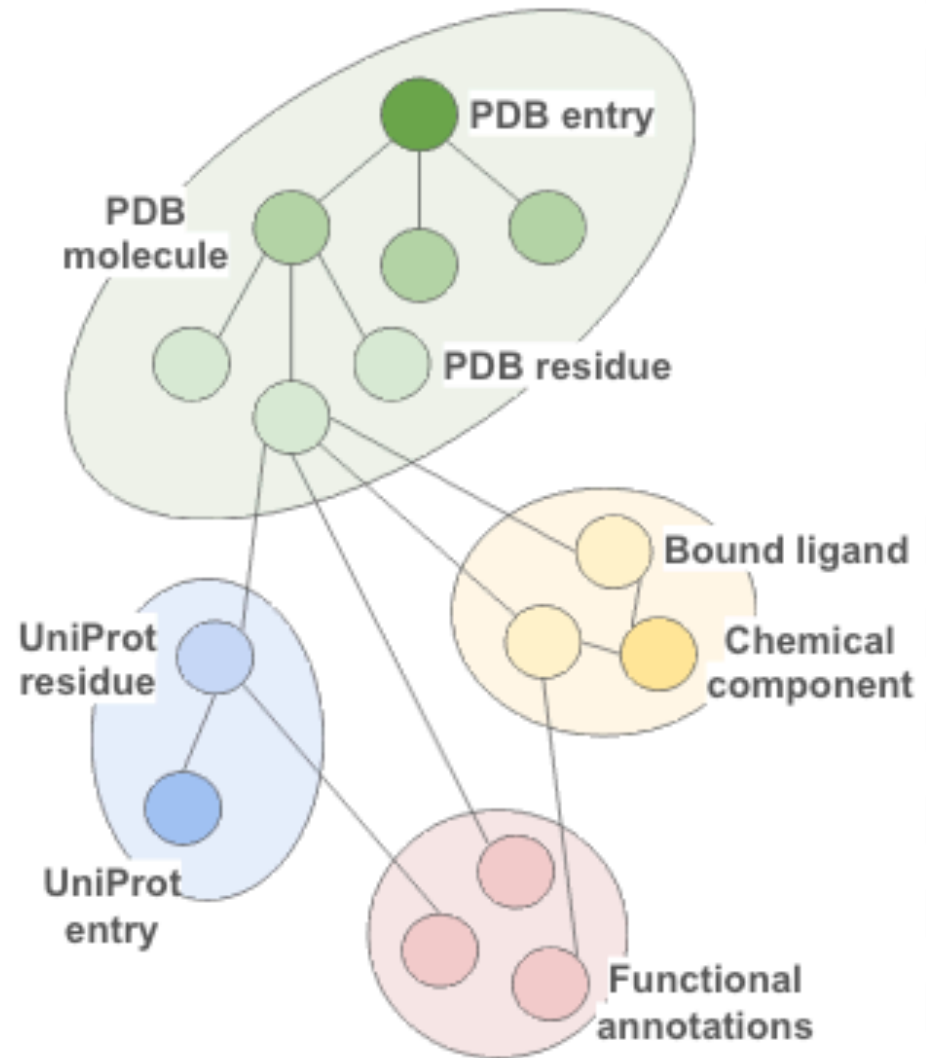
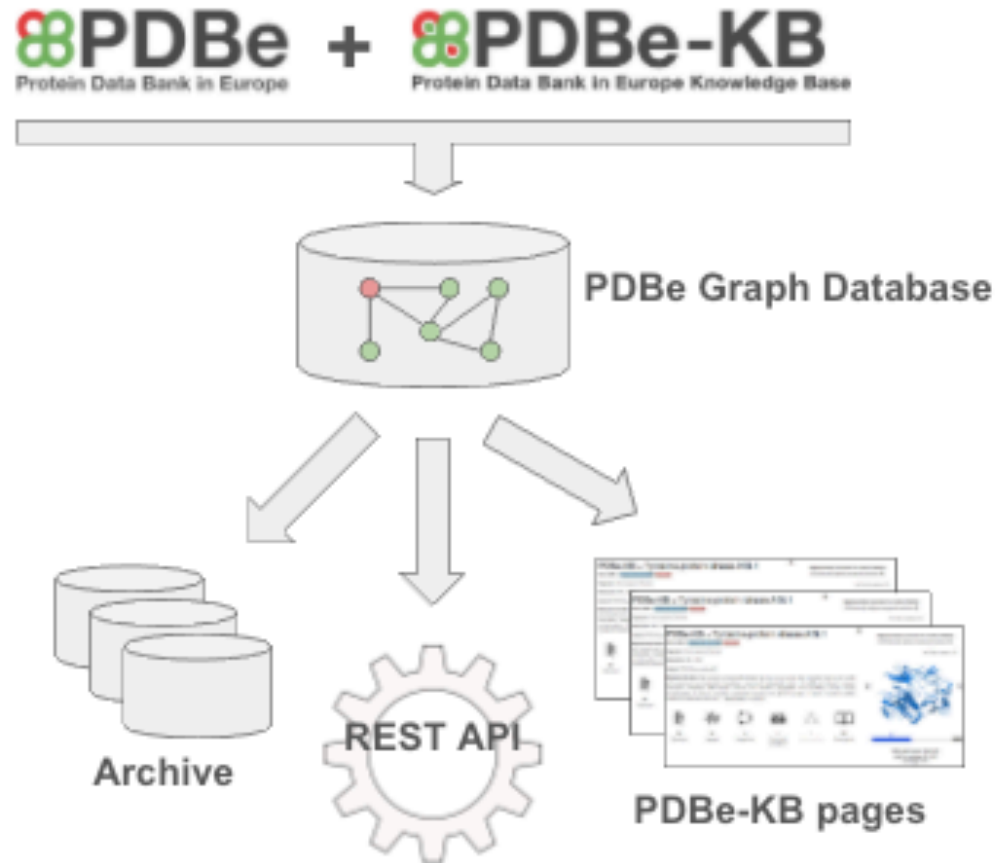


# SIFTS

- Structure Integration with Function, Taxonomy and Sequence
- Collaboration between PDBe and UniProt

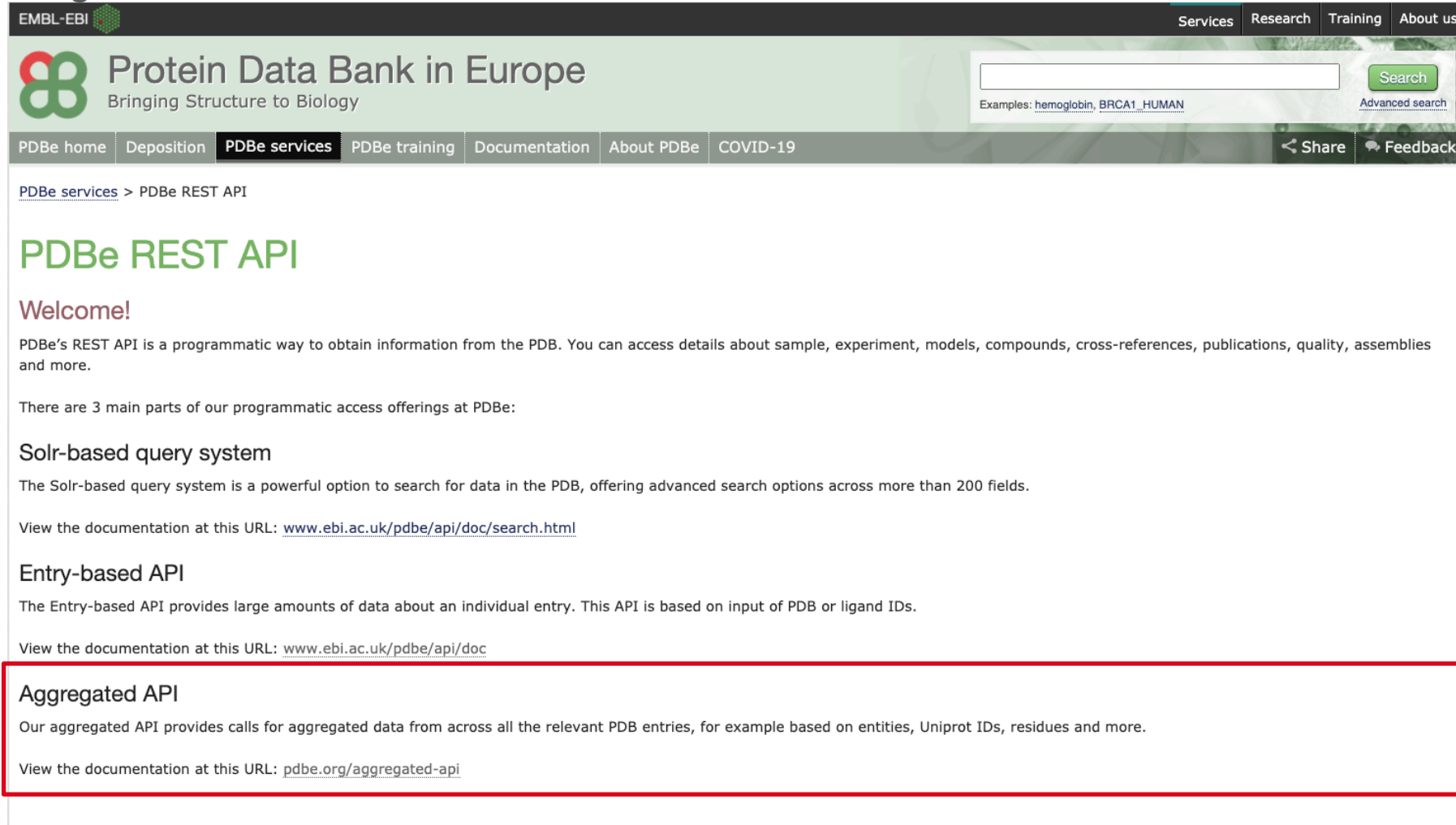


# PDBe Graph Database



# PDBe API


## Programmatic access to PDB data



The screenshot shows the PDBe REST API page. At the top, there is a navigation bar with 'EMBL-EBI' on the left and 'Services', 'Research', 'Training', and 'About us' on the right. Below this is the PDBe logo and the text 'Protein Data Bank in Europe' with the tagline 'Bringing Structure to Biology'. A search bar is present with a 'Search' button and examples: 'hemoglobin, BRCA1\_HUMAN'. Below the search bar is another navigation bar with 'PDBe home', 'Deposition', 'PDBe services' (highlighted), 'PDBe training', 'Documentation', 'About PDBe', and 'COVID-19'. On the right of this bar are 'Share' and 'Feedback' buttons. The main content area starts with a breadcrumb 'PDBe services > PDBe REST API' and a large green heading 'PDBe REST API'. Below this is a 'Welcome!' section followed by a paragraph: 'PDBe's REST API is a programmatic way to obtain information from the PDB. You can access details about sample, experiment, models, compounds, cross-references, publications, quality, assemblies and more.' This is followed by a paragraph: 'There are 3 main parts of our programmatic access offerings at PDBe:'. Then, there are three sections: 'Solr-based query system' with a paragraph and a URL 'www.ebi.ac.uk/pdbe/api/doc/search.html'; 'Entry-based API' with a paragraph and a URL 'www.ebi.ac.uk/pdbe/api/doc'; and 'Aggregated API' with a paragraph and a URL 'pdbe.org/aggregated-api'. The 'Aggregated API' section is highlighted with a red border.

EMBL-EBI

Services Research Training About us

 Protein Data Bank in Europe  
Bringing Structure to Biology

Search  
Examples: [hemoglobin](#), [BRCA1\\_HUMAN](#) [Advanced search](#)

PDBe home Deposition **PDBe services** PDBe training Documentation About PDBe COVID-19 [Share](#) [Feedback](#)

[PDBe services](#) > PDBe REST API

## PDBe REST API

### Welcome!

PDBe's REST API is a programmatic way to obtain information from the PDB. You can access details about sample, experiment, models, compounds, cross-references, publications, quality, assemblies and more.

There are 3 main parts of our programmatic access offerings at PDBe:

### Solr-based query system

The Solr-based query system is a powerful option to search for data in the PDB, offering advanced search options across more than 200 fields.

View the documentation at this URL: [www.ebi.ac.uk/pdbe/api/doc/search.html](http://www.ebi.ac.uk/pdbe/api/doc/search.html)

### Entry-based API

The Entry-based API provides large amounts of data about an individual entry. This API is based on input of PDB or ligand IDs.

View the documentation at this URL: [www.ebi.ac.uk/pdbe/api/doc](http://www.ebi.ac.uk/pdbe/api/doc)

### Aggregated API

Our aggregated API provides calls for aggregated data from across all the relevant PDB entries, for example based on entities, Uniprot IDs, residues and more.

View the documentation at this URL: [pdbe.org/aggregated-api](http://pdbe.org/aggregated-api)



# PDBe Aggregated API

- Also referred as PDBe graph API
- RESTful API
- PDBe Graph DB as backend
- Provides aggregated data across PDB entries
- ~ 80 endpoints
- Currently supports only GET request

# API Documentation

[Home](#) [Protein Aggregated View](#) [PDBe Graph API](#) [PDBe Graph Database](#) [Partners](#) [Guidelines](#)

X

[Get interface residues for an entity](#)

[Get interface residues for a UniProt accession](#)

## UniProt - Get interface residues for a UniProt accession

This call provides details on interface residues for a UniProt accession.

```
https://www.ebi.ac.uk/pdbe/graph-api/uniprot/interface_residues/:accession
```

### Parameter

Field	Type	Description
accession	String	UniProt Accession

### Success 200

Field	Type	Description
sequence	String	Sequence of the entity - available for polymeric entities only. Usually the position, but not if single-letter-code is actually multiple characters - so length field suggests.
length	Integer	Length of entities, available for polymeric entities.
dataType	String	A string denoting the type of data provided in the section.

# API Documentation

[Home](#) [Protein Aggregated View](#) [PDBe Graph API](#) [PDBe Graph Database](#) [Partners](#) [Guidelines](#)

X

Get interface residues for an entity

Get interface residues for a UniProt accession

## UniProt - Get interface residues for a UniProt accession

This call provides details on interface residues for a UniProt accession.

```
https://www.ebi.ac.uk/pdbe/graph-api/uniProt/interface_residues/:accession
```

### Parameter

Field	Type	Description
accession	String	UniProt Accession

### Success 200

Field	Type	Description
sequence	String	Sequence of the entity - available for polymeric entities only. Usually the position, but not if single-letter-code is actually multiple characters - so length field suggests.
length	Integer	Length of entities, available for polymeric entities.
dataType	String	A string denoting the type of data provided in the section.

# API Documentation

The screenshot shows the PDBe API documentation page for the endpoint `https://www.ebi.ac.uk/pdbe/graph-api/uniprot/interface_residues/:accession`. The page includes a navigation bar with links to Home, Protein Aggregated View, PDBe Graph API, PDBe Graph Database, Partners, and Guidelines. A search bar on the left contains the word "interface". The main content area is titled "UniProt - Get interface residues for a UniProt accession" and provides a description of the endpoint. Below the description is a "Send a Sample Request" section with a text input field containing the endpoint URL and a "url" label. The "Parameters" section shows a required parameter "accession" with a text input field containing "P07550" and a "String" label. A "Send" button is located to the right of the input field. The "Response" section shows a JSON response for the accession "P07550", including the protein sequence, length, data type, and interaction interfaces.

**PDBe**  
Protein Data Bank in Europe

Home Protein Aggregated View PDBe Graph API PDBe Graph Database Partners Guidelines

interface

## UniProt - Get interface residues for a UniProt accession

This call provides details on interface residues for a UniProt accession.

`https://www.ebi.ac.uk/pdbe/graph-api/uniprot/interface_residues/:accession`

Send a Sample Request

`https://www.ebi.ac.uk/pdbe/graph-api/uniprot/interface_residues/:accession` url

Parameters

accession  String

Send

Response

```
{
  "P07550": {
    "sequence":
    "MGQPNGS AFL LAPNGSHAPDHDVTQERDEVVVGMGIVMSLIVLAIVFGNVLVITAIKFERLQTVTNVFITSLACADLVMLAVVPPFGAAHILMKMWTFGNFWCEFWTSIDVLCVTASIE TLCVIAVD RYFAITSPFKYQSL LTKNKARV I I
    LMVWIVSGLTSFLPIQMHWRATHQEA INCVANETCCDFFTNQAYAIASSIVSFYVPLVIMVFVYSRVFQEA KRQLQKIDKSEGRFHVQNL SQVEQDGR TGHLRRSSKFCLKEHKAL KTLGIIMGFTFLCWL PFFIVNIVHVIQDNLIRKEYVI
    LLNWIGYVNSGFNPLIYCRSPDFRIAFQELLCLRRSSLKAYGNGYSSNGNTGEQSGYHVEQEKENKLLCEDLPGETDFVGHQGTVPSDNIDSQGRNCSTNDSSL",
    "length": 413,
    "dataType": "INTERACTION INTERFACES",
    "data": [
      {
        "name": "Camelid Antibody Fragment",
        "accession": "IG-heavy chain",
        "residues": [

```

# API Documentation

**PDBe API**

## Compounds

**category**

### Compounds - Get PDB entries that contains the compound

This set of calls returns a list of PDB entries that contain the compound defined in the PDB Chemical Component Dictionary.

```
https://www.ebi.ac.uk/pdbe/graph-api/compound/in_pdb/:hetcode
```

#### Parameter

Field	Type	Description
hetcode	String	Hetcode for the compound

Example success response JSON:

```
{  "ADP": [    "13pk",    "1a6e",    "1a9x",    "1am1",    "1amw",    "1a00",  ]}
```

# API Documentation - Compounds

The screenshot shows the PDBe API documentation page for Compounds. The page has a dark teal header with the PDBe logo and navigation links. A sidebar on the left contains a search filter and a list of API endpoints under 'Compounds' and 'PDB'. The main content area features a title 'PDBe API Compounds' and a sub-title 'Compounds - Get PDB entries that contains the compound'. Below this is a description of the API set and a highlighted URL: `https://www.ebi.ac.uk/pdbe/graph-api/compound/in_pdb/:hetcode`. A 'Parameter' table lists the 'hetcode' parameter as a String. An 'Example success response JSON' is shown in a dark box with green text, displaying a list of ADP codes.

**PDBe**  
Protein Data Bank in Europe

Home Protein Aggregated View PDBe Graph API PDBe Graph Database Partners Guidelines

Filter... X

**Compounds**

- Get PDB entries that contains the compound
- Get atoms for a compound
- Get bonds for a compound
- Get similar hetcodes
- Get similar ligands
- Get substructures for the compound
- Get summary information for the compound
- Get summary of Cofactors

**PDB**

- Get FunPDBe annotations for an entity
- Get FunPDBe resources for a PDB entry
- Get PDB Complex details
- Get Rfam domains for an entity
- Get UniProt mapping for an entity
- Get all FunPDBe annotations for a PDB entry

## PDBe API

### Compounds

#### Compounds - Get PDB entries that contains the compound

This set of calls returns a list of PDB entries that contain the compound defined in the PDB Chemical Component Dictionary.

```
https://www.ebi.ac.uk/pdbe/graph-api/compound/in_pdb/:hetcode
```

**Parameter**

Field	Type	Description
hetcode	String	Hetcode for the compound

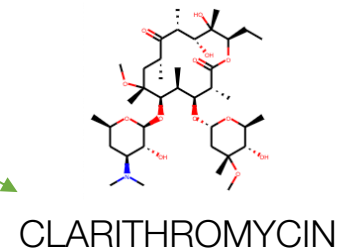
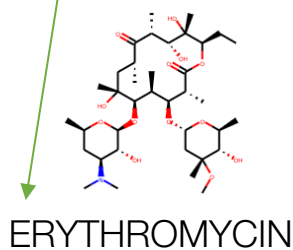
Example success response JSON:

```
{  
  "ADP": [  
    "13pk",  
    "1a6e",  
    "1a9x",  
    "1am1",  
    "1amw",  
    "1a00",  
  ]  
}
```

# API Documentation - Compounds

The screenshot shows the PDBe API interface. At the top left is the PDBe logo (Protein Data Bank in Europe). A navigation bar includes links for Home, Protein Aggregated View, PDBe Graph API, PDBe Graph Database, Partners, and Guidelines. On the left, a sidebar contains a 'Filter...' box and a 'Compounds' menu with options like 'Get PDB entries that contains the compound', 'Get atoms for a compound', 'Get bonds for a compound', 'Get similar hetcodes', 'Get similar ligands', 'Get substructures for the compound', and 'Get summary information for the compound'. The main area is titled 'Send a Sample Request' and contains a URL input field with the value 'https://www.ebi.ac.uk/pdbe/graph-api/compound/similarity/hetcode', a 'Parameters' section with a 'hetcode' field set to 'ERY', and a 'Response' section displaying a JSON object. A green 'Send' button is located to the right of the response area.

```
{  
  "ERY": [  
    {  
      "stereoisomers": [],  
      "same_scaffold": [  
        {  
          "chem_comp_id": "CTY",  
          "name": "CLARITHROMYCIN",  
          "substructure_match": [  
            "04",  
            "1610"  
          ]  
        }  
      ]  
    }  
  ]  
}
```



# API Documentation - PDB

The screenshot shows the PDB API documentation page. At the top left is the PDBe logo (Protein Data Bank in Europe). A navigation bar contains links for Home, Protein Aggregated View, PDBe Graph API, PDBe Graph Database, Partners, and Guidelines. A search filter is present. A sidebar on the left lists various API endpoints under the 'PDB' category. The main content area is titled 'PDB' and 'PDB - Get FunPDBe annotations for an entity'. It includes a description of the endpoint, a highlighted URL: `https://www.ebi.ac.uk/pdbe/graph-api/pdbe_pages/annotations/:pdbId/:entityId`, a 'Parameter' table, a 'Success 200' status, and a 'Field' table. A callout box points to the 'entityId' parameter in the parameter table, listing its associated data types.

**PDB**

**PDB - Get FunPDBe annotations for an entity**

Get FunPDBe annotations for an entity

`https://www.ebi.ac.uk/pdbe/graph-api/pdbe_pages/annotations/:pdbId/:entityId`

**Parameter**

Field	Type	Description
pdbId	String	
entityId	String	

**Success 200**

Field	Type	Description
resourceUrl	String	A URL where details on the resource can be seen.
sequence	String	Sequence of the entity - available for polymeric entities only. Usually there is one character per sequence position, but not if single-letter-code is actually multiple characters - so this string might be longer the length field suggests.
length	Integer	Length of entities, available for polymeric entities.
dataType	String	A string denoting the type of data provided in the section.
data	Object[]	A list of objects which contains the data for the corresponding data type.

**Field**

- Functional annotations from KB partners
- Sequence and structural domains
- Bound ligand interactions
- Macromolecular interactions
- Modified/mutated residues
- Secondary structures
- Sequence conservation etc.



# API Documentation - Residue

The screenshot shows the PDBe API documentation for the Residue endpoint. The page features a dark teal header with the PDBe logo and navigation links. A left sidebar contains a search filter and a list of API endpoints. The main content area displays the title 'Residue', the endpoint description 'Residue - Get FunPDBe annotations for a PDB Residue', and the API URL: `https://www.ebi.ac.uk/pdbe/graph-api/residue_mapping/funpdb_annotation/:pdbId/:entityId/:residueNumber`. Below this is a 'Parameter' table with three columns: Field, Type, and Description. The table lists parameters: `pdbId` (String, PDB Entry ID), `entityId` (String, PDB Entity ID), and `residueNumber` (String, PDB Residue Number). At the bottom, there is a 'Send a Sample Request' section with a text input field containing the same URL and a 'url' button.

**PDBe**  
Protein Data Bank in Europe

Home Protein Aggregated View PDBe Graph API PDBe Graph Database Partners Guidelines

Filter... X

**Residue**

- Get FunPDBe annotations for a PDB Residue
- Get annotations for a PDB Residue range
- Get annotations for a PDB Residue
- Get sequence conservations for a PDB Residue

**SIFTS**

- Get Best Structures for a UniProt accession
- Get Best Structures for a UniProt residue range
- Get CATH mappings for a PDB Entry ID
- Get EC mappings for a PDB Entry ID

## Residue

### Residue - Get FunPDBe annotations for a PDB Residue

Get FunPDBe annotations for a PDB Residue

```
https://www.ebi.ac.uk/pdbe/graph-api/residue_mapping/funpdb_annotation/:pdbId/:entityId/:residueNumber
```

#### Parameter

Field	Type	Description
<code>pdbId</code>	String	PDB Entry ID
<code>entityId</code>	String	PDB Entity ID
<code>residueNumber</code>	String	PDB Residue Number

#### Send a Sample Request

# API Documentation – Residue annotations

The screenshot displays the PDBe website interface. At the top left is the PDBe logo (Protein Data Bank in Europe). A navigation bar contains links for Home, Protein Aggregated View, PDBe Graph API, PDBe Graph Database, Partners, and Guidelines. On the left side, there is a sidebar with a search filter and a list of menu items under 'Residue' and 'SIFTS'. The main content area is titled 'Send a Sample Request' and contains a form with the following fields:

- url:** `https://www.ebi.ac.uk/pdbe/graph-api/residue_mapping/:pdbId/:entityId/:residueStart/:residueEnd`
- Parameters:**
  - url:** `https://www.ebi.ac.uk/pdbe/graph-api/residue_mapping/3unn/1/40/100` (highlighted with a red box)
  - pdBId:** 3unn
  - entityId:** 1
  - residueStart:** 40
  - residueEnd:** 100

A green 'Send' button is located at the bottom right of the form. Below the form, the 'Response' section shows a JSON object:

```
{
  "3unn": [
    {
      "entity_id": 1,
      "chains": [
        {
          "auth_asym_id": "A",
          "struct_asym_id": "A",
          "residues": [
```

# API Documentation – Residue annotations

The screenshot displays the PDBe API documentation for Residue annotations. The page features the PDBe logo and navigation links. A sidebar on the left contains a 'Residue' section with various API endpoints and a 'SIFTS' section. The main content area shows a 'Response' window with a JSON object representing the API response. Green arrows point from labels to specific fields in the JSON:

- Entry** points to the `"3unn": [` field.
- Entity** points to the `"entity_id": 1,` field.
- Chain** points to the `"auth_asym_id": "A",` field.
- Residue** points to the `"residue_number": 40,` field.
- Annotations** points to the `"features": {` field.

```
{
  "3unn": [
    {
      "entity_id": 1,
      "chains": [
        {
          "auth_asym_id": "A",
          "struct_asym_id": "A",
          "residues": [
            {
              "residue_number": 40,
              "author_residue_number": 65,
              "author_insertion_code": "",
              "observed": "Y",
              "features": {
                "UniProt": {
                  "Q14676-3": {
                    "identifier": "MDC1_HUMAN",
                    "name": "MDC1_HUMAN",
                    "unp_residue_number": 65,
                    "unp_one_letter_code": "A",
                    "pdb_one_letter_code": "A"
                  },
                  "Q14676-2": {
```

# API Documentation – Residue annotations

**PDBe**  
Protein Data Bank in Europe

Home Protein Aggregated View PDBe Graph API PDBe Graph Database Partners Guidelines

Filter... x

**Residue**

- Get FunPDBe annotations for a PDB Residue
- Get annotations for a PDB Residue range
- Get annotations for a PDB Residue
- Get sequence conservations for a PDB Residue

**SIFTS**

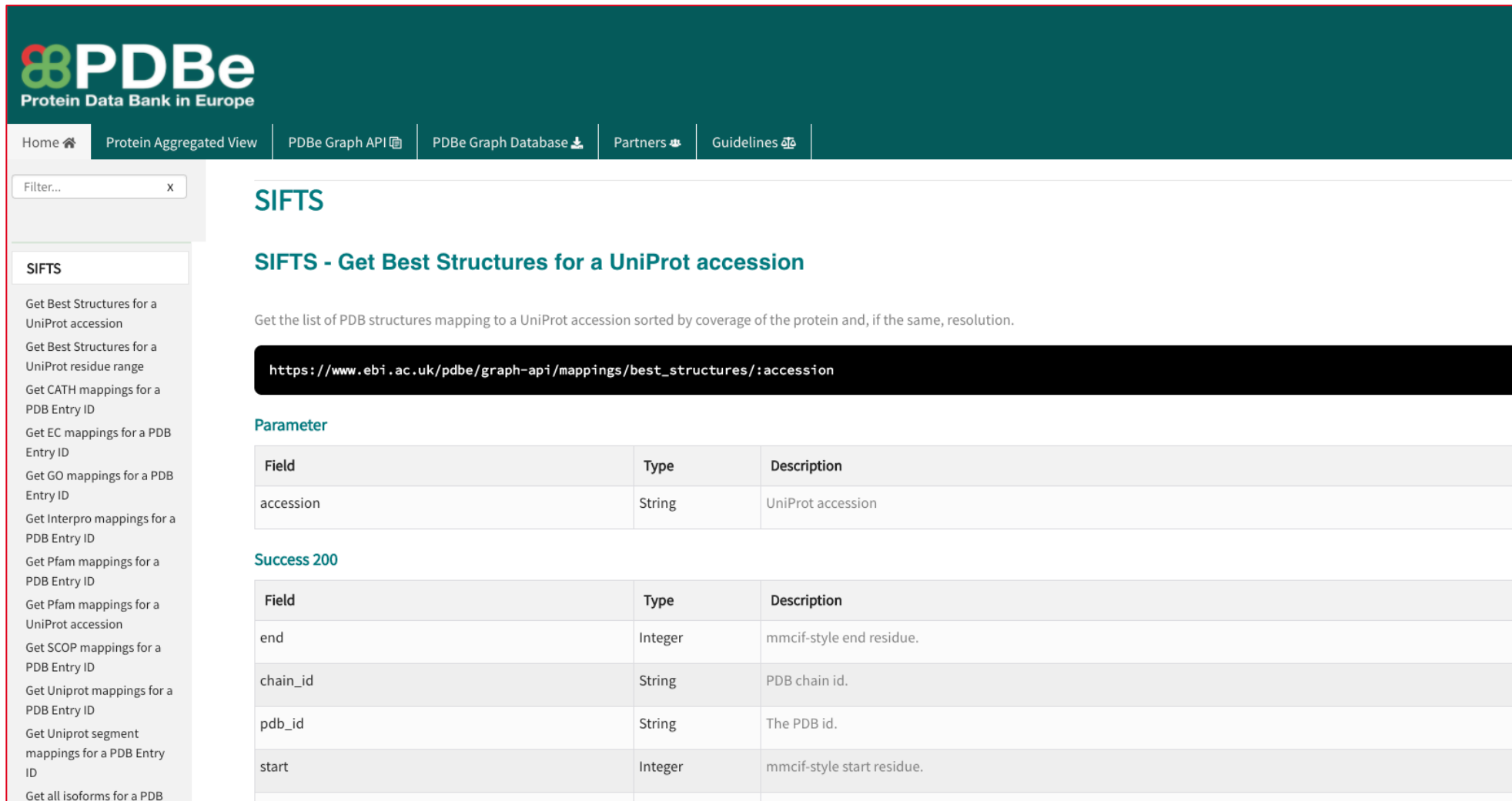
- Get Best Structures for a UniProt accession
- Get Best Structures for a UniProt residue range
- Get CATH mappings for a PDB Entry ID
- Get EC mappings for a PDB

```
"FunPDBe": [
  {
    "origin": "POPScomp_PDBML",
    "label": "total SASA [A^2]",
    "url": "https://github.com/Fraternalilab/POPScomp",
    "raw_score": 22.8527,
    "confidence_score": 0.9,
    "confidence_classification": "high",
    "evidence_codes": [
      "ECO_0000246"
    ]
  },
  {
    "origin": "POPScomp_PDBML",
    "label": "hydrophilic SASA [A^2]",
    "url": "https://github.com/Fraternalilab/POPScomp",
    "raw_score": 15.413,
    "confidence_score": 0.9,
    "confidence_classification": "high",
    "evidence_codes": [
      "ECO_0000246"
    ]
  }
]
```

Annotations from PDBe-KB partners

- Pfam
- InterPro
- CATH
- SCOP

# API Documentation – SIFTS



The screenshot shows the PDBe website interface. At the top left is the PDBe logo (Protein Data Bank in Europe). A navigation bar contains links for Home, Protein Aggregated View, PDBe Graph API, PDBe Graph Database, Partners, and Guidelines. A search filter box is present. A sidebar on the left lists various API endpoints, with 'SIFTS' selected. The main content area is titled 'SIFTS' and 'SIFTS - Get Best Structures for a UniProt accession'. It includes a description: 'Get the list of PDB structures mapping to a UniProt accession sorted by coverage of the protein and, if the same, resolution.' Below this is a code block showing the API endpoint: `https://www.ebi.ac.uk/pdbe/graph-api/mappings/best_structures/:accession`. A 'Parameter' table follows, and a 'Success 200' table shows the response structure.

**PDBe**  
Protein Data Bank in Europe

Home Protein Aggregated View PDBe Graph API PDBe Graph Database Partners Guidelines

Filter... x

**SIFTS**

- Get Best Structures for a UniProt accession
- Get Best Structures for a UniProt residue range
- Get CATH mappings for a PDB Entry ID
- Get EC mappings for a PDB Entry ID
- Get GO mappings for a PDB Entry ID
- Get Interpro mappings for a PDB Entry ID
- Get Pfam mappings for a PDB Entry ID
- Get Pfam mappings for a UniProt accession
- Get SCOP mappings for a PDB Entry ID
- Get Uniprot mappings for a PDB Entry ID
- Get Uniprot segment mappings for a PDB Entry ID
- Get all isoforms for a PDB

## SIFTS

### SIFTS - Get Best Structures for a UniProt accession

Get the list of PDB structures mapping to a UniProt accession sorted by coverage of the protein and, if the same, resolution.

```
https://www.ebi.ac.uk/pdbe/graph-api/mappings/best_structures/:accession
```

**Parameter**

Field	Type	Description
accession	String	UniProt accession

**Success 200**

Field	Type	Description
end	Integer	mmcif-style end residue.
chain_id	String	PDB chain id.
pdb_id	String	The PDB id.
start	Integer	mmcif-style start residue.

# API Documentation – SIFTS

The screenshot displays the PDBe website's API documentation for SIFTS. The page title is "Send a Sample Request". The URL bar shows the endpoint: `https://www.ebi.ac.uk/pdbe/graph-api/mappings/best_structures/:accession`. The "Parameters" section includes an "accession" parameter with the value "P0DTD1". The "Response" section shows a JSON object with the following structure:

```
{
  "P0DTD1": [
    {
      "end": 933,
      "entity_id": 1,
      "chain_id": "A",
      "pdb_id": "7bv2",
      "start": 1,
      "unp_end": 5324,
      "coverage": 0.131,
      "unp_start": 4392,
      "resolution": 2.5,
      "experimental_method": "Electron Microscopy",
      "tax_id": 2697049,
      "preferred_assembly_id": 1
    },
    {
      "end": 932,
      "entity_id": 1,
      "chain_id": "A",
      "pdb_id": "7aap",
      "start": 1,

```

The response is titled "Replicase polyprotein 1ab 2019-nCoV".

# API Documentation – SIFTS

**PDBe**  
Protein Data Bank in Europe

Home [Protein Aggregated View](#) [PDBe Graph API](#) [PDBe Graph Database](#) [Partners](#) [Guidelines](#)

Filter... x

**SIFTS**

- Get Best Structures for a UniProt accession
- Get Best Structures for a UniProt residue range**
- Get CATH mappings for a PDB Entry ID
- Get EC mappings for a PDB Entry ID
- Get GO mappings for a PDB Entry ID
- Get Interpro mappings for a PDB Entry ID
- Get Pfam mappings for a PDB Entry ID
- Get Pfam mappings for a UniProt accession
- Get SCOP mappings for a PDB Entry ID
- Get Uniprot mappings for a

### Send a Sample Request

url:

Parameters

accession:  String

unpStart:  String

unpEnd:  String

Replicase polyprotein 1ab 2019-nCoV

Response

```
{
  "P0DTD1": [
    {
      "end": 40,
      "entity_id": 1,
      "chain_id": "A",
      "pdb_id": "7k3n",
      "start": 30,
      "unp_end": 40,
      "coverage": 1,
      "unp_start": 30,

```

# API Documentation – UniProt

The screenshot shows the PDBe API documentation page for UniProt. The page has a dark green header with the PDBe logo and navigation links: Home, Protein Aggregated View, PDBe Graph API, PDBe Graph Database, Partners, and Guidelines. A sidebar on the left contains a search filter and a list of API endpoints under the 'UniProt' category. The main content area is titled 'UniProt - Get PDB structure mappings for a UniProt accession' and includes a description, an example API URL, a parameter table, and a success 200 response table.

**PDBe**  
Protein Data Bank in Europe

Home Protein Aggregated View PDBe Graph API PDBe Graph Database Partners Guidelines

Filter... x

**UniProt**

- Get PDB structure mappings for a UniProt accession
- Get SIFTS mappings for a UniProt residue
- Get all PDB structures for a UniProt accession
- Get all chain superposition matrices for a UniProt accession
- Get annotations for a UniProt accession
- Get interface residues for a UniProt accession
- Get ligand binding residues for a UniProt accession
- Get list of complexes in which the protein interacts
- Get non-overlapping structures for a UniProt accession
- Get processed protein details for a UniProt accession
- Get secondary structure mappings for a UniProt

## UniProt - Get PDB structure mappings for a UniProt accession

This call provides details on mapped PDB structures for a UniProt accession.

```
https://www.ebi.ac.uk/pdbe/graph-api/uniprot/unipdb/:accession
```

### Parameter

Field	Type	Description
accession	String	UniProt Accession

### Success 200

Field	Type	Description
sequence	String	Sequence of the entity - available for polymeric entities only. Usually there is one character per sequence position, but not if single-letter-code is actually multiple characters - so this string might be longer the length field suggests.
length	Integer	Length of entities, available for polymeric entities.
dataType	String	A string denoting the type of data provided in the section.
data	Object[]	A list of objects which contains the data for the corresponding data type.
name	String	Name of the resource, annotation, etc.
accession	String	A unique identifier for the resource, annotation, etc.



# API Documentation – Validation

The screenshot shows the PDBe API documentation page for Validation. The page has a dark teal header with the PDBe logo and navigation links: Home, Protein Aggregated View, PDBe Graph API, PDBe Graph Database, Partners, and Guidelines. A left sidebar contains a search filter and a list of API endpoints, with 'Validation' selected. The main content area is titled 'Validation' and includes a sub-section 'Validation - Get Entry-wide validation metrics'. Below this, a text block explains that metrics are recommended by the validation task force and provides a URL: `https://www.ebi.ac.uk/pdbe/graph-api/validation/global-percentiles/entry/:pdbId`. Two tables are present: 'Parameter' and 'Success 200'. The 'Parameter' table has one row for 'pdbId' (String, PDB Entry ID). The 'Success 200' table has five rows for different metrics: 'percent-RSRZ-outliers' (Object), 'relative' (Float), 'rawvalue' (Float), 'absolute' (Float), and 'clashscore' (Object).

**PDBe**  
Protein Data Bank in Europe

Home Protein Aggregated View PDBe Graph API PDBe Graph Database Partners Guidelines

Filter... x

conservations for a UniProt accession  
Get similar proteins for a UniProt accession for a given sequence identity  
Get superposition details for a UniProt accession

**Validation**

Get Entry-wide validation metrics  
Get Ramachandran status for a PDB Entry ID  
Get SIFTS backbone and sidechain outliers for a PDB Entry ID  
Get Suite and pucker outliers in RNA chains  
Get X-Ray refine data stats  
Get a list of outlier types found in residues  
Get key validation stats  
Get residues with geometric outliers in protein, DNA, RNA chains  
Get summary of global absolute percentiles

## Validation

### Validation - Get Entry-wide validation metrics

Metrics here are the ones recommended by validation task force. Global is against whole PDB archive and relative is against entries of comparable resolution.

```
https://www.ebi.ac.uk/pdbe/graph-api/validation/global-percentiles/entry/:pdbId
```

#### Parameter

Field	Type	Description
pdbId	String	PDB Entry ID

#### Success 200

Field	Type	Description
percent-RSRZ-outliers	Object	Percentile based on percent RSRZ outliers (calculated on standard amino acid residues or nucleotides in protein, DNA, RNA chains).
relative	Float	This percentile is based on entries in the PDB archive that are comparable to the entry, e.g. similar resolution for X-ray entries.
rawvalue	Float	The raw value of the metric.
absolute	Float	This percentile is based on all possible entries in the PDB archive.
clashscore	Object	Percentile based on clash score calculated by Molprobit component of the wwPDB validation pipeline.

# Where do we use it?

## Aggregated views of proteins

EMBL-EBI Services Research Training About us

**PDBe-KB**  
Protein Data Bank in Europe Knowledge Base

Home Aggregated Views of Proteins PDBe Graph API PDBe Graph Database Partners Guidelines Contact Feedback

### What are the Aggregated Views of Proteins?

Structures Small-molecules Macromolecular Interactions Functional Annotations

The PDBe-KB aggregated view of proteins provides a comprehensive overview of structural data available in PDB for a full-length protein sequence. Either PDB or UniProt identifiers can be used to display all the available data, and in particular all the PDB entries related to the protein sequence, all the observed small-molecules interacting with the protein, all the macromolecular interaction sites and partners, and additional functional annotations, such as sequence conservation and druggable sites. [Learn more about PDBe-KB...](#)

Explore PDBe-KB Aggregated Views of Proteins

Search by PDB accession or UniProt accession...

Examples: [2etx](#) [Q14676](#)

### Latest updates

- Added functionality to view superposed structure clusters of a protein
- Added functionality to view all the ligands superposed for a protein
- Added annotations for peptides and antibodies

26/08/2020

# Aggregated views of proteins

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Ex. - hemoglobin, BRCA1\_HUMAN

**PDBe-KB**  
Protein Data Bank in Europe Knowledge Base

Summary Structures (103) Ligands (91) Interactions (12) Functional annotations (4) Similar proteins (2) Publications (72)

## PDBe-KB > CREB-binding protein

Gene: CREBBP Enzyme: EC 2.3.1.48 Disease

Organism: *Homo sapiens* (Human)

Synonyms: CBP

Uniprot: Q92793 [go to UniProt]

**Biological function:** Acetylates histones, giving a specific tag for transcriptional activation (PubMed:24616510). Also acetylates non-histone proteins, like DDX21, FBL, IRF2, MAFG, NCOA3, POLR1E/PAF53 and FOXO1 (PubMed:10490106, PubMed:11154691, PubMed:12738767, PubMed:12929931, PubMed:9707565, PubMed:24207024, PubMed:28790157, PubMed:30540930). Binds specifically to phosphorylated CREB and enhances its transcriptional activity toward ... [show more] [go to UniProt]

103 Structures  
Download View structure clusters

91 Ligands  
Download View all ligands

12 Interactions  
Download

4 Functional annotations

2 Similar proteins  
Download

72 Publications

Representative structures for UniProt Q92793  
PDB chains with highest data quality, coverage and best resolution  
Click to view in 3D

PDB chain shown: 4nr7 A  
UniProt residues 1081 - 1197  
Coverage: 5%  
View structure clusters for segment 3

What structural data available for my protein?

How many ligands known to bind to this protein?

CREB-binding protein, structures available in PDB

# Representative structures

## UniProt - Get non-overlapping best structures for a UniProt accession

This call provides details on non-overlapping PDB chains with the highest number of observed residues for the UniProt accession.

```
https://www.ebi.ac.uk/pdbe/graph-api/uniprot/best_non_overlapping_structures/:accession
```

### Parameters

accession

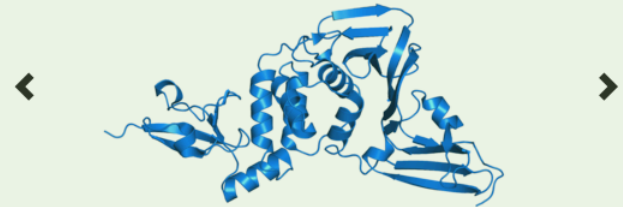
### Response

```
{
  "P0DTD1": [
    {
      "experimental_method": "X-ray diffraction",
      "tax_id": 2697049,
      "resolution": 1.66,
      "pdb_id": "6wx4",
      "chain_id": "A",
      "entity_id": 1,
      "preferred_assembly_id": 1,
      "observed_regions": [
        {

```

Representative structures for UniProt P0DTD1  
PDB chains with highest data quality, coverage and best resolution ⓘ

👁️ Click to view in 3D



PDB chain shown: 6wx4 A [🔗](#)

UniProt residues 1562 - 1879

Coverage: 4%

[View structure clusters for segment 3](#) 👁️

# Interface residues

**PDBe-KB**  
Protein Data Bank in Europe Knowledge Base

Ex. - hemoglobin, BRCA1\_HUMAN

Summary | Structures (419) | Ligands (303) | **Interactions (48)** | Functional annotations (3) | Similar proteins (35) | Publications (2756) | Feedback

## PDBe-KB > Prothrombin

Gene: F2 [Enzyme: EC 3.4.21.5](#) [Disease](#)

Organism: *Homo sapiens (Human)*

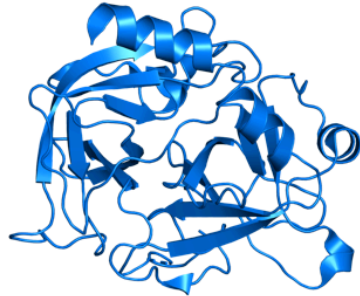
Uniprot: P00734 [\[go to UniProt\]](#)

**Biological function:** Thrombin, which cleaves bonds after Arg and Lys, converts fibrinogen to fibrin and activates factors V, VII, VIII, XIII, and, in complex with thrombomodulin, protein C. Functions in blood homeostasis, inflammation and wound healing [\[go to UniProt\]](#)

What's new?

Representative structures for UniProt P00734  
PDB chains with highest data quality, coverage and best resolution

Click to view in 3D



419 Structures | 303 Ligands | **48 Interactions** | 3 Functional annotations | 35 Similar proteins | 2756 Publications

Download | Download | Download | Download

View structure clusters | View all ligands

**Processed Proteins (2):**

Protein Name	Representative Structures <small>Click on a box for 3D view</small>	Available Structural Data	Navigate
Thrombin light chain		393 Structures, 230 Ligands, 3 Interactions	<a href="#">View Page</a>
Thrombin heavy chain		411 Structures, 241 Ligands, 47 Interactions	<a href="#">View Page</a>

PDB chain shown: 4ud9 A  
UniProt residues 364 - 622  
Coverage: 41%

[View structure clusters for segment 1](#)

Thrombin (pdbe-kb.org/protein/P00734)

# Interface residues

Summary Structures (419) Ligands (303) Interactions (48) Functional annotations (3) Similar proteins (35) Publications (2756) Feedback

## Interface Residues

The sequence viewer below shows residues that are directly interacting with macromolecular interaction partners.

Select File Format: CSV  JSON  [Download](#)

Select a file format and press "Download" to get the data displayed below.

Interaction interfaces

- Prothrombin (self) (P00734)
- Hirudin variant-1 (P01050)
- Proteinase-activated receptor 1 (P25116)
- Other

Domains : Pfam domains CATH domains InterPro annotations

# Interface residues

The screenshot shows the PDBe website interface. At the top left is the PDBe logo (Protein Data Bank in Europe). A navigation bar contains links for Home, Protein Aggregated View, PDBe Graph API, PDBe Graph Database, Partners, and Guidelines. On the left side, there is a sidebar with a search filter and a list of API endpoints. The selected endpoint is "Get interface residues for a UniProt accession". The main content area displays the title "UniProt - Get interface residues for a UniProt accession", a brief description, the API URL in a black box, a parameter table, and a success response table.

**UniProt - Get interface residues for a UniProt accession**

This call provides details on interface residues for a UniProt accession.

```
https://www.ebi.ac.uk/pdbe/graph-api/uniProt/interface_residues/:accession
```

**Parameter**

Field	Type	Description
accession	String	UniProt Accession

**Success 200**

Field	Type	Description
sequence	String	Sequence of the entity - available for polymeric entities only. Usually there is one character per sequence position, but not if single-letter-code is actually multiple characters - so this string might be longer the length field suggests.
length	Integer	Length of entities, available for polymeric entities.
dataType	String	A string denoting the type of data provided in the section.
data	Object[]	A list of objects which contains the data for the corresponding data type.
name	String	Name of the resource, annotation, etc.

# Interface residues

**PDBe**  
Protein Data Bank in Europe

Home Protein Aggregated View PDBe Graph API PDBe Graph Database Partners Guidelines

Filter... x

matrices for a uniprot accession  
Get annotations for a UniProt accession  
Get interface residues for a UniProt accession  
Get ligand binding residues for a UniProt accession  
Get list of complexes in which the protein interacts  
Get non-overlapping structures for a UniProt accession  
Get processed protein details for a UniProt accession  
Get secondary structure mappings for a UniProt accession  
Get sequence and structural domains for a UniProt accession  
Get sequence conservations for a UniProt Residue  
Get sequence conservations for a UniProt accession  
Get similar proteins for a UniProt accession

### Send a Sample Request

url:

Parameters

accession:  String

Send

### Response

```
{
  "P00734": {
    "sequence":
    "MAHVRGLQLPGCLALAAALCSLVHSQHVFLAPQARSLLRVRRANTFLEEVRKGNLERECVEETCSYEEAFELESSTATDVFMAKYTACETARTPRDKLAACLEGNCAEGLGTNYRGHVNITRSGIECQLWRSRYPHKPEINSTTHPGADLQENFCRNPDSSTTGPWC
    YTTDPTVRRQECIPVGGQDQVTAMTPRSEGSSVNLSPLEQCVDRGQQYQGR LAVTTHTGLPCLAWASQAQAKALSKHQDFNSAVQLVENFCRNPDDGDEGVWCYVAGKPGDFGYCDLNYCEEAVEEETGDGLDESDRAIEGRTATSEYQTFNPRTFGSGEADCGLR
    PLFEKKSLEDKTERELLESYIDGRIVEGSDAEIGMSPQWMLFRKSPQELLGGASLISDRWVLTAAHCLLYPPWDKNFTENDLLVRIGKHSRTRYERNIEKISMLEKIYIHPRYNWRNLDRIALMKLKKPVAFSDYIHPVCLPDRETAASLLQAGYKGRVTGWGNLKE
    TWTANVGKGPVSVLQVNLPIVERPVCKDSTRITRITDNMFCAGYKPEGKRGDACEGDSGGPFVMKSPFNRRWYQMGIVSWGEGCDRDGKYGFYTHVFRLLKKWIQKVIDQFGE",
    "length": 622,
    "dataType": "INTERACTION INTERFACES",
    "data": [
      {
        "name": "Prothrombin",
        "accession": "P00734",
        "residues": [
          {
            "startIndex": 230,
            "endIndex": 230,
            "startCode": "HIS",
            "endCode": "HIS",
            "indexType": "UNIPROT",
            "interactingPDBEntries": [
              {
                "pdbId": "6px5",
                "entityId": 2,
                "chainIds": "B"
              }
            ]
          }
        ]
      }
    ]
  }
}
```



# Ligand binding residues

**PDBe-KB**  
Protein Data Bank in Europe Knowledge Base

Ex. - hemoglobin, BRCA1\_HUMAN

Summary | Structures (419) | **Ligands (303)** | Interactions (48) | Functional annotations (3) | Similar proteins (35) | Publications (2756) | Feedback

## PDBe-KB > Prothrombin

Gene: F2 [Enzyme: EC 3.4.21.5](#) [Disease](#)

Organism: *Homo sapiens (Human)*

Uniprot: P00734 [\[go to UniProt\]](#)

**Biological function:** Thrombin, which cleaves bonds after Arg and Lys, converts fibrinogen to fibrin and activates factors V, VII, VIII, XIII, and, in complex with thrombomodulin, protein C. Functions in blood homeostasis, inflammation and wound healing [\[go to UniProt\]](#)

419 Structures | **303 Ligands** | 48 Interactions | 3 Functional annotations | 35 Similar proteins | 2756 Publications

Download | Download | Download | Download

View structure clusters | View all ligands

**Processed Proteins (2):**

Protein Name	Representative Structures <small>Click on a box for 3D view</small>	Available Structural Data			Navigate
Thrombin light chain		393	230	3	<a href="#">View Page</a>
Thrombin heavy chain		411	241	47	<a href="#">View Page</a>

Representative structures for UniProt P00734  
PDB chains with highest data quality, coverage and best resolution

Click to view in 3D

PDB chain shown: 4ud9 A  
UniProt residues 364 - 622  
Coverage: 41%

[View structure clusters for segment 1](#)

Thrombin (pdbe-kb.org/protein/P00734)

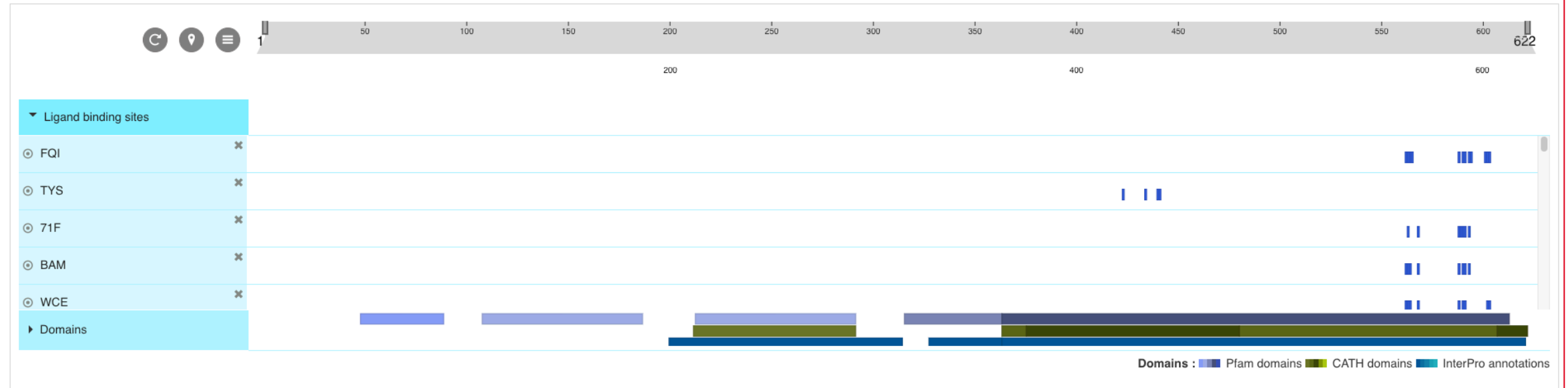
# Ligand binding residues

## Ligand Binding Residues

The sequence viewer below shows residues that are directly interacting with small molecules, when this data is available.

Select File Format:  CSV  JSON  [Download](#) 

 Select a file format and press "Download" to get the data displayed below.



# Ligand binding residues

The screenshot shows the PDBE website interface. At the top left is the PDBE logo (Protein Data Bank in Europe). A navigation bar contains links for Home, Protein Aggregated View, PDBE Graph API, PDBE Graph Database, Partners, and Guidelines. A sidebar on the left lists various API endpoints, with 'Get ligand binding residues for a UniProt accession' highlighted in green. The main content area is titled 'UniProt - Get ligand binding residues for a UniProt accession'. It includes a description: 'This call provides details on ligand binding residues for a UniProt accession.' Below this is a black box containing the API endpoint: `https://www.ebi.ac.uk/pdbe/graph-api/uniprot/ligand_sites/:accession`. There are two tables: one for 'Parameter' and one for 'Success 200'. Both tables have columns for Field, Type, and Description.

**UniProt - Get ligand binding residues for a UniProt accession**

This call provides details on ligand binding residues for a UniProt accession.

```
https://www.ebi.ac.uk/pdbe/graph-api/uniprot/ligand_sites/:accession
```

**Parameter**

Field	Type	Description
accession	String	UniProt Accession

**Success 200**

Field	Type	Description
sequence	String	Sequence of the entity - available for polymeric entities only. Usually there is one character per sequence position, but not if single-letter-code is actually multiple characters - so this string might be longer the length field suggests.
length	Integer	Length of entities, available for polymeric entities.
dataType	String	A string denoting the type of data provided in the section.
data	Object[]	A list of objects which contains the data for the corresponding data type.
name	String	Name of the resource, annotation, etc.

# Ligand binding residues

**PDBe**  
Protein Data Bank in Europe

Home Protein Aggregated View PDBe Graph API PDBe Graph Database Partners Guidelines

Filter... x

Get all chain superposition matrices for a UniProt accession  
Get annotations for a UniProt accession  
Get interface residues for a UniProt accession  
**Get ligand binding residues for a UniProt accession**  
Get list of complexes in which the protein interacts  
Get non-overlapping structures for a UniProt accession  
Get processed protein details for a UniProt accession  
Get secondary structure mappings for a UniProt accession  
Get sequence and structural domains for a UniProt accession  
Get sequence conservations for a UniProt Residue  
Get sequence conservations for a UniProt accession

### Send a Sample Request

url:

Parameters

accession:  String

Send

### Response

```
{
  "P00734": {
    "sequence":
    "MAHVRGLQLPGCLLAAALCSLVHSQHVFLAPQQRASLLQRVRRANTFLEEVRKGNLERECVEETCSYEEAFEALLESSTADTVFWAKYACETARTPRDKLAACLEGNCAEGLTNYRGHVNIITRSGIECQLWRSRYPHKPEINSTTHPGADLQENFCRNPDSSTTGPWC
    YTTDPTVRRQECVIPVCGDQVTVAMTPRSEGSVNLSPPLEQCVPDRGQYQGR LAVTTHTGLPCLAWASQAQAKLSKHQDFNSAVQLVFNFCRNPDGDEEGWCVYAGKPGDFGYCDLNYCEEAVEEETGDGLDESDRAIEGRATSEVQTF FNPRTFGSGEADCGLR
    PLFEKKSLEDKTERELLESYIDGRIVEGSDAEIGMSPWQVMLFRKSPQELLCCGASLISDRVWLTAACHLLYPPWDKNTENDLVRIGKHSRTRYERNIEKISMLEKIYIHPRYNWRNLRDIALMMLKKPVAFSDYIHPVCLPDRETAASLLQAGYKGRVTGWGNLKE
    TWTANVGKQPSVLQVNLPIVERPVCKDSTRITDNMFCAGYKPDGKRGDACEGDSGGPFVMSPFNRRWYQMGIVSWGEGCDRDGKYGFYTHVFLRKKWIQKVIDQFGE",
    "length": 622,
    "dataType": "LIGAND BINDING SITES",
    "data": [
      {
        "name": "5-CHLORO-2-THIOPHENECARBOXAMIDE",
        "accession": "FQI",
        "residues": [
          {
            "startIndex": 562,
            "endIndex": 562,
            "startCode": "ASP",
            "endCode": "ASP",
            "indexType": "UNIPROT",
            "interactingPDBEntries": [
              {
                "pdbId": "4ud9",
                "entityId": 1,
                "chainIds": "H"
              }
            ]
          }
        ]
      }
    ]
  }
}
```

# What can I learn about protein-protein interactions from the available structure data?



- Some residues are involved in ligand binding and macromolecular interactions
- Some of these ligands and proteins are known inhibitors

High-affinity receptor-binding region 551-573

# Ligand environment

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**Protein Data Bank in Europe**  
Bringing Structure to Biology

Search  [Advanced search](#)

Examples: [hemoglobin](#), [BRCA1\\_HUMAN](#)

[Feedback](#)

## PDBe > 4r7i



**Crystal structure of FMS kinase domain with a small molecular inhibitor, GLEEVEC**  
**Source organism:** *Homo sapiens*

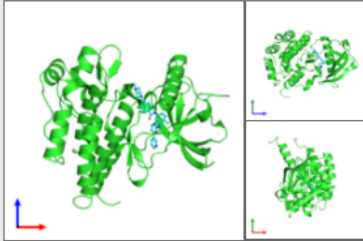
**Primary publication:**  
[Structure-Guided Blockade of CSF1R Kinase in Tenosynovial Giant-Cell Tumor.](#)

Tap WD, Wainberg ZA, Anthony SP, Ibrahim PN, Zhang C, Healey JH, Chmielowski B, Staddon AP, Cohn AL, Shapiro GI, Keedy VL, Singh AS, Puzanov I, Kwak EL, Wagner AJ, Von Hoff DD, Weiss GJ, Ramanathan RK, Zhang J, Habets G, Zhang Y, Burton EA, Visor G, Sanftner L, Severson P, Nguyen H, Kim MJ, Marimuthu A, Tsang G, Shellooe R, Gee C, West BL, Hirth P, Nolop K, van de Rijn M, Hsu HH, Peterfy C, Lin PS, Tong-Starksen S, Bollag G  
*N. Engl. J. Med.* **373** 428-37 (2015)  
PMID: 26222558

**X-ray diffraction**  
**2.75Å resolution**

**Released:** 12 Aug 2015  
**DOI:** [10.2210/pdb4r7i/pdb](https://doi.org/10.2210/pdb4r7i/pdb)

Model geometry   
Fit model/data 



**Quick links**

- 4r7i overview**
- Citations
- Structure analysis
- Function and Biology
- Ligands and Environments
- Experiments and Validation

View  
Downloads  
3D Visualisation

**Function and Biology** [Details](#)

**Reaction catalysed:**

ATP + a [protein]-L-tyrosine = ADP + a [protein]-L-tyrosine phosphate

**Biochemical function:**

- ATP binding

**Biological process:**

- transmembrane receptor protein tyrosine kinase signaling pathway

**Cellular component:**

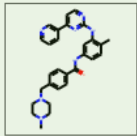
- not assigned

**Sequence domains:**

- Serine-threonine/tyrosine-protein kinase, catalytic domain

**Ligands and Environments**

**1 bound ligand:**



1 x STI

**No modified residues**

**Experiments and Validation** [Details](#)

**Citations**


**39 review citations**

[Harnessing tumor-associated macrophages as aids for cancer immunotherapy.](#)  
Li et al. (2019)

[38 more](#)

**PDB-REDO**

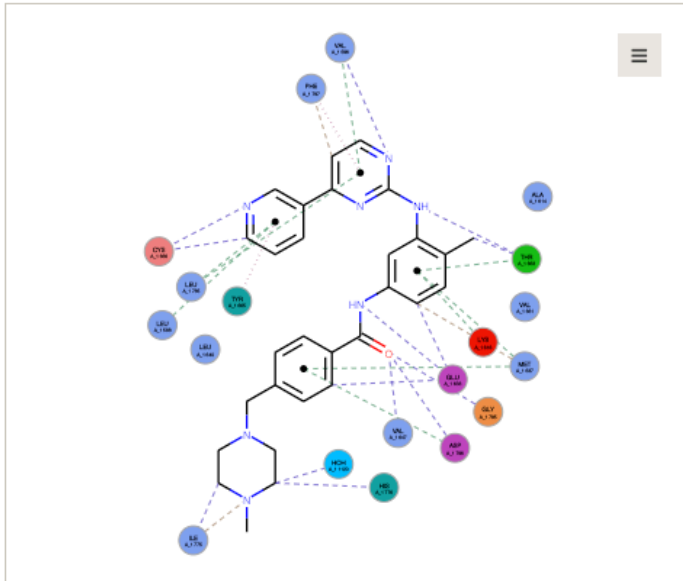
The sliders below show the change in model quality between original PDB entry and the PDB-REDO entry

Model Geometry 

FMS Kinase domain with Gleevec (PDB 4r7i)

# Ligand environment

STI 1001 bound to chain A\_1



<https://www.ebi.ac.uk/pdbe/entry/pdb/4r7i/bound/STI>

## PDB - Get bound ligand interactions

Get interactions for a bound ligand found in the entry.

```
https://www.ebi.ac.uk/pdbe/graph-api/pdb/bound_ligand_interactions/:pdbId/:chain/:seqId
```

Send a Sample Request

url

Parameters

pdbid  String

chain  String

seqid  Integer

Response

```
{
  "4r7i": [
    {
      "ligand": {
        "author_residue_number": 1001,
        "chain_id": "A_1",
        "chem_comp_id": "STI",
        "author_insertion_code": " "
      },
      "interactions": [
        {
          "ligand_stoms": [
            "C1",
            "C2",
            "C4",
            "C5",
            "C6",
            "N3"
          ],
          "end": {
            "chain_id": "A_1",
            "author_residue_number": 588,

```

# Use case

## Accessible residues for a PDB structure

### Send a Sample Request

[https://www.ebi.ac.uk/pdbe/graph-api/pdb/funpdb\\_annotation/:origin/:pdbId](https://www.ebi.ac.uk/pdbe/graph-api/pdb/funpdb_annotation/:origin/:pdbId)

### Parameters

origin 3Dcomplex

pdbid 3pxe

### Response

```
    },
    {
      "site_id": 2,
      "label": "ASA_alone",
      "site_residues": [
        {
          "entity_id": 1,
          "chain_id": "A",
          "residue_number": 2,
          "author_residue_number": 1647,
          "chem_comp_id": "ASN",
          "author_insertion_code": "",
          "raw_score": 208.5,
```

label = ASA\_alone  
raw\_score > 0

### PDB - Get all FunPDBe annotations for a PDB entry from a specific resource

This call provides details of all FunPDBe annotations for a PDB entry from a specific resource.

[https://wwwdev.ebi.ac.uk/pdbe/graph-api/pdb/funpdb\\_annotation/:origin/:pdbId](https://wwwdev.ebi.ac.uk/pdbe/graph-api/pdb/funpdb_annotation/:origin/:pdbId)

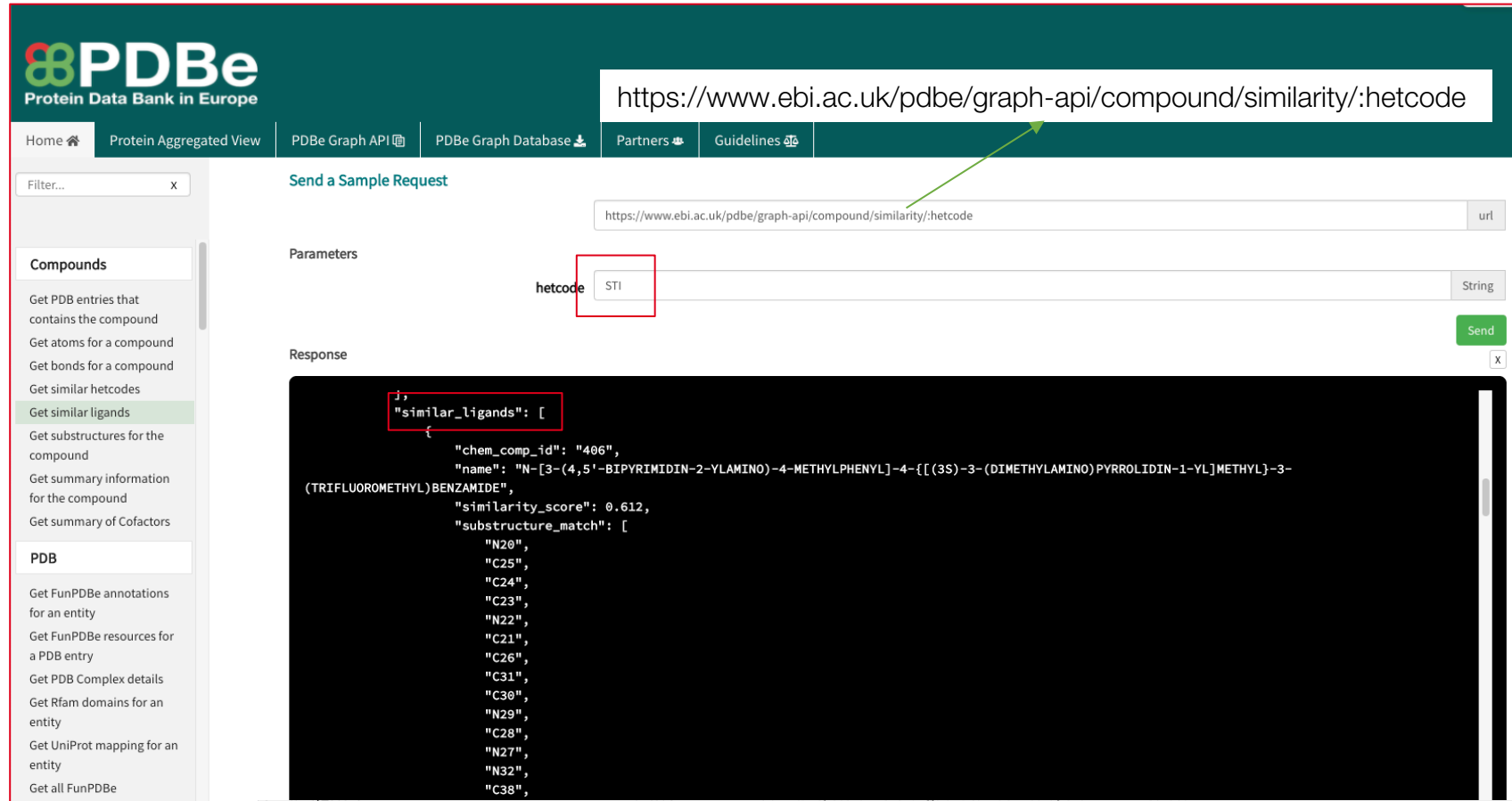
### Parameter

Field	Type	Description
origin	String	Origin/Resource Allowed values: "cath-funsites", "14-3-3-pred", "3Dcomplex", "akid", "3dligandsite", "camkinet", "canSAR", "ChannelsDB", "depth", "dynamine", "FoldX", "MetalPDB", "M-CSA", "p2rank", "Missense3D", "POPScomp_PDBML", "ProKin0"
pdbid	String	PDB Entry ID



# Use case

## Ligands similar to drug Imatinib (STI)




The screenshot shows the PDBe website interface. At the top, the URL `https://www.ebi.ac.uk/pdbe/graph-api/compound/similarity/:hetcode` is displayed. Below the navigation bar, the 'Send a Sample Request' form is visible. The 'url' field contains the same URL, and the 'hetcode' field is set to 'STI'. A green arrow points from the URL in the top bar to the 'url' field in the form. The 'Response' section shows a JSON object with a 'similar\_ligands' array. The first element in the array is a JSON object for Imatinib, with a similarity score of 0.612. The 'substructure\_match' array lists atom IDs: N20, C25, C24, C23, N22, C21, C26, C31, C30, N29, C28, N27, N32, and C38.

```
{
  "similar_ligands": [
    {
      "chem_comp_id": "406",
      "name": "N-[3-(4,5'-BIPYRIMIDIN-2-YLAMINO)-4-METHYLPHENYL]-4-[[ (3S)-3-(DIMETHYLAMINO)PYRROLIDIN-1-YL]METHYL]-3-(TRIFLUOROMETHYL) BENZAMIDE",
      "similarity_score": 0.612,
      "substructure_match": [
        "N20",
        "C25",
        "C24",
        "C23",
        "N22",
        "C21",
        "C26",
        "C31",
        "C30",
        "N29",
        "C28",
        "N27",
        "N32",
        "C38"
      ]
    }
  ]
}
```

# Teaching resources

PDBe API webinar series



1.0

Introduction to PDBe programmatic access

- Searching with the PDBe API
- Creating complex PDBe API queries

Using the PDBe Graph API

- Introduction
- Usecases
  - PDBe tools in github
  - Data visualisation at PDBe

» Using the PDBe Graph API [View page source](#)

## Using the PDBe Graph API

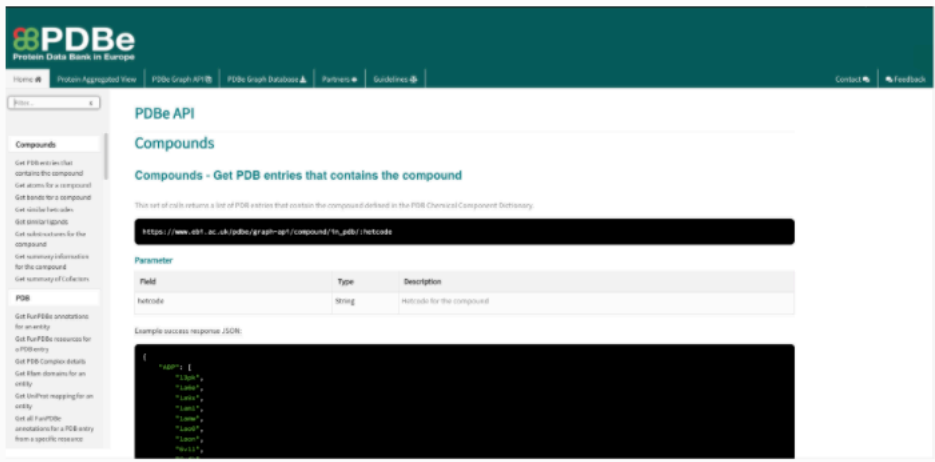
### Introduction

PDBe Graph API (also referred as **Aggregated API**) is a RESTful API using PDBe Graph Database as backend. It currently supports only **GET** requests and provides aggregated data across all relevant PDB entries, for eg. based on entities, UniProt IDs, residues and more.

API documentation can be accessed here [pdbe.org/graph-api](http://pdbe.org/graph-api)

### Using the documentation

The documentation is a web based application to work with the API.




The screenshot shows the PDBe API documentation interface. The main heading is 'PDBe API' and the sub-heading is 'Compounds'. Below this, there is a description: 'Compounds - Get PDB entries that contains the compound'. A text box contains the URL: `https://www.ebi.ac.uk/pdbe/graph-api/compound/{id}/httpcode`. A table lists the parameters for the API call:

Field	Type	Description
httpcode	String	Httpcode for the compound

Below the table, there is an 'Example success response (JSON):' section with a code block showing a JSON array of objects.

# Teaching resources – worked out examples

PDBe API webinar series



1.0

Introduction to PDBe programmatic access

- Searching with the PDBe API
- Creating complex PDBe API queries

Using the PDBe Graph API

- Introduction
- Usecases
  - Predicated ligand binding sites in interaction interface
    - 1) Get the annotations data for UniProt accession P61626
    - 2) Filter the data for providers p2rank and 3dligandsite
    - 3) Get interacting residues for the UniProt accession
    - 4) Filter interface\_data on common residues
  - Accessible residues for a PDB structure

PDBe tools in github

Data visualisation at PDBe

» Using the PDBe Graph API » Predicated ligand binding sites in interaction interface

[View page source](#)

## Predicated ligand binding sites in interaction interface

If you have a protein of interest and want to know the predicted ligand binding sites of it which are also in a protein-protein interaction, you can first make use of the annotations API for a UniProt accession to get all annotations from PDBe-KB partners for the protein.

The predicted ligand site annotations are provided by `p2rank` and `3dligandsite`. Post process this response to filter the `accession` field for these providers. This gives all UniProt residues which are annotated as a predicted ligand binding site.

### UniProt - Get annotations for a UniProt accession

This call provides details on annotations for a UniProt accession.

```
https://www.ebi.ac.uk/pdbe/graph-api/uniProt/annotations/:accession
```

Send a Sample Request

url:

Parameters

accession:  String

Send

Response

```
{
  "P61626": {
    "sequence":
      "MKALIVLGLVLLSVTVQGVKVFERCELARTLKRLLGNDGVRGISLAMWCLAKWESGVNTRATNYNAGDRSTDYGFQINSRYWCNDGKTPGAVNACH
      LSCSALLQDNIADAVACAKRVVDRDPQGIAMVAMRNRCQNRDVRQYVQGGCV",
    "length": 348,
    "dataType": "ANNOTATIONS",
  }
}
```

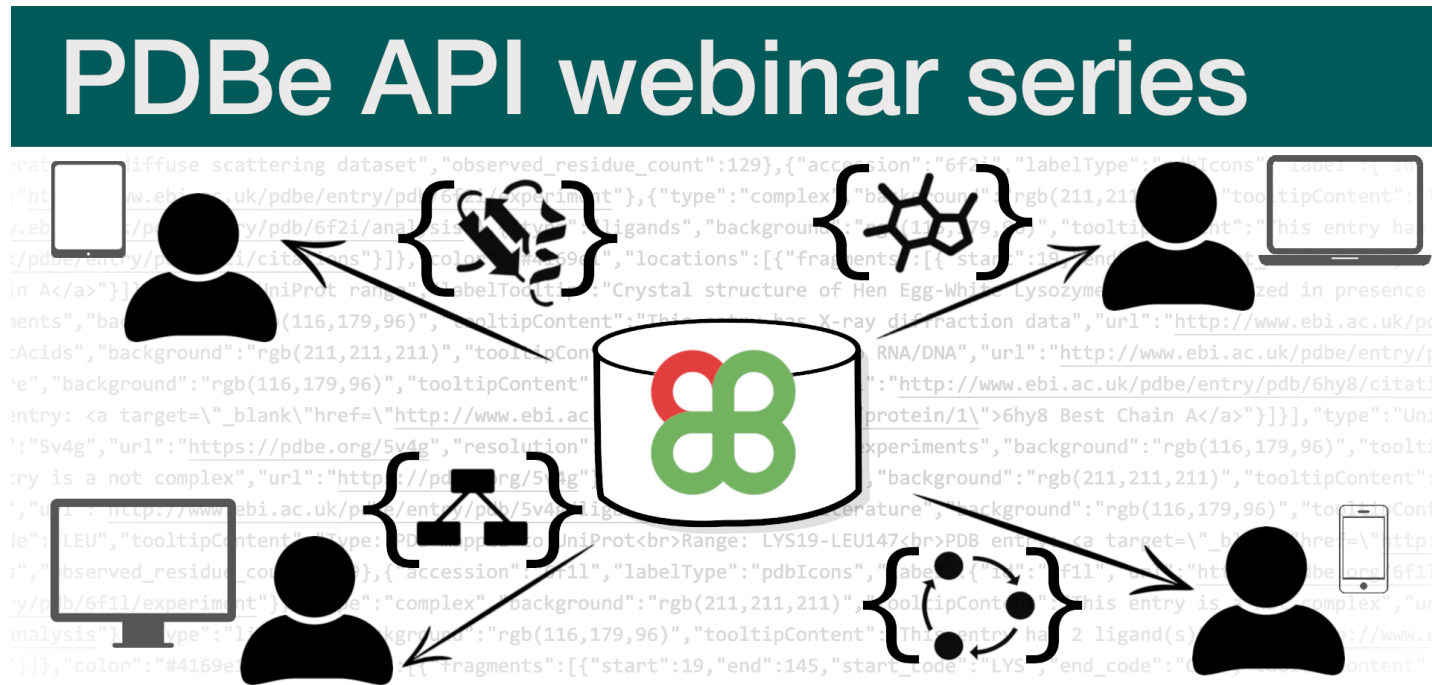
# PDBe API webinar series

- Sep 15th Introduction to PDBe programmatic access
- Sep 22nd Searching with the PDBe API
- Sep 29th Creating complex PDBe API queries
- Oct 6th Using the PDBe graph API
- Oct 13th PDBe tools in github**
- Oct 20th Data visualisation at PDBe



# To register for future webinars in the series

- See the full list of upcoming webinars at [bit.ly/PDBe\\_API\\_webinars](http://bit.ly/PDBe_API_webinars)
- Or visit the PDBe events pages at [PDBe.org/events](http://PDBe.org/events)
- Remember to register for each webinar individually!!!



Thank you for your attention!  
Any questions?

[PDBe.org/graph-api](https://pdbe.org/graph-api)



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