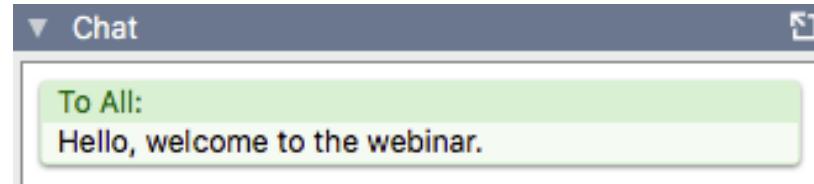


Welcome - webinar instructions

- 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



Sreenath Nair



-  pdbhelp@ebi.ac.uk
-  [proteindatabank](#)
-  [@PDBeurope](#)
-  [proteindatabank](#)
-  [pdbeurope](#)
-  [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

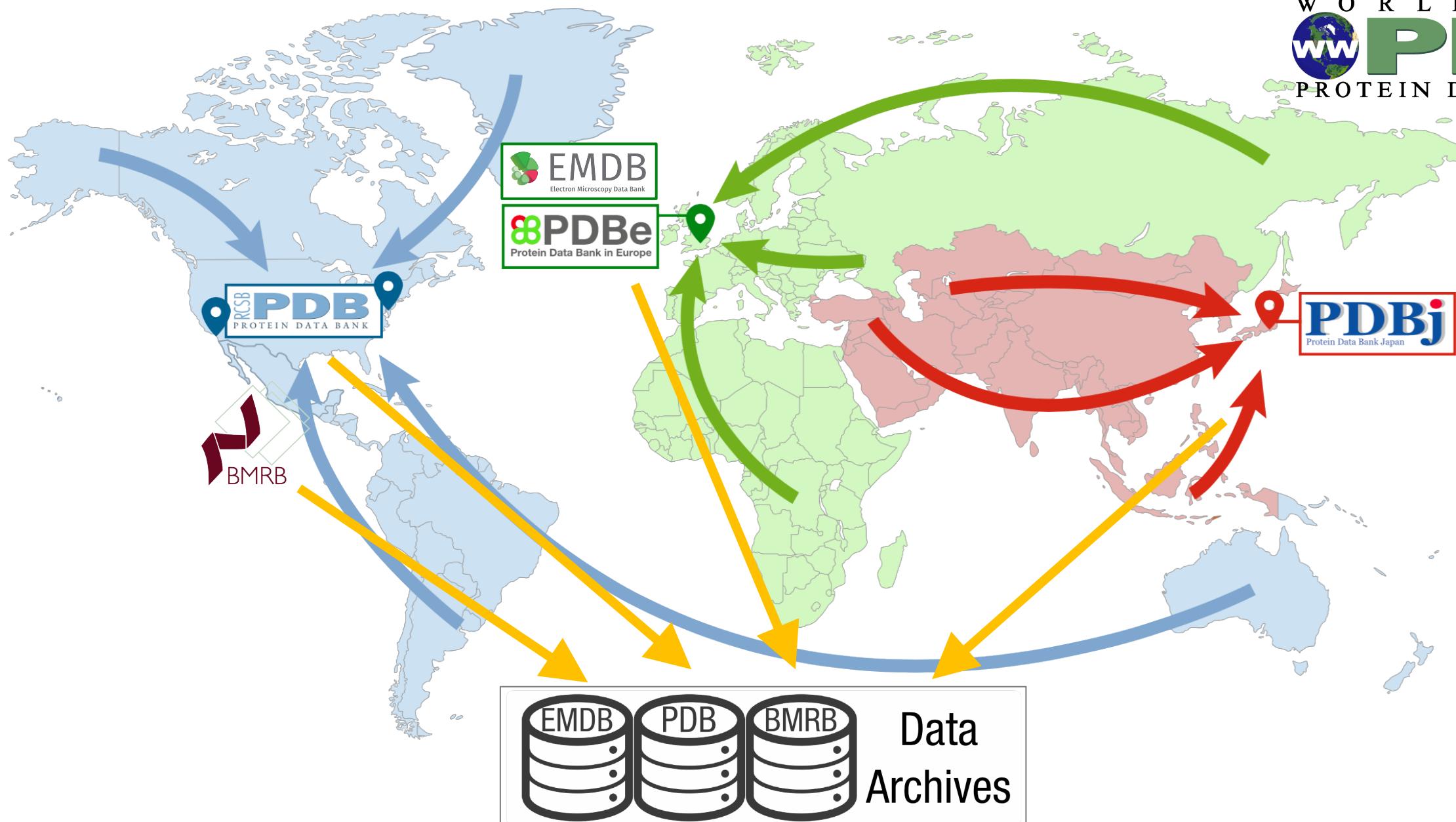
Oct 6th Using the PDBe graph API

Oct 13th PDBe tools in github

Oct 20th Data visualisation at PDBe

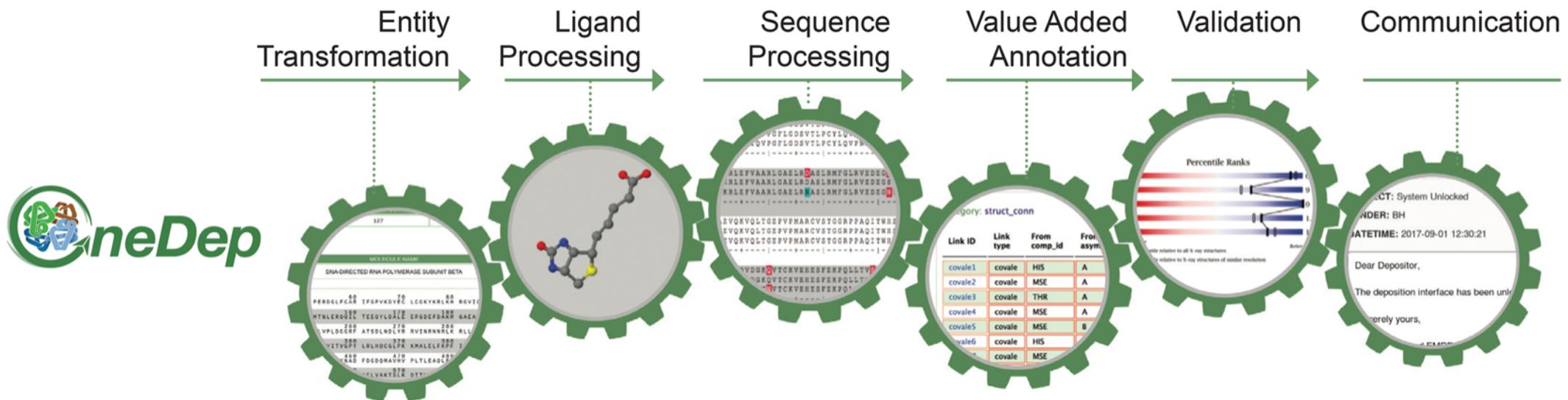
Summary of the webinar

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

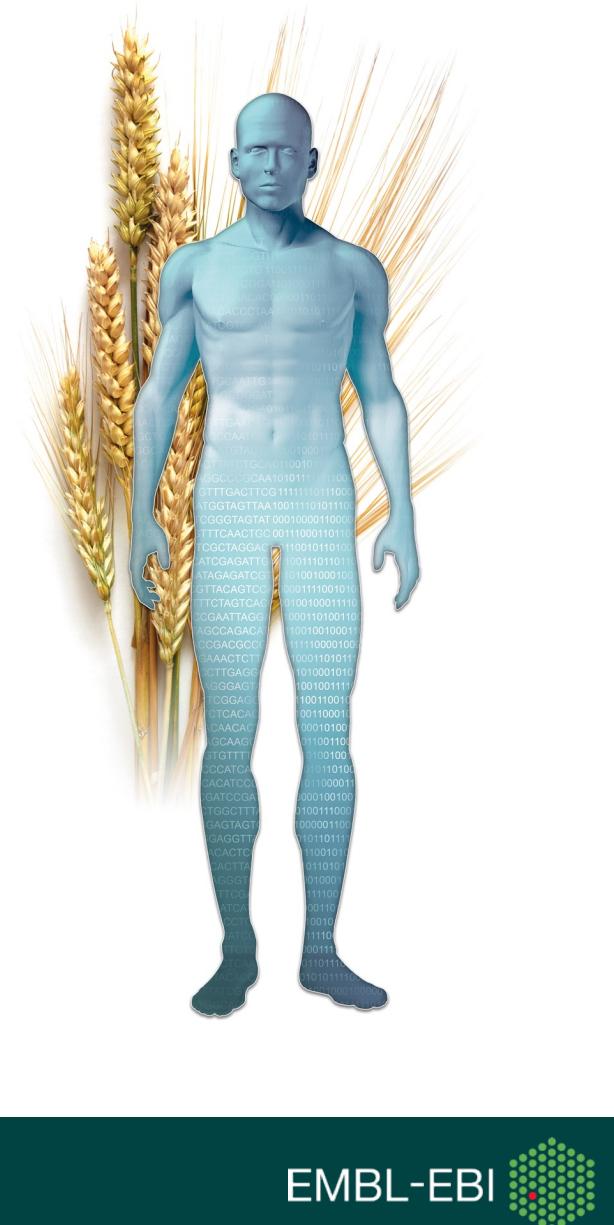
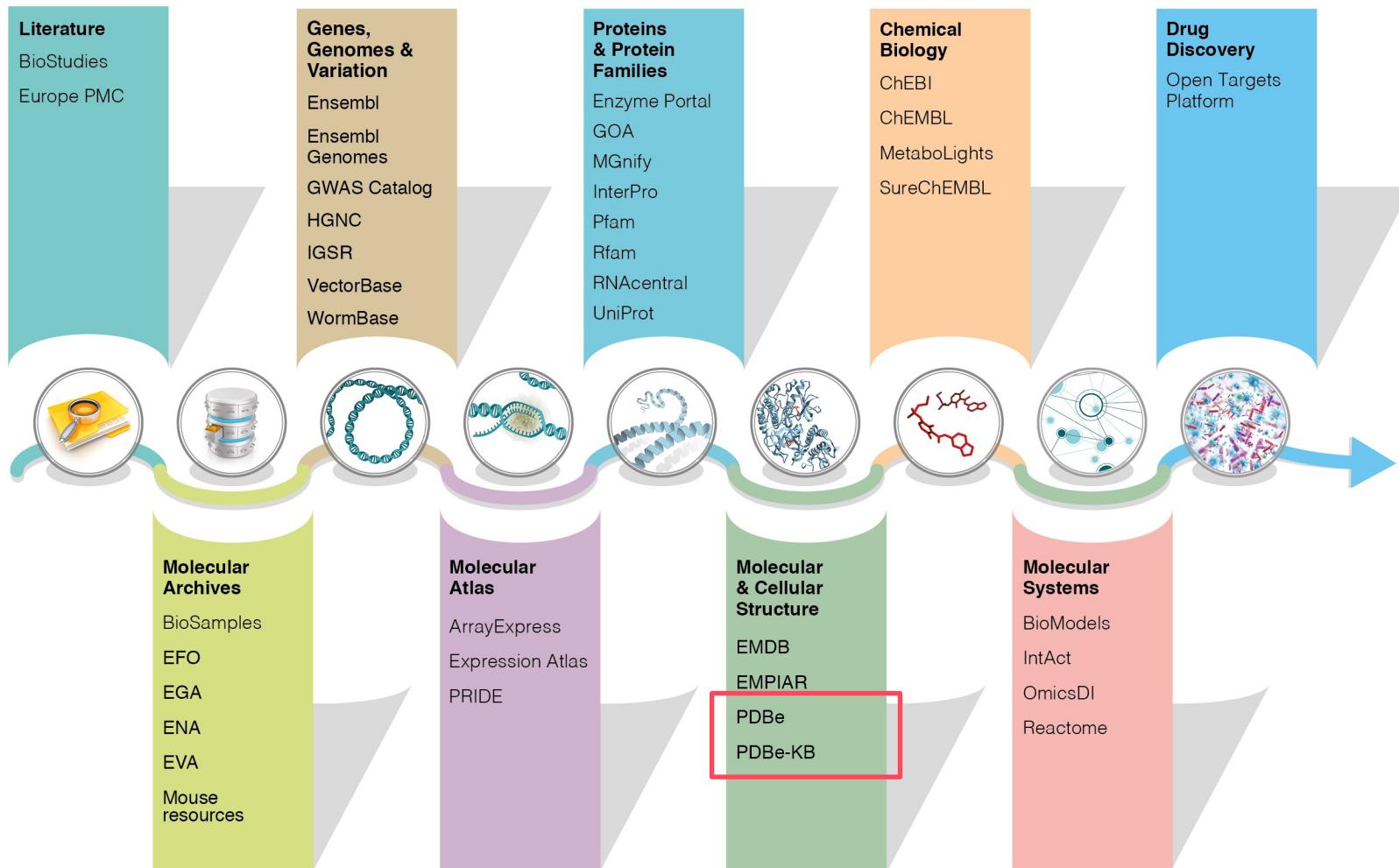


Data added through deposition

- 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



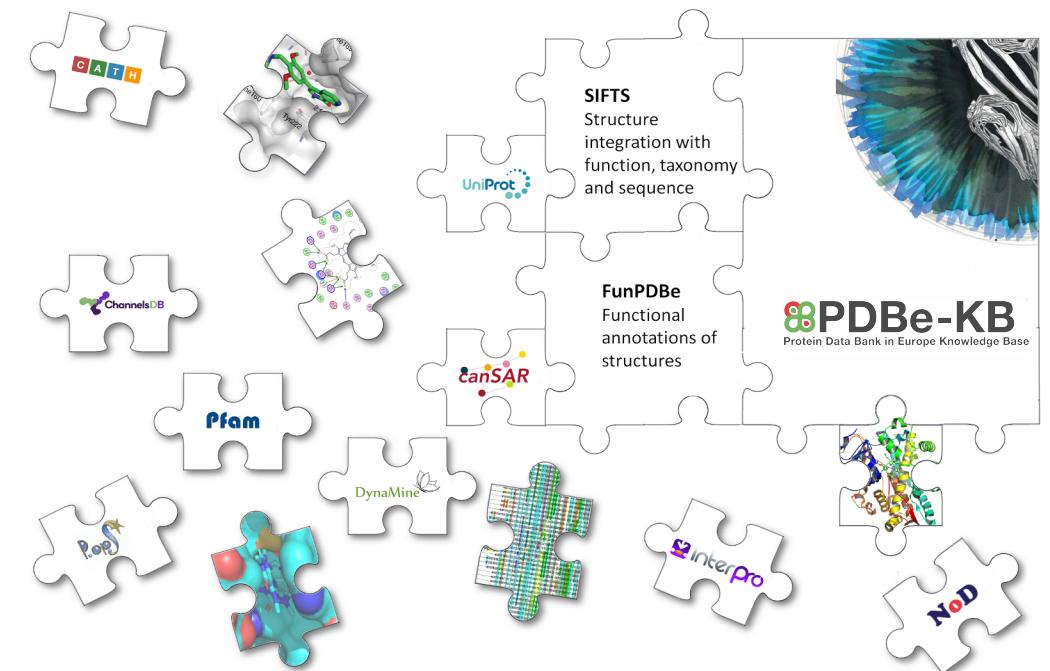
At the heart of EMBL-EBI resources



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

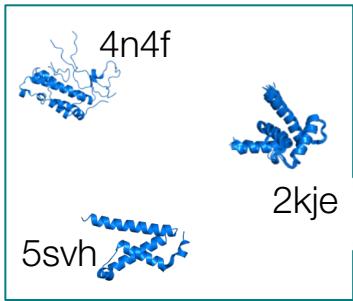
- Data standards
- Data access mechanisms
- Reduce fragmentation



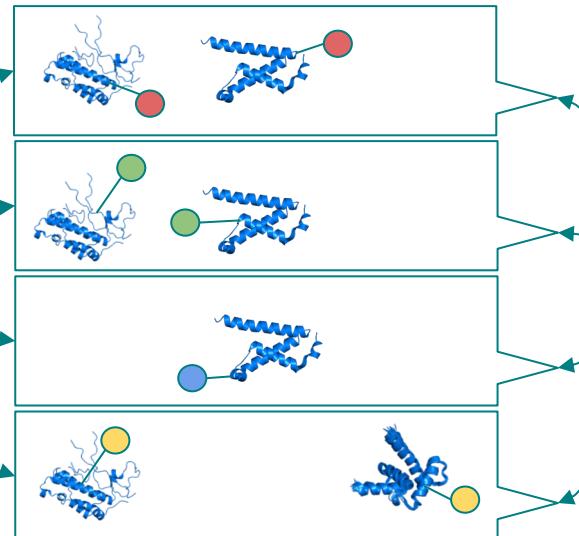
Data enrichment and integration in PDBe-KB

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

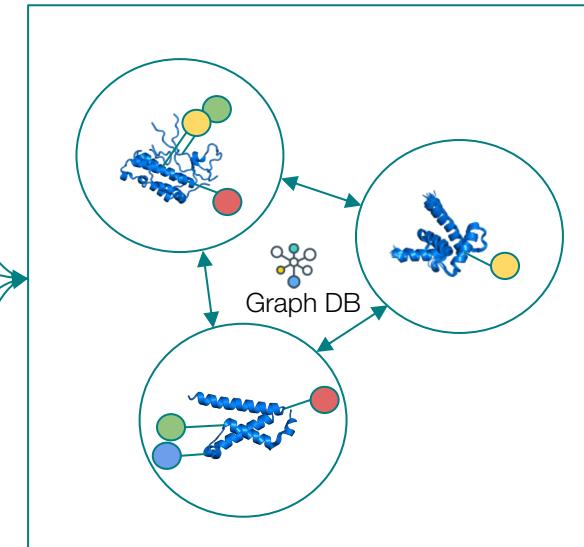
PDB entries



Specialist databases
annotating PDB entries



Interconnected,
annotated PDB entries



Data is exposed using
novel, aggregated views

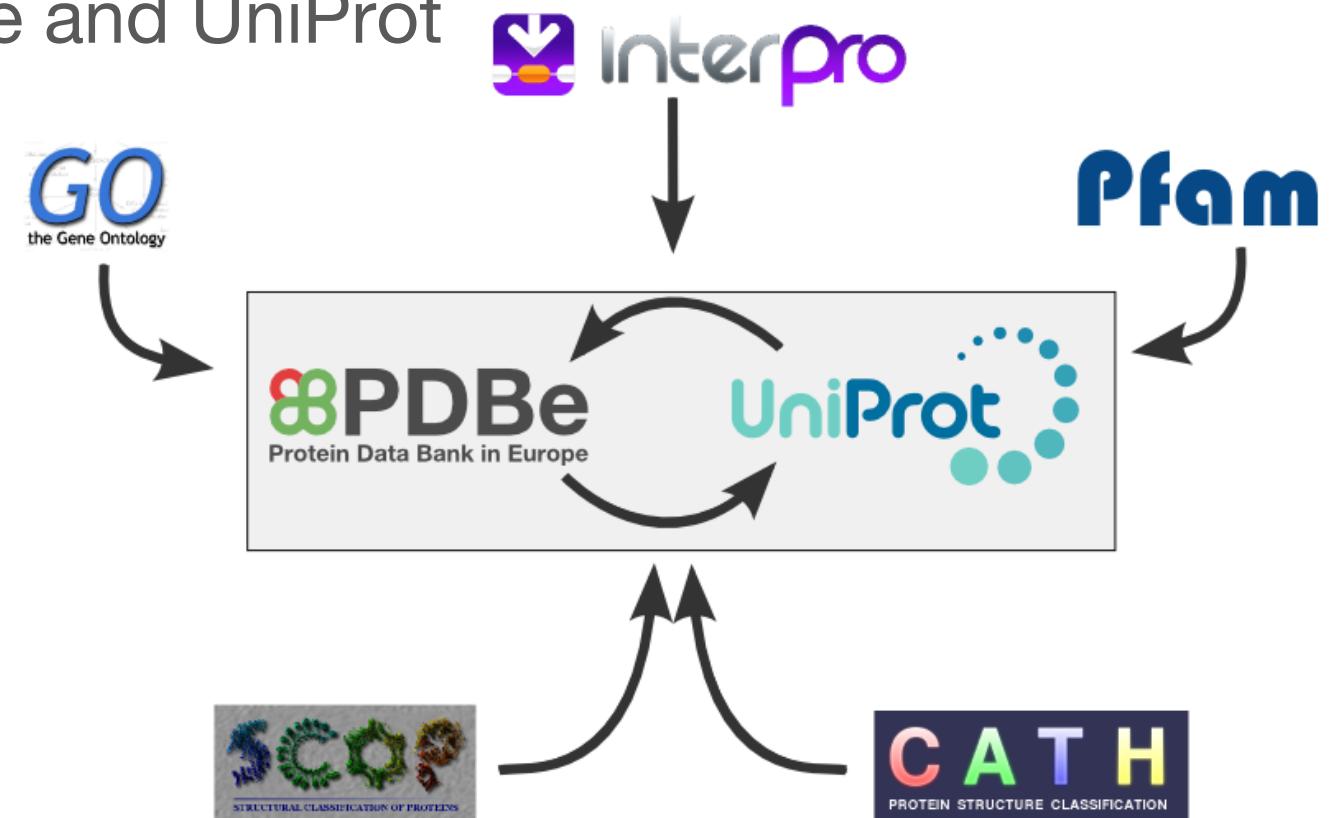


- Domains
- Rfam classification
- Functional sites (e.g. ligand binding)
- Post-translational modifications
- Physico-chemical parameters (residue depth, flexibility, etc.)
- Interacting residues/interfaces

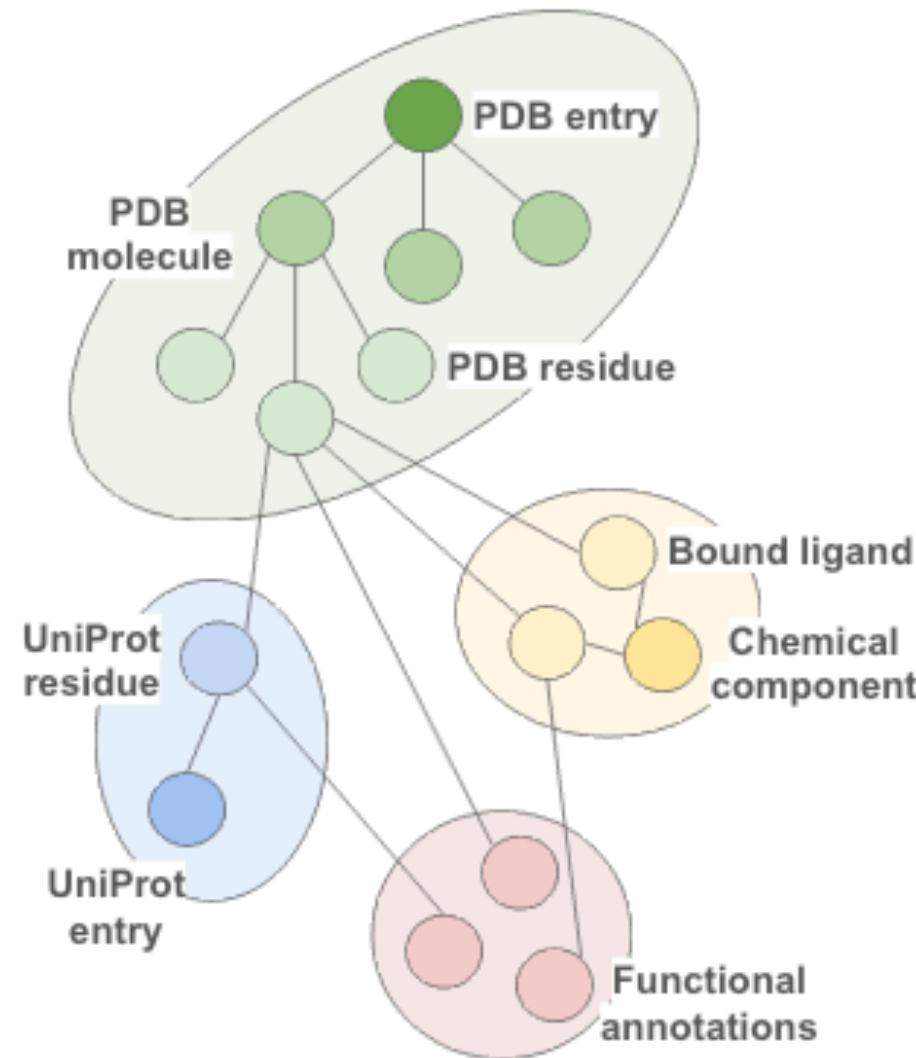
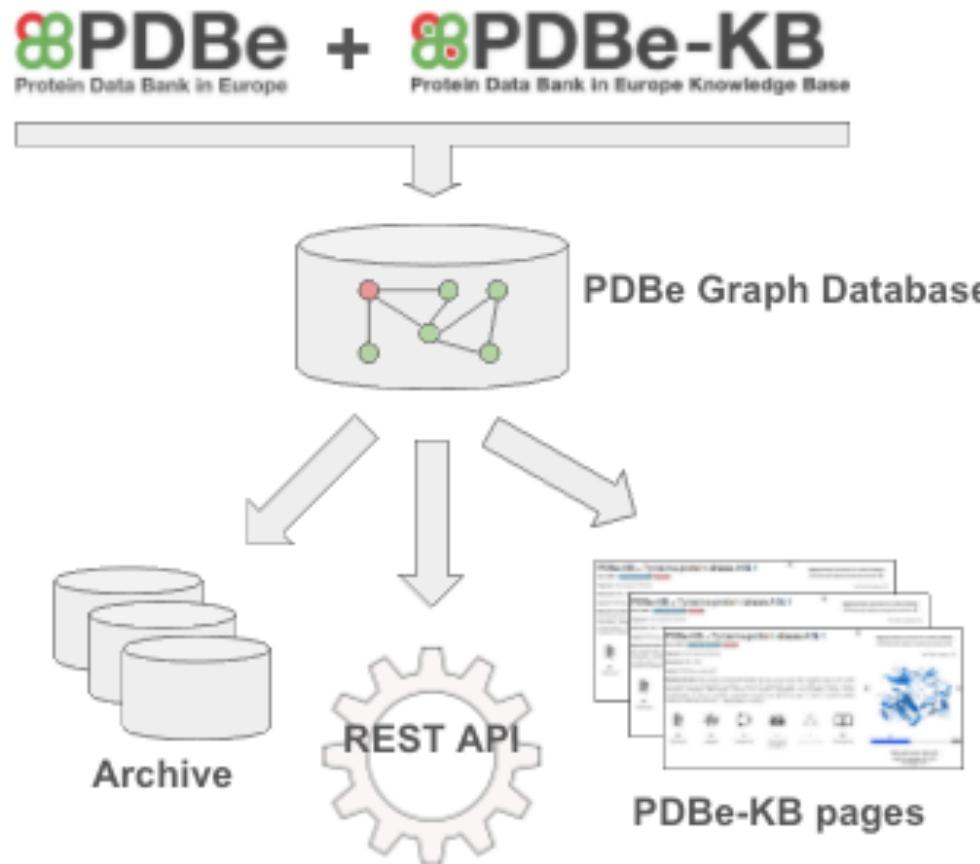
PDBe-KB
Protein Data Bank in Europe Knowledge Base

SIFTS

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

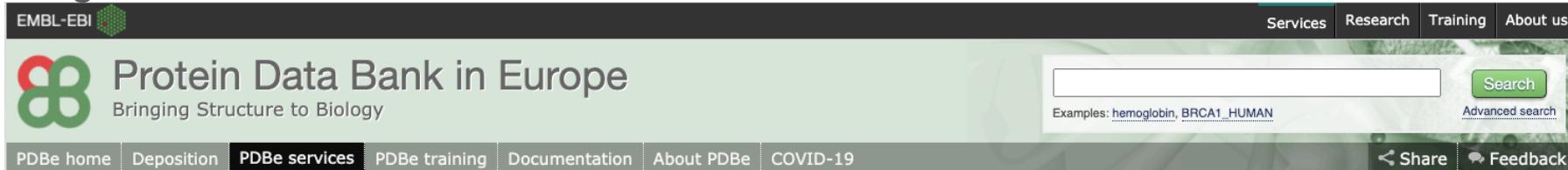


PDBe Graph Database



PDBe API

Programmatic access to PDB data



The screenshot shows the PDBe homepage with a dark header containing the EMBL-EBI logo, a search bar with examples like "hemoglobin, BRCA1_HUMAN", and a "Search" button. Below the header is a navigation bar with links for PDBe home, Deposition, PDBe services (which is highlighted), PDBe training, Documentation, About PDBe, COVID-19, Share, and 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

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

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

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 

interface 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 

interface 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 for the "UniProt - Get interface residues for a UniProt accession" endpoint. The page has a dark green header with the PDBe logo and navigation links for Home, Protein Aggregated View, PDBe Graph API, PDBe Graph Database, Partners, and Guidelines.

The main content area has a search bar with the placeholder "interface" and an "X" button. To the left, there are two buttons: "Get interface residues for an entity" and "Get interface residues for a UniProt accession". The second button is highlighted in green.

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

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

Parameters:

accession	P07550	String
-----------	--------	--------

Send

Response

```
{  
    "P07550": {  
        "sequence": "  
MGQPGNGSAFLAPNGSHAPDHVTQERDEVWVGMGIVMSLIVLAIVFGNVLVITAIAKFERLQTVNYFITSLACADLVMGLAVVPGAAHILMKMWTFGNFCEFWTSIDVLCVTAISETLCVIAVDRYFAITSPFKYQSLLTKNKARVII  
LMWIVVSGLTSFLPIQMHWYRATHQEAEAINCYANETCCDFTNQAYAIAASSIVSFVYPLIVMFVYSRVFQEAKRQLQKIDKSEGRFHVNLSQVEQDGRTGHLRRSSKFCLEHKALKTLGIIMGFTLCWLPPFIVNIVHVIQDNLIRKEVYI  
LLNWIGYVNSGFNPLIYCRSPDFRIAFCQELLCLRRSSLKAYGNGYSSNGNTGEQSGYHVEQEKENKLLEDLPGTEDFVGHQGTVPDSNIDSQGRNCSTNDSSL",  
        "Length": 413,  
        "dataType": "INTERACTION INTERFACES",  
        "data": [  
            {  
                "name": "Camelid Antibody Fragment",  
                "accession": "IG-heavy chain",  
                "residues": [  
                    {  
                        "start": 1, "end": 413, "residues": "P07550"}  
                ]  
            }  
        ]  
    }  
}
```

API Documentation

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



API Documentation - Compounds

API Documentation - Compounds

PDBe
Protein Data Bank in Europe

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

Filter... X

Send a Sample Request

url: <https://www.ebi.ac.uk/pdbe/graph-api/compound/similarity/:hetcode>

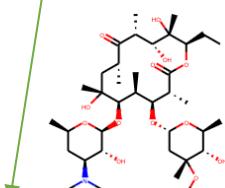
Parameters

hetcode: ERY String

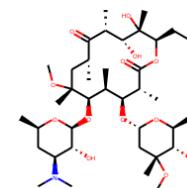
Response

Send X

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



ERYTHROMYCIN



CLARITHROMYCIN

API Documentation - PDB

The screenshot shows the PDBe API documentation for the PDB section. The top navigation bar includes links for Home, Protein Aggregated View, PDBe Graph API, PDBe Graph Database, Partners, and Guidelines. A search bar labeled 'Filter...' is present. On the left, a sidebar lists various API endpoints under the 'PDB' category. The main content area is titled 'PDB - Get FunPDBe annotations for an entity'. It describes the endpoint for getting annotations for a specific entity, provides the URL (https://www.ebi.ac.uk/pdbe/graph-api/pdbe_pages/annotations/:pdbId/:entityId), and details the parameters:

Parameter	Description
Field	Functional annotations from KB partners
pdbId	Sequence and structural domains
entityId	Bound ligand interactions
	Macromolecular interactions
	Modified/mutated residues
	Secondary structures
	Sequence conservation etc.

The 'entityId' parameter is highlighted with a green arrow pointing to its description. Below this, a 'Success 200' status section shows the response structure:

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.

API Documentation - Residue

PDBe
Protein Data Bank in Europe

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

Filter...

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/funpdbe_annotation/:pdbId/:entityId/:residueNumber

Parameter

Field	Type	Description
pdbId	String	PDB Entry ID
entityId	String	PDB Entity ID
residueNumber	String	PDB Residue Number

Send a Sample Request

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

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

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 Entry ID
- Get GO mappings for a PDB Entry ID

Send a Sample Request

Parameters

url: https://www.ebi.ac.uk/pdbe/graph-api/residue_mapping/:pdbId/:entityId/:residueStart/:residueEnd

https://www.ebi.ac.uk/pdbe/graph-api/residue_mapping/3unn/1/40/100

pdbId: 3unn String

entityId: 1 String

residueStart: 40 String

residueEnd: 100 String

Send X

Response

```
{  
  "3unn": [  
    {  
      "entity_id": 1,  
      "chains": [  
        {  
          "auth_asym_id": "A",  
          "struct_asym_id": "A",  
          "residues": [  
            {  
              "residue_id": "40",  
              "atom_ids": ["40A1", "40A2", "40A3", "40A4", "40A5", "40A6", "40A7", "40A8", "40A9", "40A10", "40A11", "40A12", "40A13", "40A14", "40A15", "40A16", "40A17", "40A18", "40A19", "40A20", "40A21", "40A22", "40A23", "40A24", "40A25", "40A26", "40A27", "40A28", "40A29", "40A30", "40A31", "40A32", "40A33", "40A34", "40A35", "40A36", "40A37", "40A38", "40A39", "40A40"],  
              "atom_labels": ["C", "H", "O", "N", "S"]  
            }  
          ]  
        }  
      ]  
    }  
  ]  
}
```

API Documentation – Residue annotations

The screenshot shows the PDBe API documentation interface. On the left, there's a sidebar with sections for "Residue" and "SIFTS". The "Residue" section contains links like "Get FunPDBe annotations for a PDB Residue", "Get annotations for a PDB Residue range", and "Get sequence conservations for a PDB Residue". The "SIFTS" section contains links for UniProt accessions and residue ranges. The main content area is titled "Response" and displays a JSON object with annotations pointing to its components:

```
{  
  "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": {  
                    "identifier": "MDC1_HUMAN",  
                    "name": "MDC1_HUMAN",  
                    "unp_residue_number": 65,  
                    "unp_one_letter_code": "A",  
                    "pdb_one_letter_code": "A"  
                  }  
                ]  
              }  
            }  
          ]  
        }  
      ]  
    }  
  ]  
}
```

Annotations in the JSON output point to the following components:

- An arrow points from the first "3unn" entry to the label "Entry".
- An arrow points from the "entity_id" field to the label "Entity".
- An arrow points from the "chains" array to the label "Chains".
- An arrow points from the "residues" array to the label "Residues".
- An arrow points from the "features" object to the label "Annotations".

API Documentation – Residue annotations

The screenshot shows the PDBe API documentation for residue annotations. The top navigation bar includes links for Home, Protein Aggregated View, PDBe Graph API, PDBe Graph Database, Partners, and Guidelines. A sidebar on the left lists various API endpoints under 'Residue' and 'SIFTS'. The main content area displays a JSON response for residue annotations, with a green arrow pointing from the 'Annotations from PDBe-KB partners' text to the 'origin' field of the first object. To the right of the JSON, logos for Pfam, InterPro, CATH, and SCOP are displayed.

```
"FunPDBe": [ { "origin": "POPScomp_PDBML", "label": "total SASA [A^2]", "url": "https://github.com/Fraternallilab/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/Fraternallilab/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

PDBe
Protein Data Bank in Europe

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

Filter... X

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 shows the PDBe API documentation interface. On the left, there's a sidebar with a navigation menu under the 'SIFTS' section, including options like 'Get Best Structures for a UniProt accession'. The main area is titled 'Send a Sample Request' and contains a form. The URL field contains 'https://www.ebi.ac.uk/pdbe/graph-api/mappings/best_structures/:accession'. The 'accession' parameter is set to 'P0DTD1'. The response section shows the JSON output for this request:

```
{  
  "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,  
      "unp_end": 5324,  
      "coverage": 0.131,  
      "unp_start": 4392,  
      "resolution": 2.5,  
      "experimental_method": "Electron Microscopy",  
      "tax_id": 2697049,  
      "preferred_assembly_id": 1  
    }  
  ]  
}
```

API Documentation – SIFTS

The screenshot shows the PDBe API documentation interface. On the left, there's a sidebar with a 'SIFTS' section containing various API endpoints. The 'Get Best Structures for a UniProt residue range' endpoint is highlighted with a green background. The main area has a 'Send a Sample Request' section. It shows a URL input field with the value https://www.ebi.ac.uk/pdbe/graph-api/mappings/best_structures/:accession/:unpStart/:unpEnd. Below it, three parameters are defined: 'accession' set to 'P0DTD1', 'unpStart' set to '30', and 'unpEnd' set to '40'. A 'Response' section shows the JSON output for the sample request, which includes the protein name 'Replicase polyprotein 1ab 2019-nCoV' and a detailed mapping object for the P0DTD1 entry.

PDBe
Protein Data Bank in Europe

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

Filter...

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

Parameters

url

accession P0DTD1 String

unpStart 30 String

unpEnd 40 String

Response

Send

Replicase polyprotein 1ab 2019-nCoV

```
{  
  "P0DTD1": [  
    {  
      "end": 40,  
      "entity_id": 1,  
      "chain_id": "A",  
      "pdb_id": "7k3n",  
      "start": 30,  
      "unp_end": 40,  
      "coverage": 1,  
      "unp_start": 30,  
      "residues": [  
        {  
          "aa": "A",  
          "pos": 30, "unp_pos": 30},  
        {  
          "aa": "A",  
          "pos": 31, "unp_pos": 31},  
        {  
          "aa": "A",  
          "pos": 32, "unp_pos": 32},  
        {  
          "aa": "A",  
          "pos": 33, "unp_pos": 33},  
        {  
          "aa": "A",  
          "pos": 34, "unp_pos": 34},  
        {  
          "aa": "A",  
          "pos": 35, "unp_pos": 35},  
        {  
          "aa": "A",  
          "pos": 36, "unp_pos": 36},  
        {  
          "aa": "A",  
          "pos": 37, "unp_pos": 37},  
        {  
          "aa": "A",  
          "pos": 38, "unp_pos": 38},  
        {  
          "aa": "A",  
          "pos": 39, "unp_pos": 39},  
        {  
          "aa": "A",  
          "pos": 40, "unp_pos": 40}  
      ]  
    }  
  ]  
}
```

API Documentation – UniProt

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

PDBe
Protein Data Bank in Europe

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

Filter...

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 Molprobity component of the wwPDB validation pipeline

Where do we use it?

Aggregated views of proteins

The screenshot shows the PDBe-KB homepage with a dark teal header and a white main content area. The header includes the EMBL-EBI logo, navigation links for Services, Research, Training, About us, a search bar, and the PDBe-KB logo. The main content features a title 'What are the Aggregated Views of Proteins?' above four categories: 'Structures' (molecule icon), 'Small-molecules' (lightbulb icon), 'Macromolecular Interactions' (circular arrows icon), and 'Functional Annotations' (book icon). Below this is a text block about aggregated views and a search bar. The bottom section has a teal background with the text 'Latest updates' and a list of recent changes.

EMBL-EBI Services Research Training About us EMBL-EBI

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

26/08/2020

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

Latest updates

Aggregated views of proteins

Ex. - hemoglobin, BRCA1_HUMAN

PDBe-KB Protein Data Bank in Europe Knowledge Base

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

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 91 Ligands 12 Interactions 4 Functional annotations 2 Similar proteins 72 Publications

Download Download Download Download Download

View structure clusters View all ligands

How many ligands known to bind to this protein?

What structural data available for my protein?

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

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

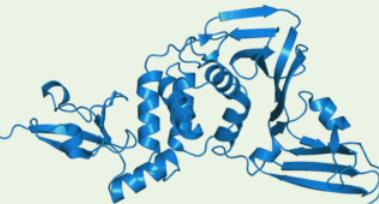
accession

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": [  
        {  
          "start": 1562,  
          "end": 1879  
        }  
      ]  
    }  
  ]  
}
```

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 | [What's new?](#) | [?](#)

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]

Key statistics:

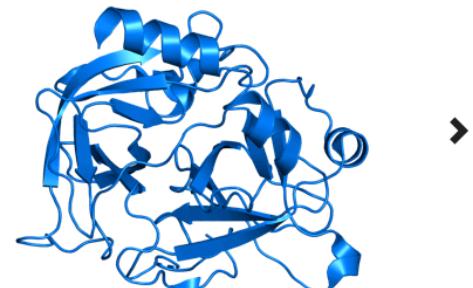
419 Structures	303 Ligands	48 Interactions	3 Functional annotations	35 Similar proteins	2756 Publications
Download	Download	Download	Download	View structure clusters	View all ligands

Processed Proteins (2):

Protein Name	Representative Structures Click on a box for 3D view	Available Structural Data	Navigate
Thrombin light chain		393 230 3	View Page
Thrombin heavy chain		411 241 47	View Page

Representative structures for UniProt P00734
PDB chains with highest data quality, coverage and best resolution [?](#)

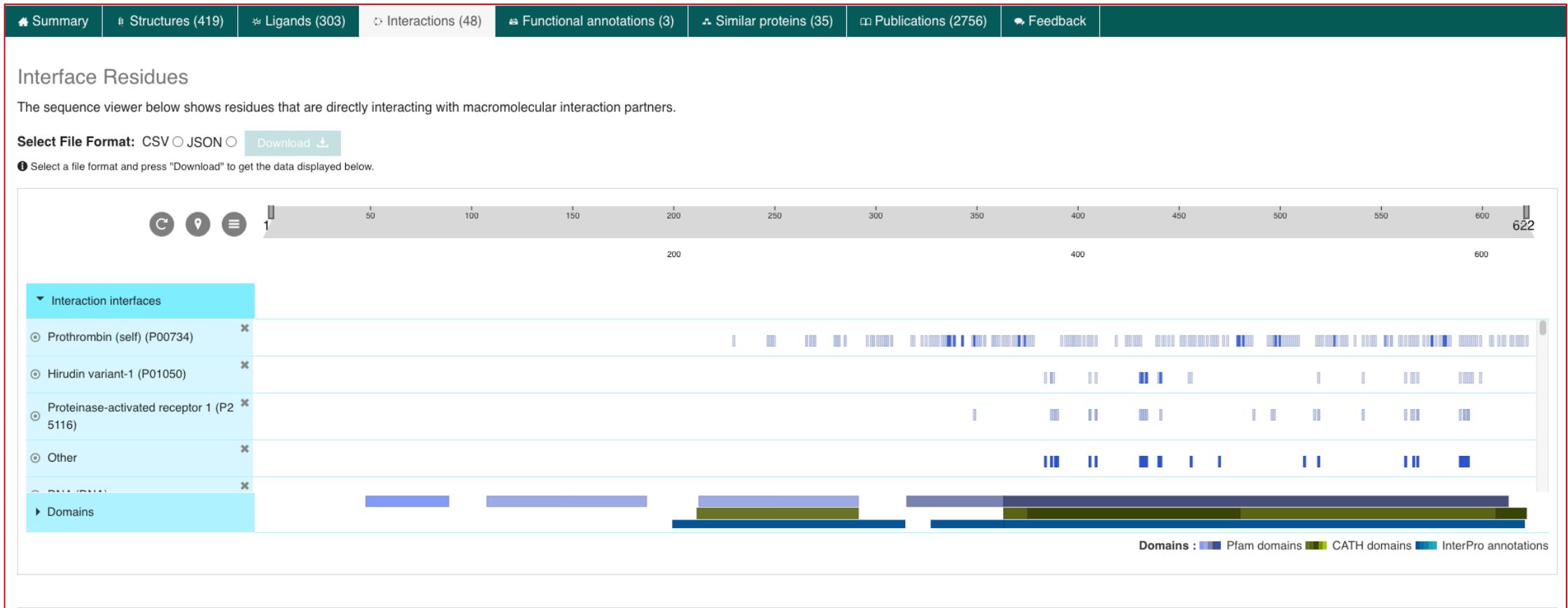
[Click to view in 3D](#)



PDB chain shown: 4ud9 A
UniProt residues 364 - 622
Coverage: 41%
[View structure clusters for segment 1](#)

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

Interface residues



Interface residues

PDBe
Protein Data Bank in Europe

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

Filter...

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

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... Send a Sample Request

matrices for a UniProt accession
Get annotations for a UniProt accession
Get interface residues 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

Parameters

accession **P00734** url String

Response

```
{  
    "P00734": {  
        "sequence": "  
MAHVRGLQLPGCLALAALCSLVHSQHVFLAPQQARSLLQRVRRANTFLEEVRKGNLERECEVEETCSYEEAFAELESSTATDVFWAKYTACETARTPRDKLAACLEGNCAGLGTNYRGHVNITRSGIECQLWRSRYPHKPEINSTTHPGADLQENFCRNPDSTS  
TGPWCYTTDPTVRRQECSTPVGODQVTAMTPRSEGSVNLSPPLEQCVPRDRGQQYQGRЛАVTTHGLPCA  
WASAAQAKALSKHQDFNSAVLQVLENFCRNPDGDEEGVWCYVAGKPGDFGYCDLNCEEA  
VEETGDGLDEDSRAIEGRATSEYQTFFNPRTFGSGEADCGLR  
PLFEKKSL  
EDKTERELLESYIDGRIVEGSDAEIGMSPWQMLFRKSPQELLCGASLISDRWLTAHCLLYPPWDKNFTENDLLVRIGKHSRTRYERNIEKISM  
LEKIVIHPRYNWRENLDRLDIALMKLKPVAFSDYIHPVCLPDRETAASLLQAGYKGRVTGWNLKE  
WTANVGKGQPSVLQVNVLP  
I  
VERPVCKDSTRITDN  
MFCA  
GK  
YK  
P  
DEKG  
R  
G  
D  
ACE  
GS  
GG  
F  
V  
M  
K  
S  
P  
F  
N  
R  
W  
Y  
Q  
M  
G  
I  
V  
S  
W  
E  
G  
C  
D  
R  
D  
G  
K  
Y  
F  
Y  
T  
H  
V  
F  
R  
L  
K  
W  
I  
Q  
K  
V  
I  
D  
Q  
F  
G  
E",  
        "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"  
                            }  
                        ]  
                    }  
                ]  
            }  
        ]  
    }  
}
```

pdbe.org/aggregated-api

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]

Key statistics:

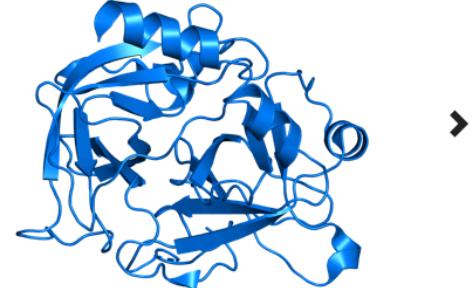
419 Structures	303 Ligands	48 Interactions	3 Functional annotations	35 Similar proteins	2756 Publications
Download	Download	Download	Download		
View structure clusters	View all ligands				

Processed Proteins (2):

Protein Name	Representative Structures Click on a box for 3D view	Available Structural Data	Navigate
Thrombin light chain		393 230 3	View Page
Thrombin heavy chain		411 241 47	View Page

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)

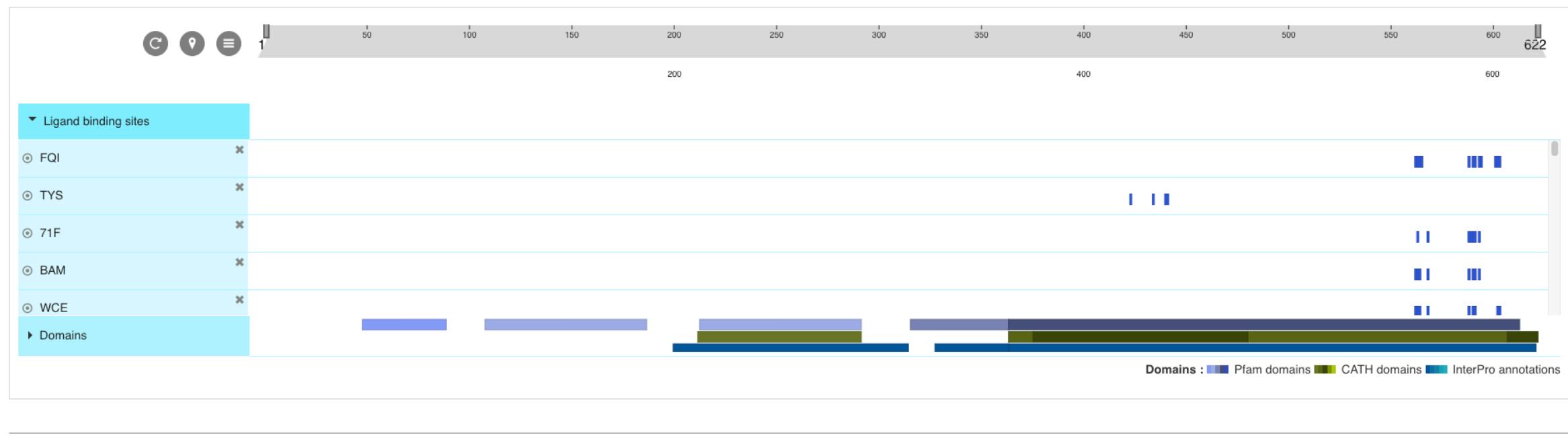
Ligand binding residues

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

PDBe
Protein Data Bank in Europe

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

Filter...

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 **(selected)**
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

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

The screenshot shows the PDBe Aggregated View interface. On the left, a sidebar lists various protein-related services, with "Get ligand binding residues for a UniProt accession" highlighted. The main area is titled "Send a Sample Request" and contains a form. The URL field is set to https://www.ebi.ac.uk/pdbe/graph-api/uniprot/ligand_sites/:accession. The "Parameters" section has a single entry: "accession" with the value "P00734", which is highlighted with a red box. A "Send" button is visible to the right. The "Response" section displays a JSON object representing the ligand binding residues for the specified UniProt accession. The JSON starts with:

```
{  
  "P00734": {  
    "sequence": "  
MAHVVRGLQLPGCLALAALCSLVHSQHVFLAPQQARSLLQRVRRANTFLEEVRKGNLERECVEETCSYEEAFELESSTATDVFWAKYTACETARTPRDKLAACLEGNCAGLGTNYRGHVNITRSGIECQLWRSRYPHKPEINSTTHPGADLQENFCRNPDSSTTGPWC  
YTTDPTRRQECISIPVCGQDQVTAMTPRSEGSVNLSPPLEQCVPDRQQYQGRALAVTTHGLPCLAWSAQAKALSKHQDFNSAVQLVENFCRNPDGDEEGVWCYVAGKPGDFGYCDLNCEEAVEEETDGDLDEDSDRAIEGRTATSEYQTFFNRTFGSEADCGLR  
PLFEKKSLIEDKTERELLESYIDGRIVEGSDAEIGMPSPWQVMLFRKSPQELLCGASLISDRWVLTAHHCLLYPPWDKNFTENDLLVIRIGKHSRTRYERNIEKISMLEKIYIHPRYNWRENLDRDIALMKLKKPVAFSDYIHPVCLPDRETAASLLQAGYKGRVTGWGNLKE  
TWTANVGKQGQPSVLQVNVLPIVERPVCKDSTRIRITDNMFCAGYKPDGKRDACEGDGGPFVKSPFNNRWYQMGIVSWGEGCDRGKYGFYTHVFRKKWIKVIDQFGE",  
    "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": "4uds",  
                "entityId": 1,  
                "chainIds": "H"  
              }  
            ]  
          }  
        ]  
      }  
    ]  
  }  
}
```

pdbe.org/aggregated-api

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

EMBL-EBI 

Protein Data Bank in Europe
Bringing Structure to Biology

Services Research Training About us

Examples: hemoglobin, BRCA1_HUMAN Search Advanced search 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.

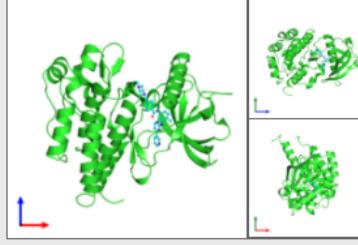
Tap WD, Wainberg ZA, Anthony SP, Ibrahim PN, Zhang C, Healey JH, Chmielowski B, Staddon AP, Cohn AL, Shapiro GI, Keedy VL, Singh AS, Puzanov I, Kwak EL, Wagner AJ, Von Hoff DD, Weiss GJ, Ramanathan RK, Zhang J, Habets G, Zhang Y, Burton EA, Visor G, Sanftner L, Severson P, Nguyen H, Kim MJ, Marimuthu 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 

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 

PDB-REDO

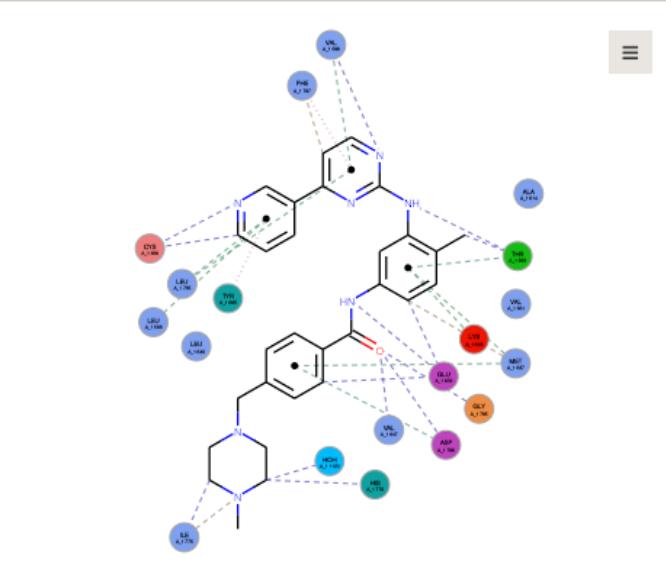
The sliders below show the change in model quality between original PDB entry and the PDB-REDO entry

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

Parameters

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

pdbId: 4r7i

chain: A_1

seqId: 1001

Response

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

Use case

Accessible residues for a PDB structure

Send a Sample Request

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"
    }
  ]
}
```

PDB - Get all FunPDB annotations for a PDB entry from a specific resource

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

https://wwwdev.ebi.ac.uk/pdbe/graph-api/pdb/funpdbe_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

label = ASA_alone
raw_score > 0

Use case

Ligands similar to drug Imatinib (STI)

The screenshot shows the PDBe website interface. On the left, there's a sidebar with various menu items under 'Compounds' and 'PDB'. The 'Get similar ligands' item is highlighted with a green box. The main area has a title bar with the URL <https://www.ebi.ac.uk/pdbe/graph-api/compound/similarity/:hetcode>. Below this, a 'Send a Sample Request' section contains a text input field with the same URL, a parameter input field with 'hetcode STI', and a 'Send' button. The response section displays a JSON-like code block:

```
j,
  "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",
        "C22"
      ]
    }
  ]
```

pdbe.org/aggregated-api

Teaching resources

PDBe API webinar series

PDBe

Protein Data Bank in Europe

1.0

Search docs

Introduction to PDBe programmatic access

Searching with the PDBe API

Creating complex PDBe API queries

Using the PDBe Graph API

Introduction

Use cases

PDBe tools in github

Data visualisation at PDBe

» Using the PDBe Graph API

View page source

Using the PDBe Graph API

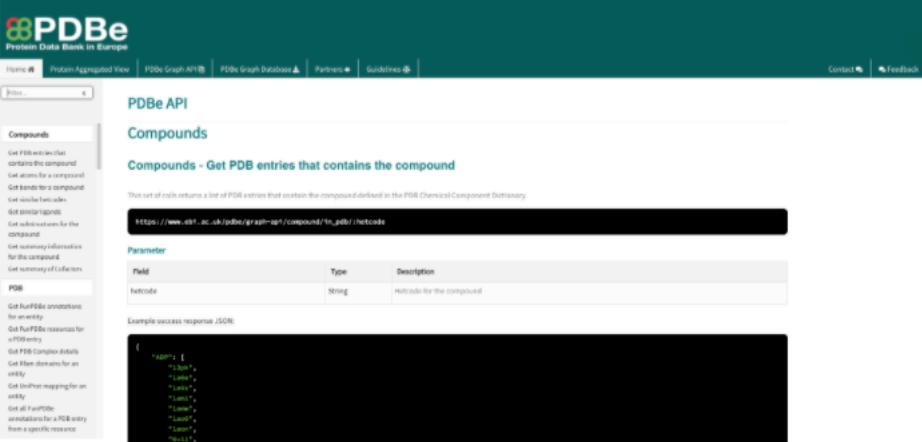
Introduction

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

Using the documentation

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



bit.ly/PDBe_API_webinars

Teaching resources – worked out examples

The screenshot shows a webpage from the PDBe API webinar series. The left sidebar contains navigation links for various topics like 'Introduction to PDBe programmatic access', 'Searching with the PDBe API', and 'Using the PDBe Graph API'. Under 'Using the PDBe Graph API', the 'Usecases' section is expanded, and the 'Predicated ligand binding sites in interaction interface' example is selected. This example is highlighted with a red border. The main content area has a title 'Predicated ligand binding sites in interaction interface' and a paragraph explaining how to use the annotations API to find predicted ligand binding sites. It includes a code snippet for a UniProt annotation request and a JSON response.

PDBe API webinar series

PDBe
Protein Data Bank in Europe

1.0

Search docs

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

Parameters

accession: P61626

Response

```
{  
  "P61626": [  
    {"sequence": "  
      \"MKALIVLGLVLLSVTVQGKIVFERCELARTLKRLGMDGYRGISLANWNLAKWESGYNTRATNYNAGDRSTOYQIFQINSRYWCNDGKTPGAVNACH  
      LSCSALLQDNIAIAWACAKRVRDPGIRAWVAMRNRCQNRDVRQYVQGCGV\",  
    \"length\": 148,  
    \"dataType\": \"ANNOTATIONS\",  
    \"id\": \"P61626_1\"}  
  ]}
```

bit.ly/PDBe_API_webinars

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**

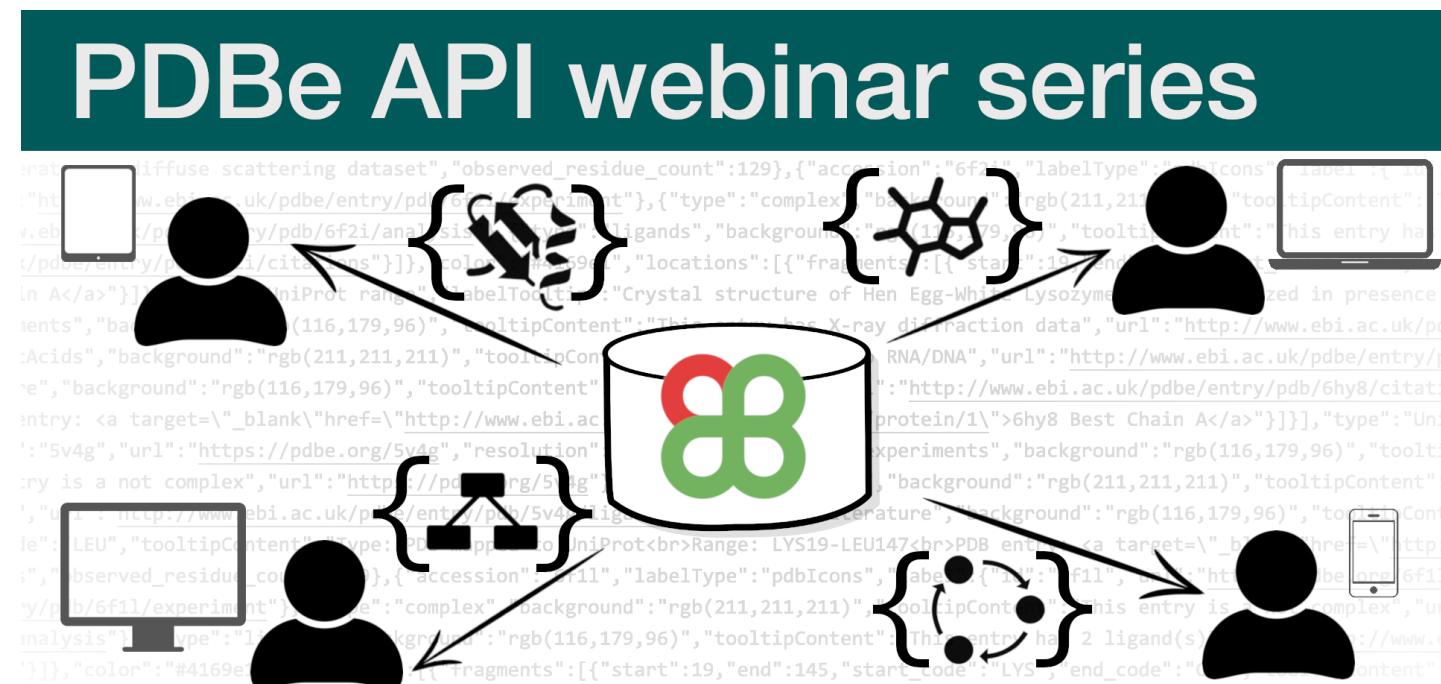
Oct 13th **PDBe tools in github**

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
- Or visit the PDBe events pages at PDBe.org/events
- Remember to register for each webinar individually!!!



bit.ly/PDBe_API_webinars

Thank you for your attention!

Any questions?

PDBe.org/graph-api



Sreenath Nair