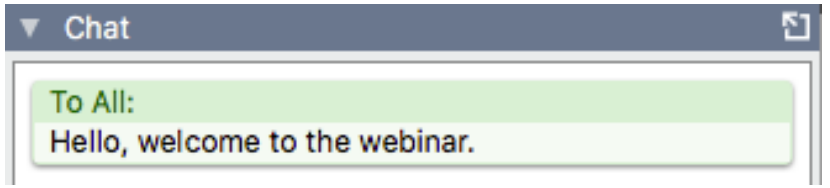
Welcome - webinar instructions

- 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

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proteindatabank
@PDBeurope
proteindatabank
pdbeurope
pdbart

PDBe
Protein Data Bank in Europe

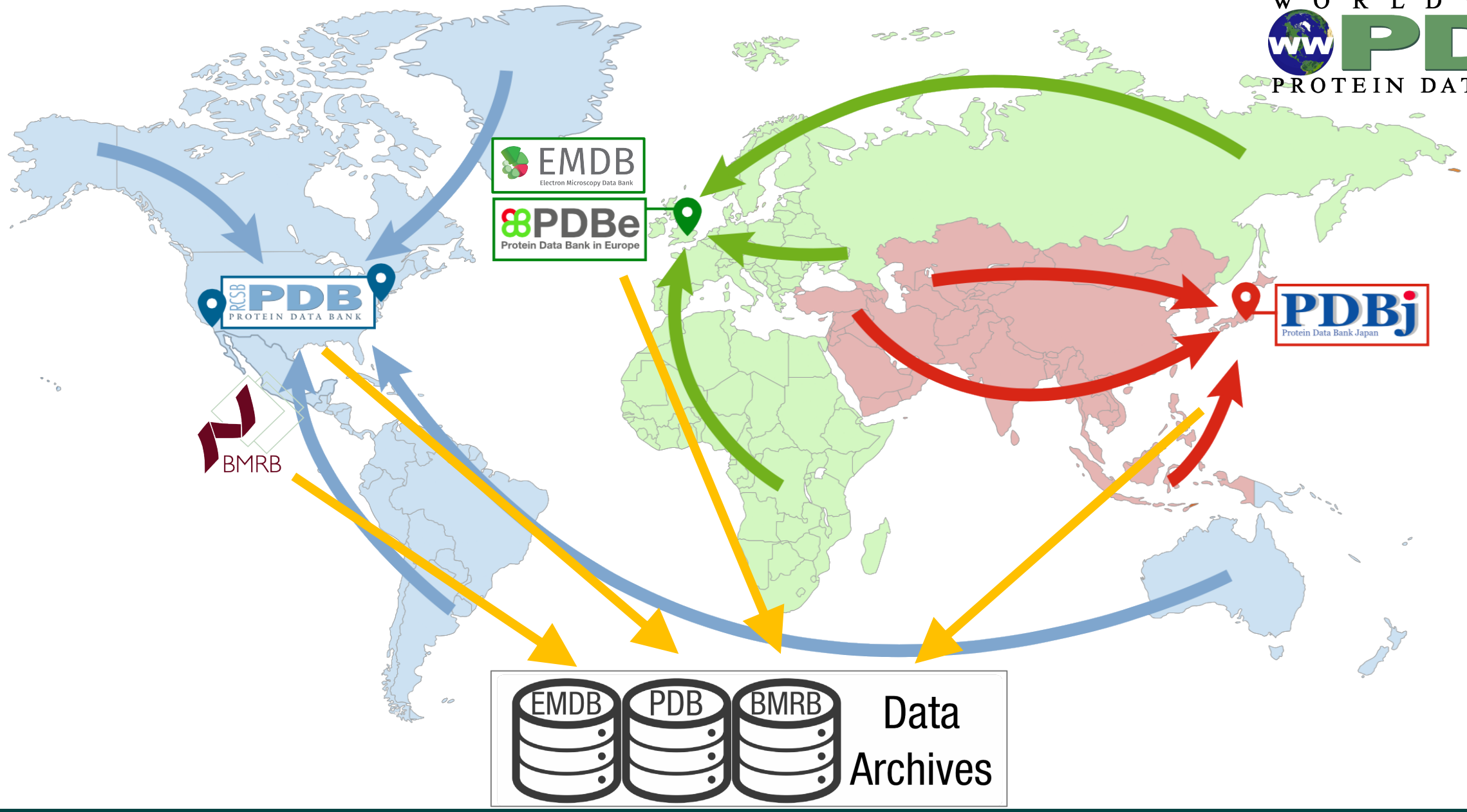
EMBL-EBI

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

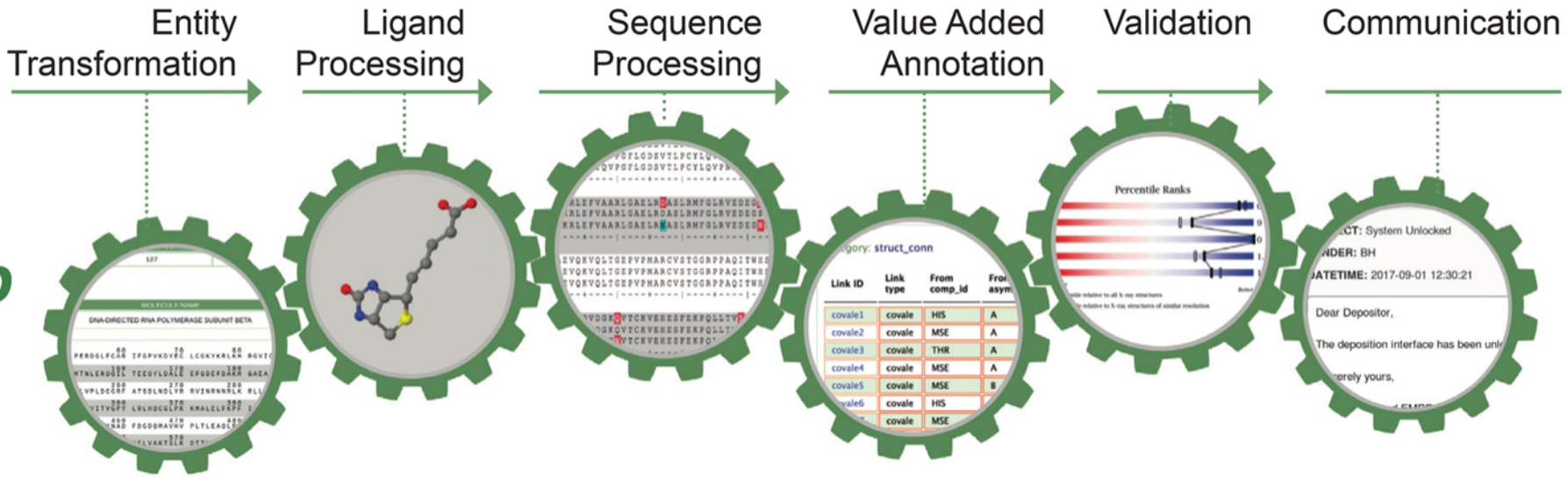
Summary of the webinar

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

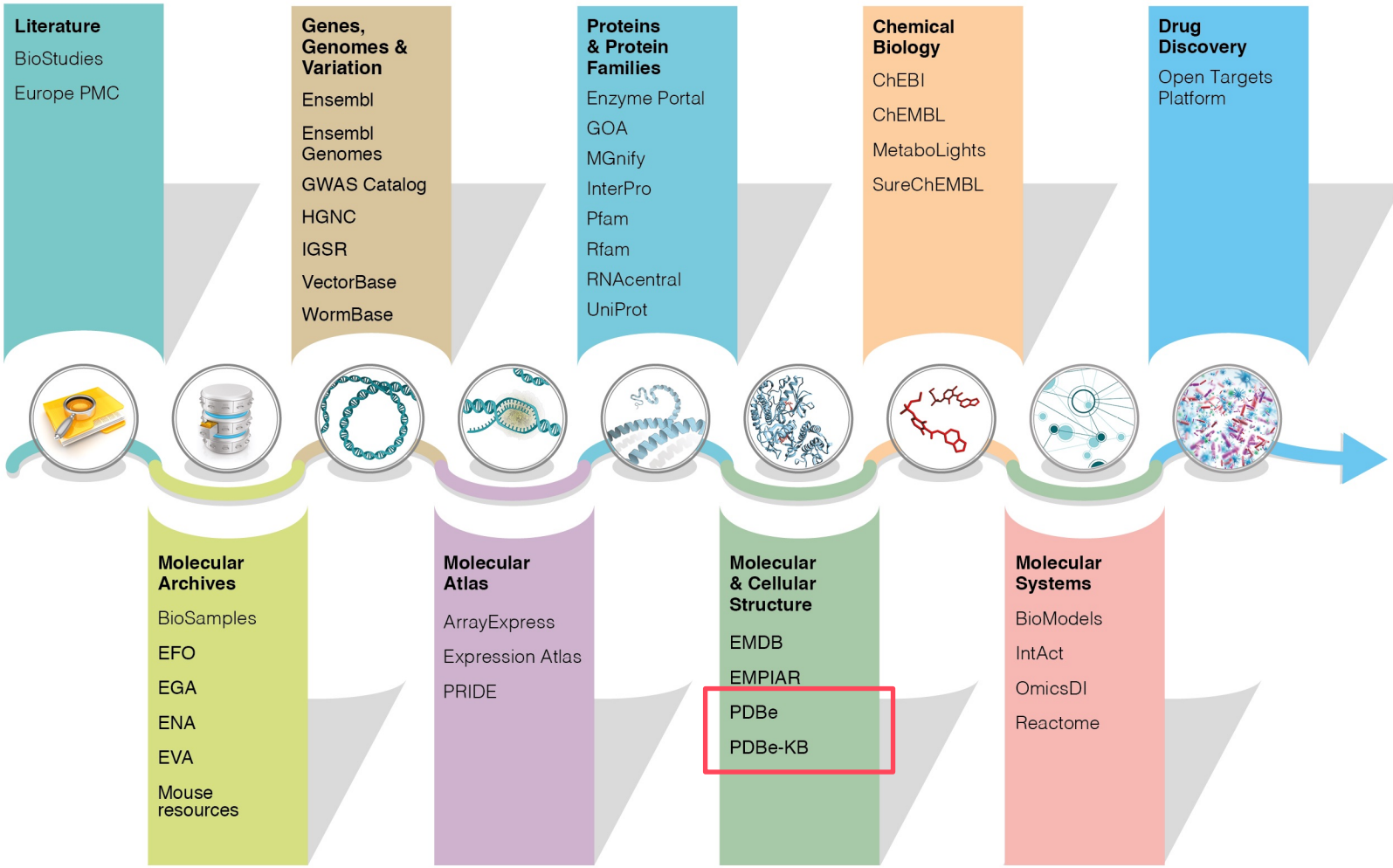

WORLDWIDE PDB
PROTEIN DATA BANK
EMDB
Electron Microscopy Data Bank
PDBe
Protein Data Bank in Europe
RCSB PDB
PROTEIN DATA BANK
PDBj
Protein Data Bank Japan
BMRB
EMDB
PDB
BMRB
Data Archives

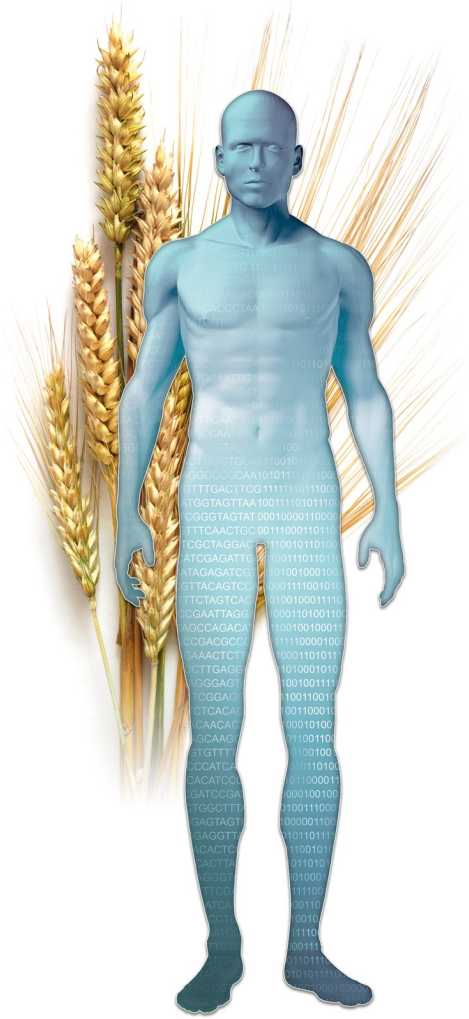
Data added through deposition

- 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

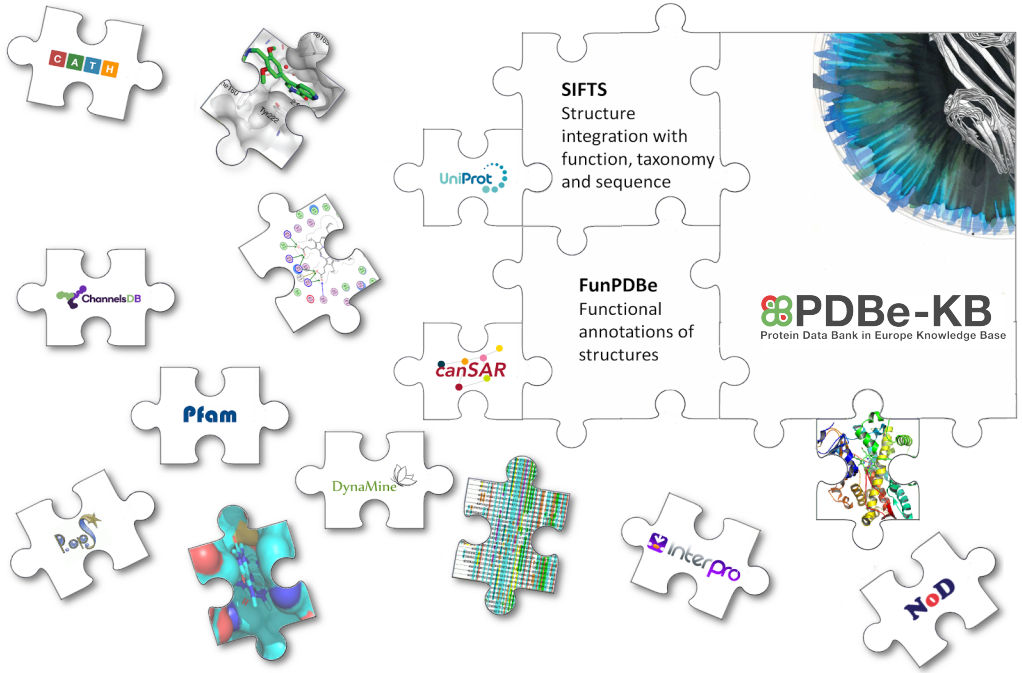




Protein Data Bank in Europe - Knowledge Base (PDBe-KB)

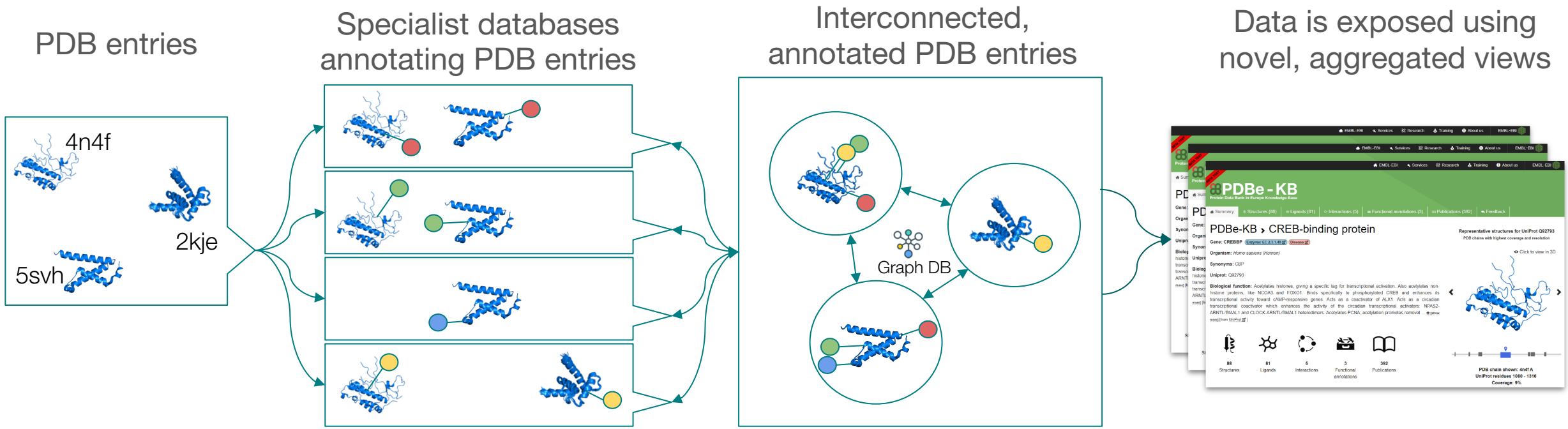
Placing macromolecular structure data in their biological context by establishing a community-driven, integrated resource for structural annotations to promote basic and applied research

- 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



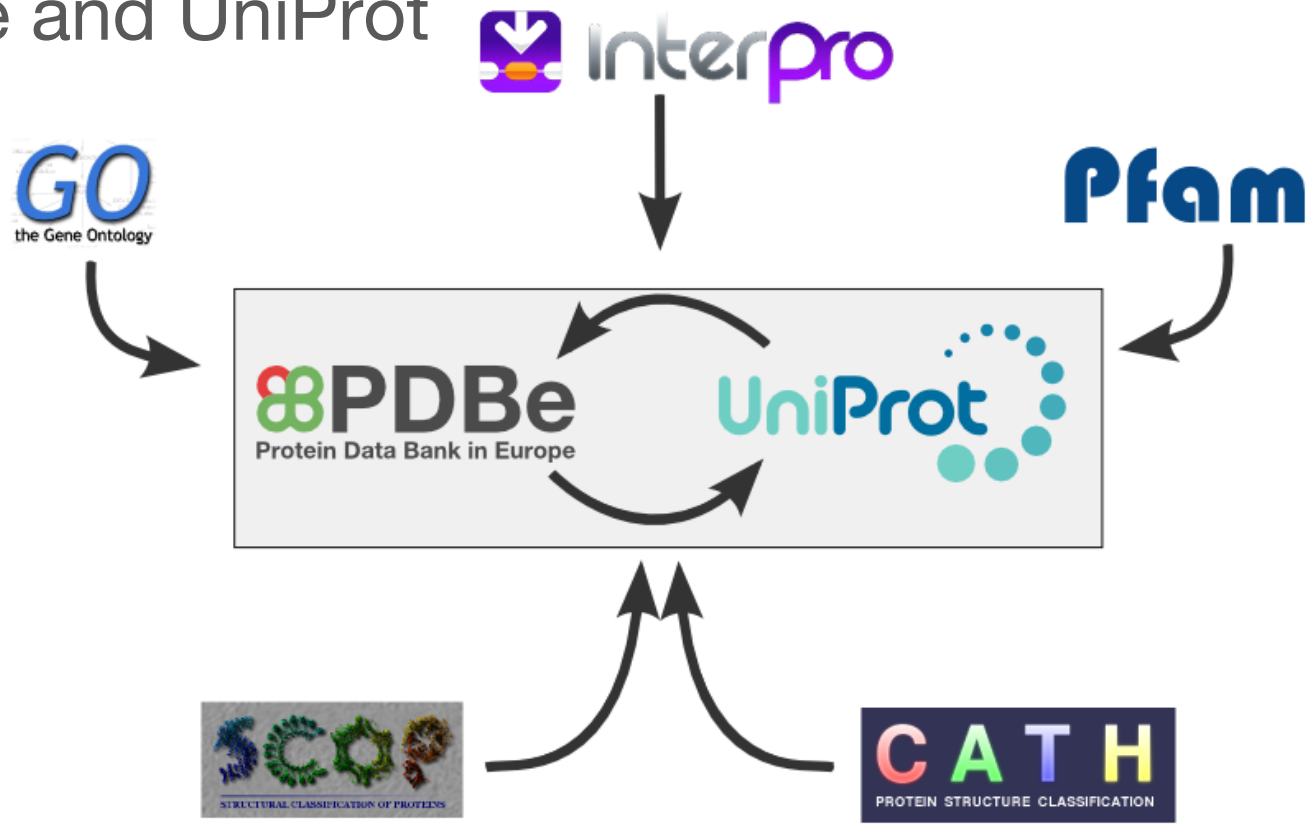
- Domains
- Rfam classification
- Functional sites (e.g. ligand binding)
- Post-translational modifications
- Physico-chemical parameters (residue depth, flexibility, etc.)
- Interacting residues/interfaces

WORLDWIDE PDB PROTEIN DATA BANK

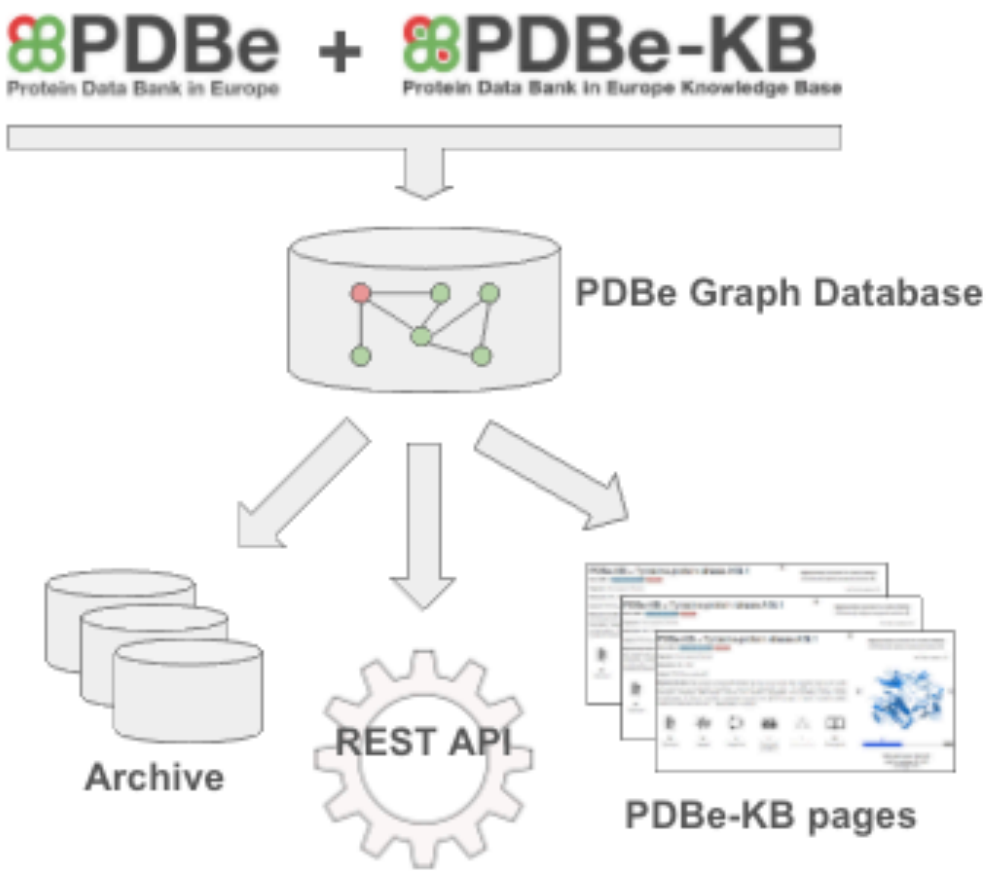
PDBe-KB
Protein Data Bank in Europe Knowledge Base

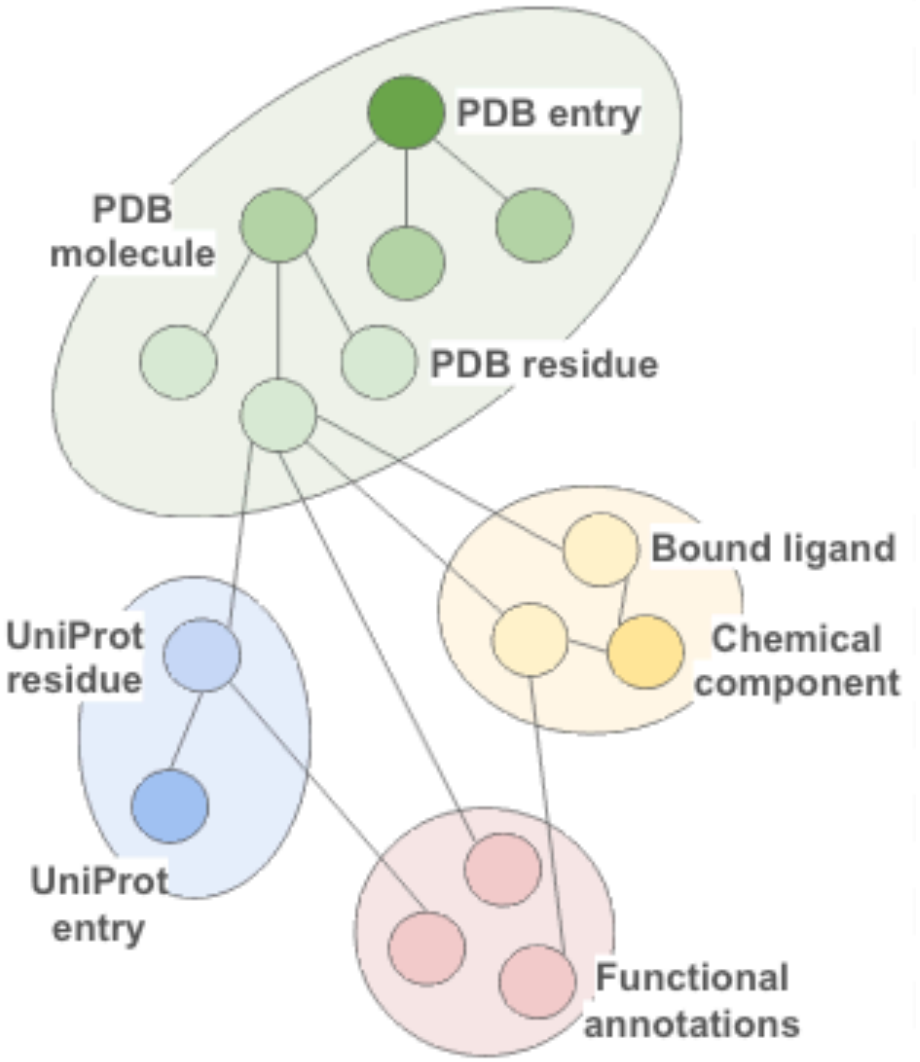
SIFTS

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



PDBe Graph Database



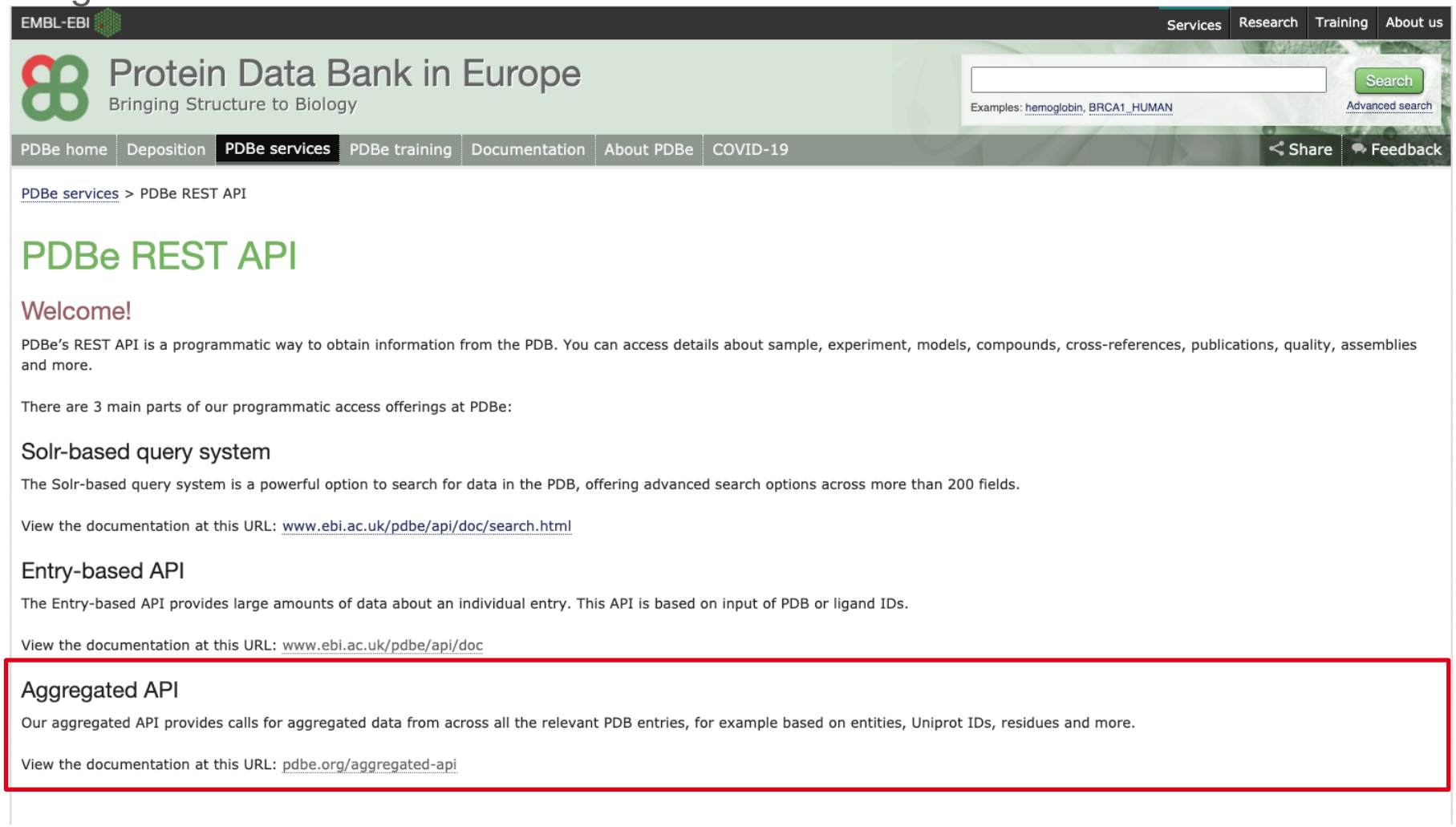


PDBe.org/graph-download

EMBL-EBI

PDBe API

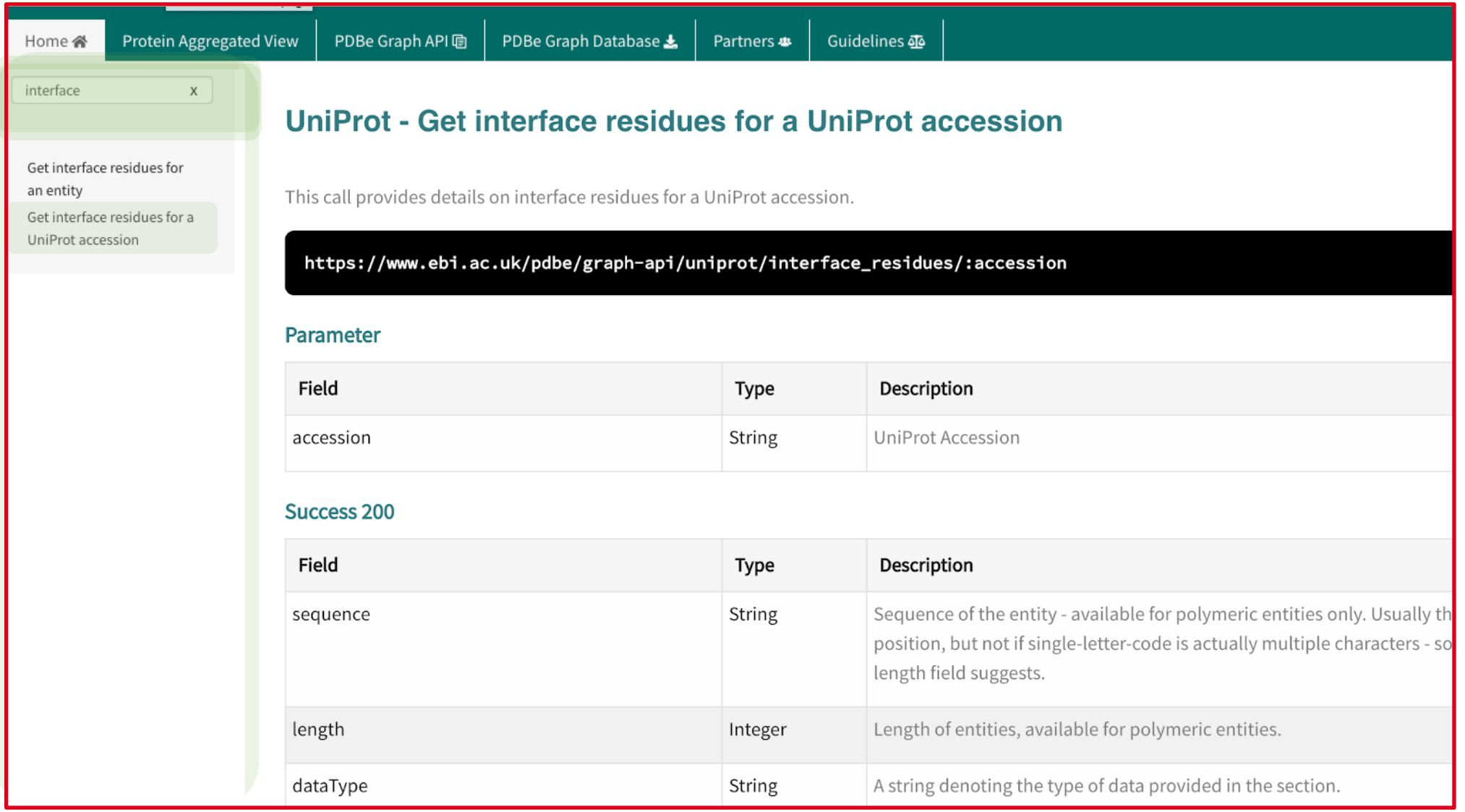
Programmatic access to PDB data



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



PDBe.org/ aggregated-api

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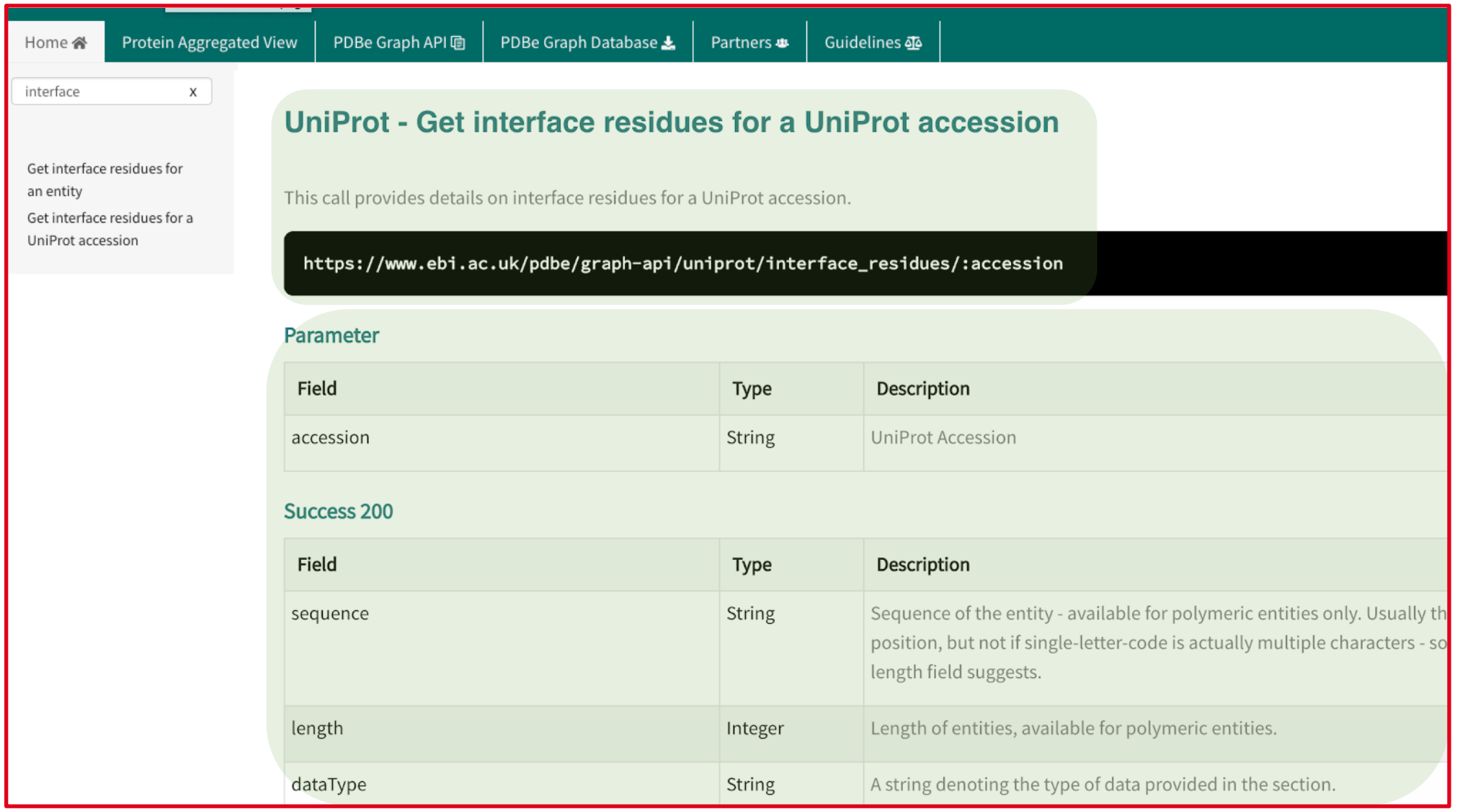
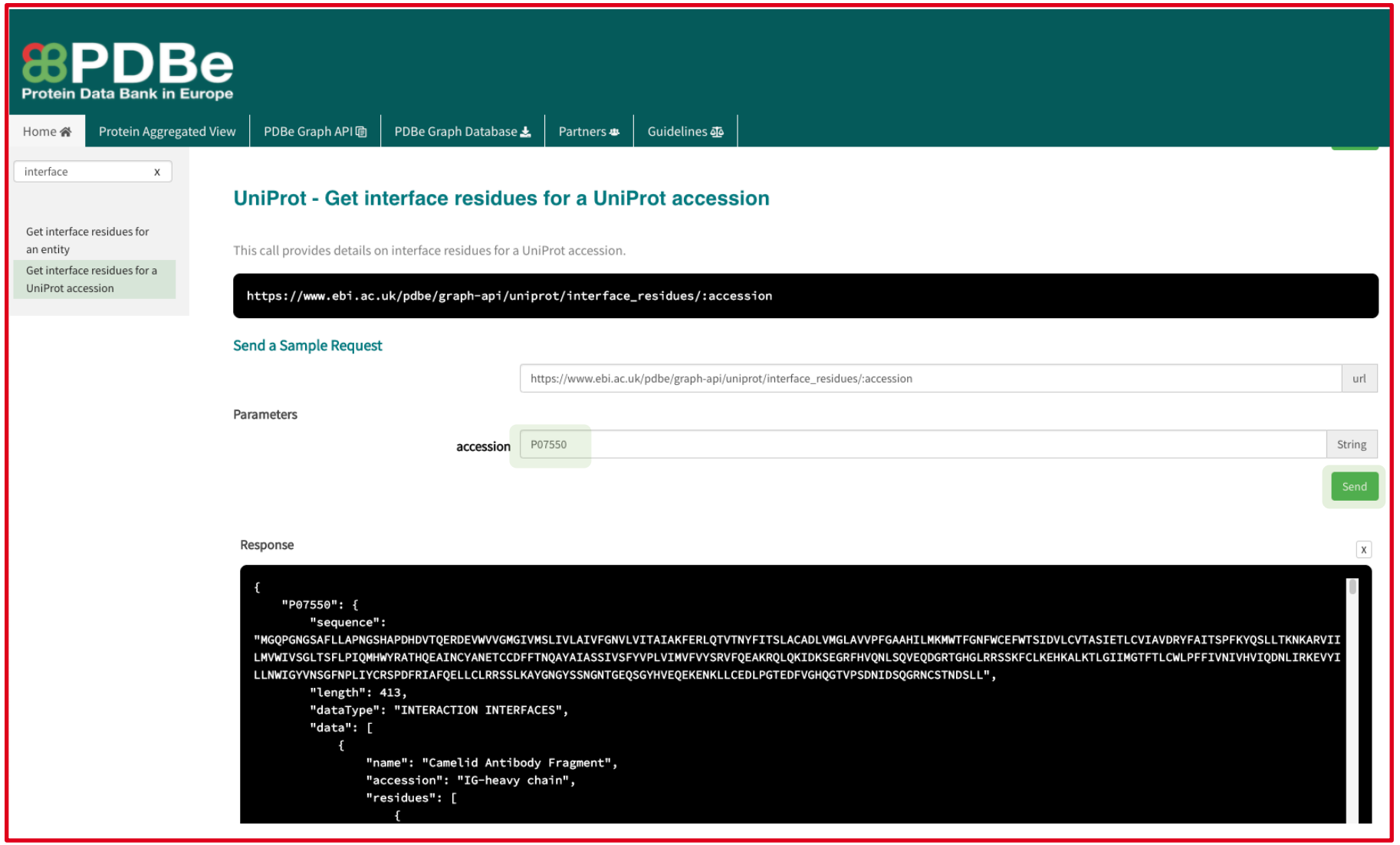
API Documentation



API Documentation



PDBe.org/ aggregated-api

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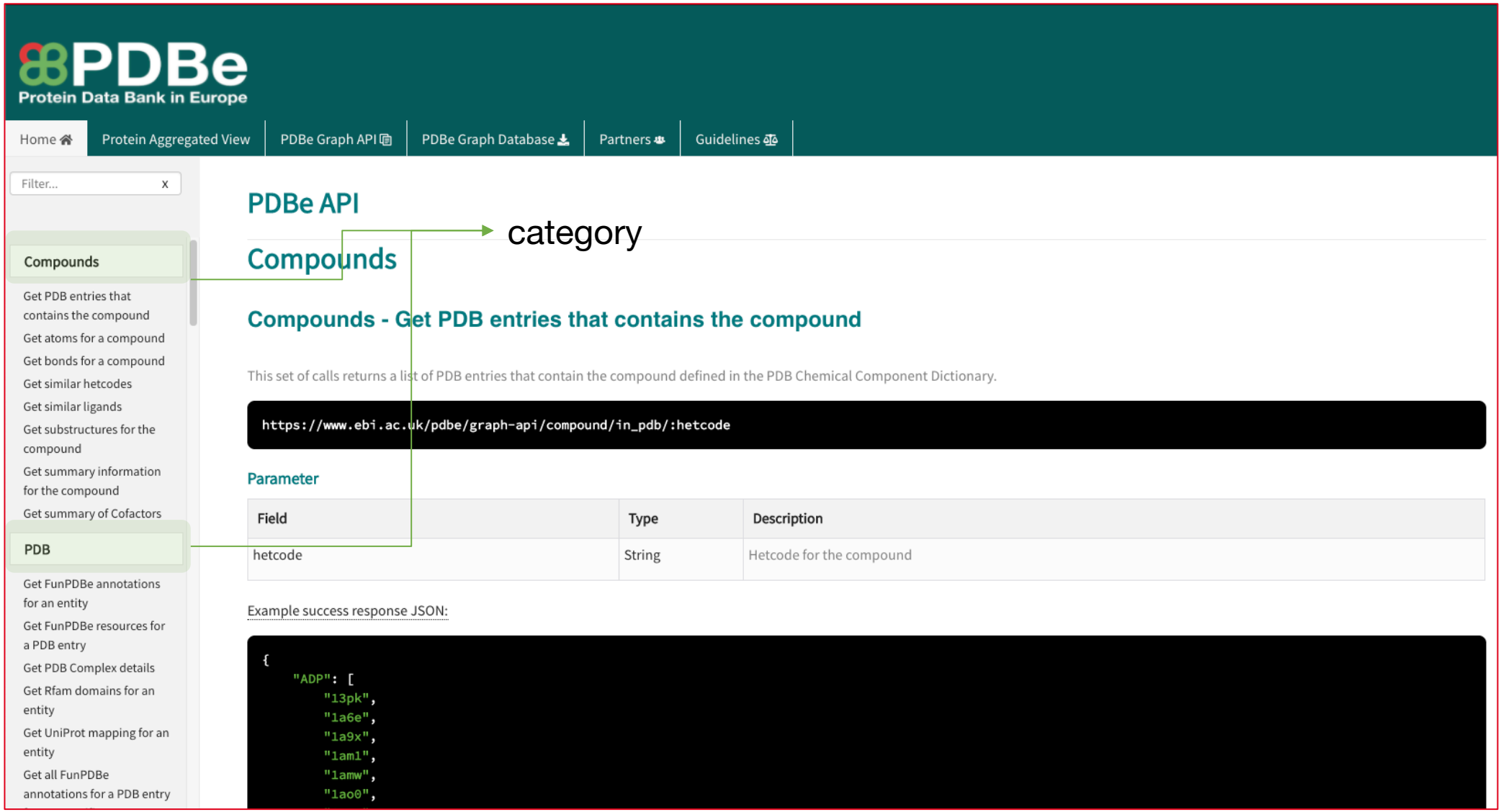
API Documentation



PDBe.org/ aggregated-api

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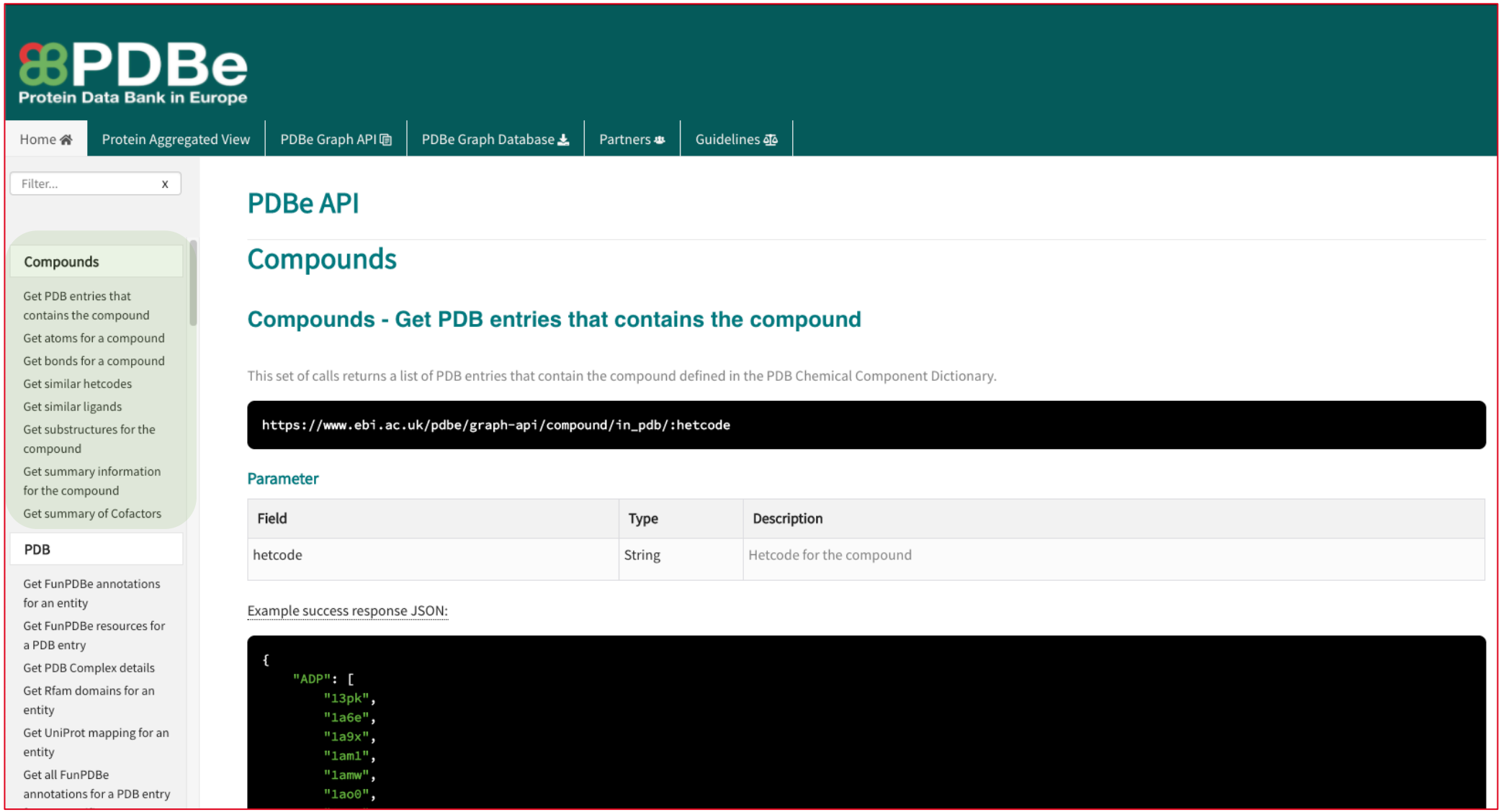
API Documentation - Compounds



PDBe.org/ aggregated-api

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API Documentation - Compounds

PDBe
Protein Data Bank in Europe

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

Filter...

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

Send a Sample Request

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

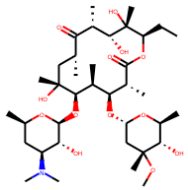
Parameters

hetcode ERY String

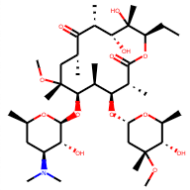
Send

Response


```
{
    "ERY": [
        {
            "stereoisomers": [],
            "same_scaffold": [
                {
                    "chem_comp_id": "CTY",
                    "name": "CLARITHROMYCIN",
                    "substructure_match": [
                        "O4",
```

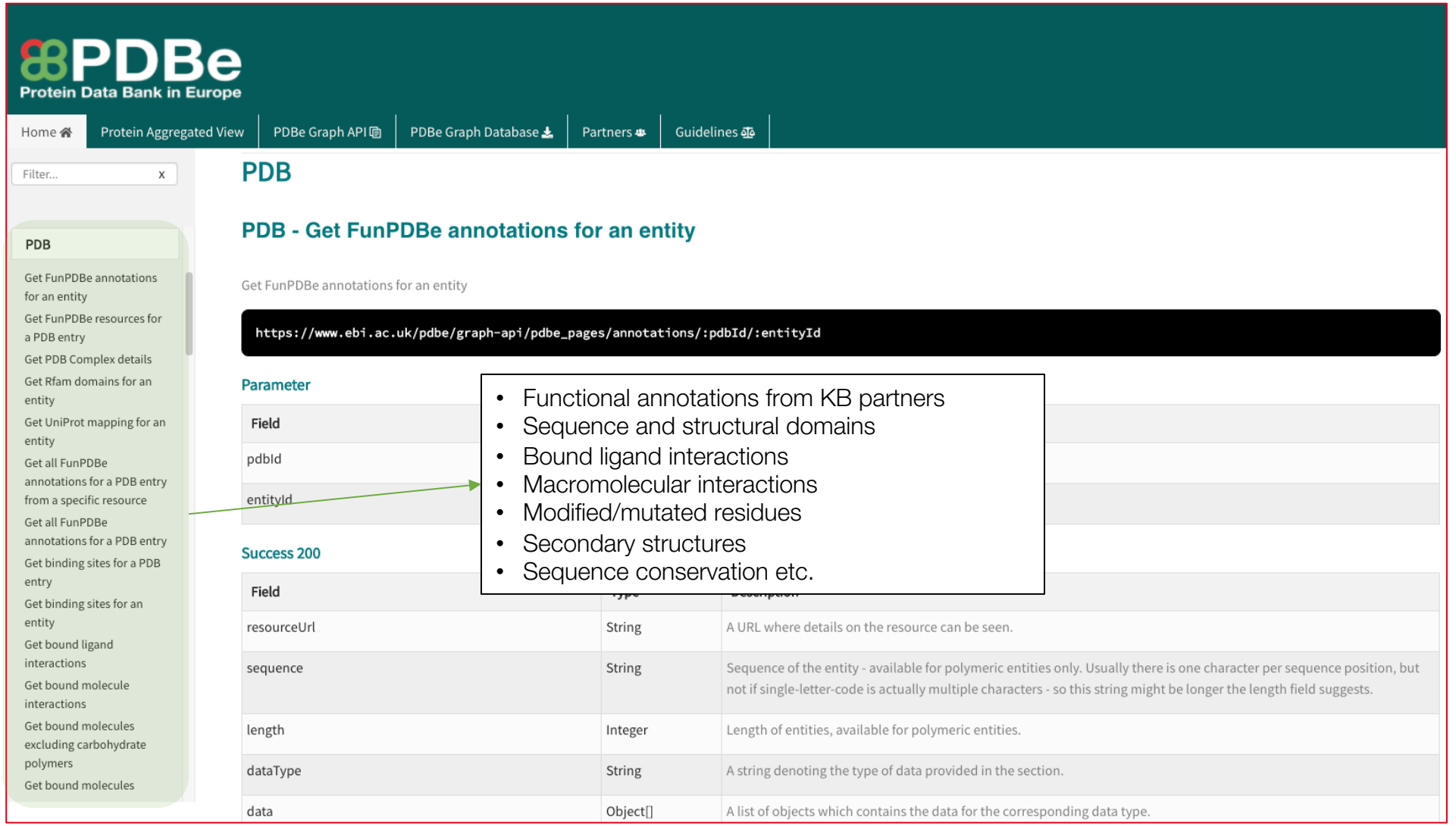



ERYTHROMYCIN



CLARITHROMYCIN

API Documentation - PDB



PDBe.org/ aggregated-api

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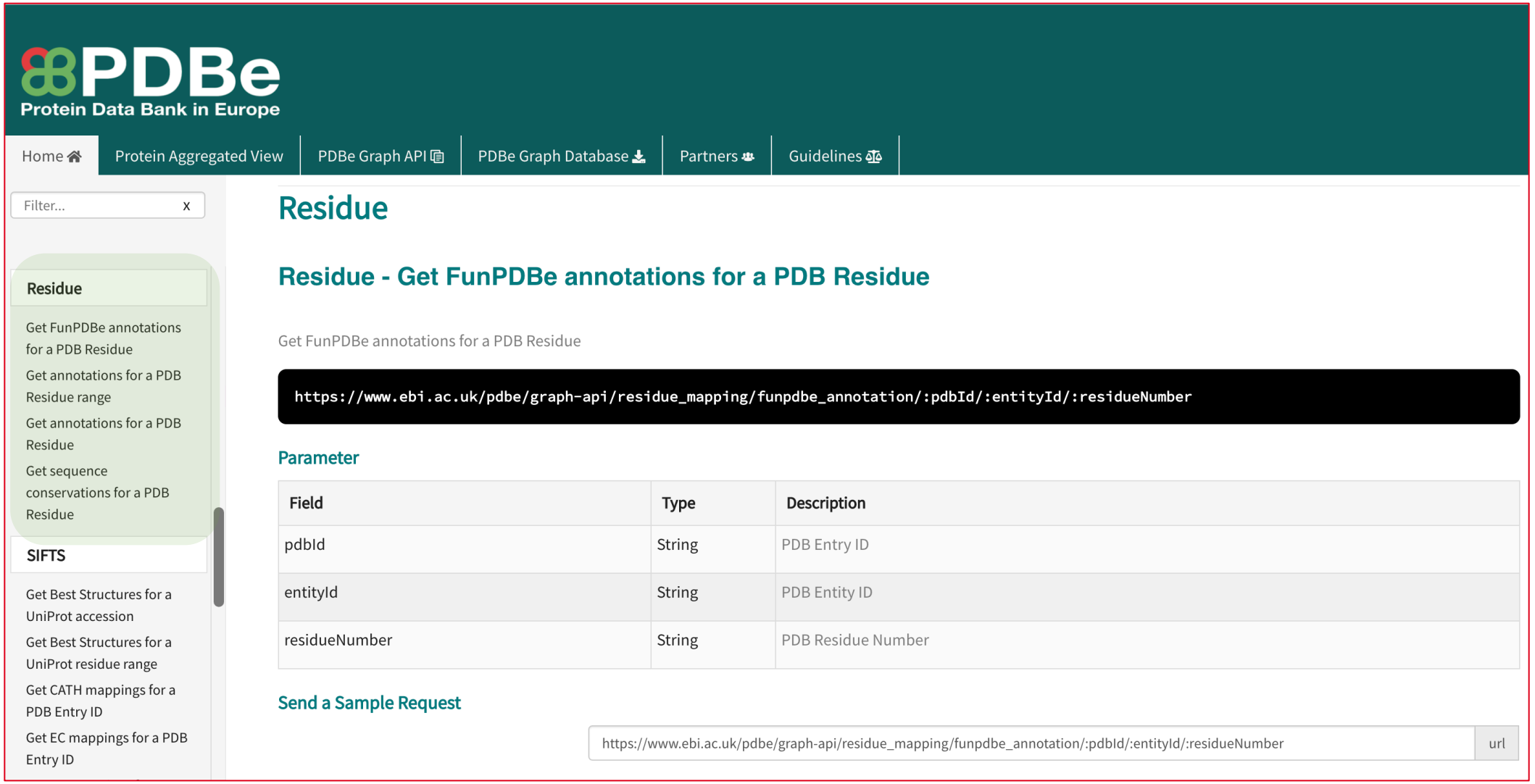
API Documentation - Residue



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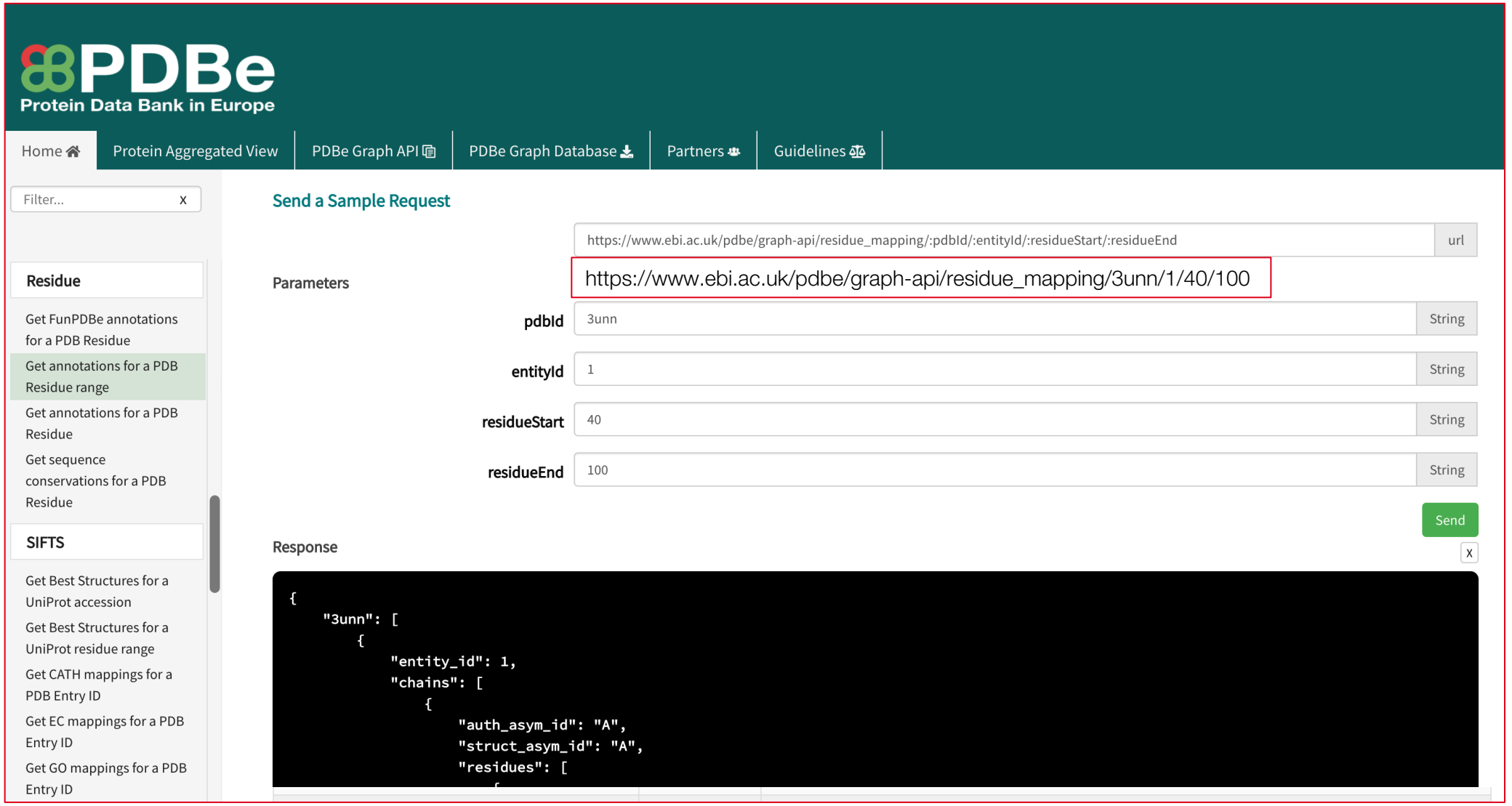
API Documentation – Residue annotations



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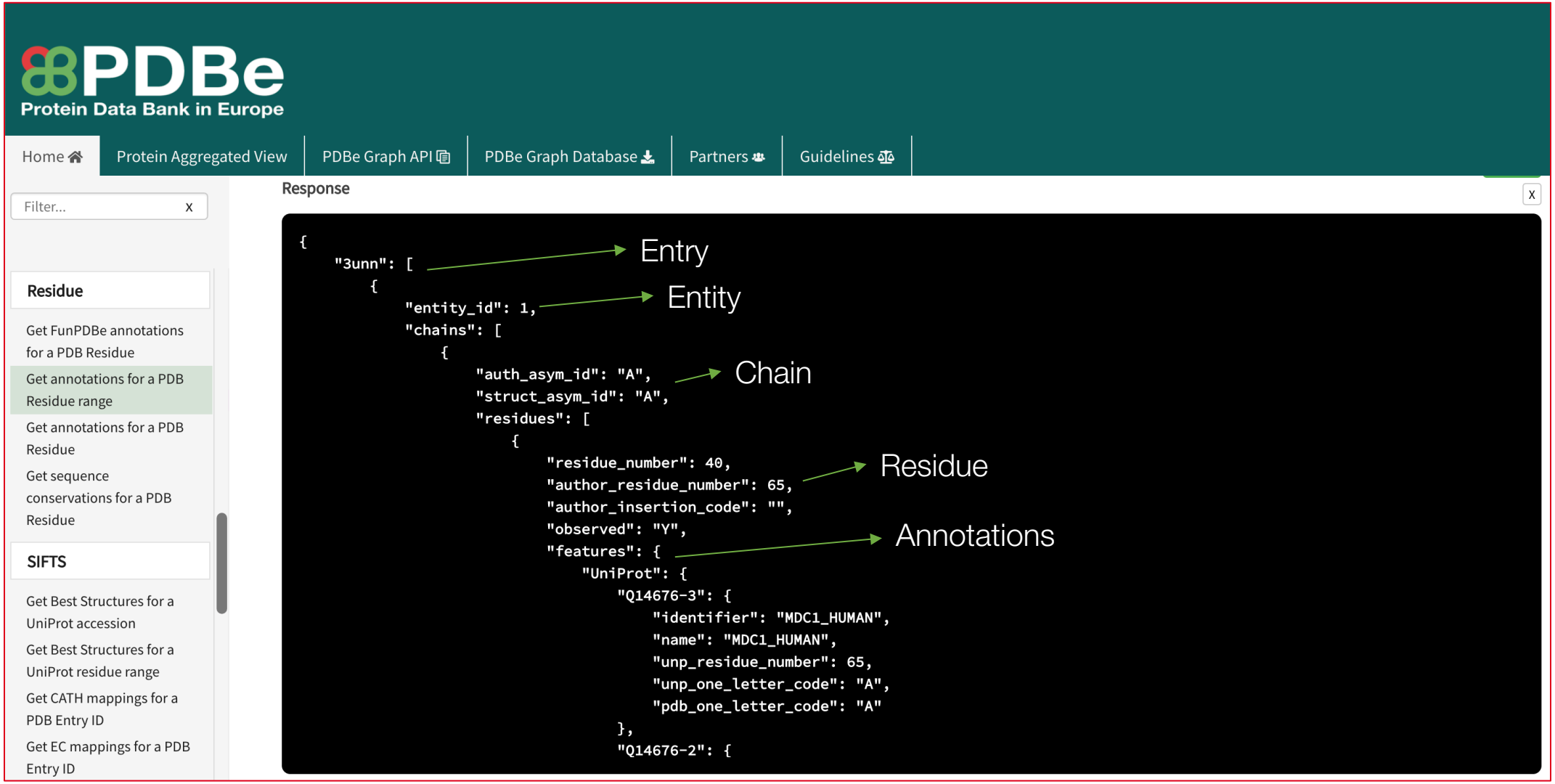
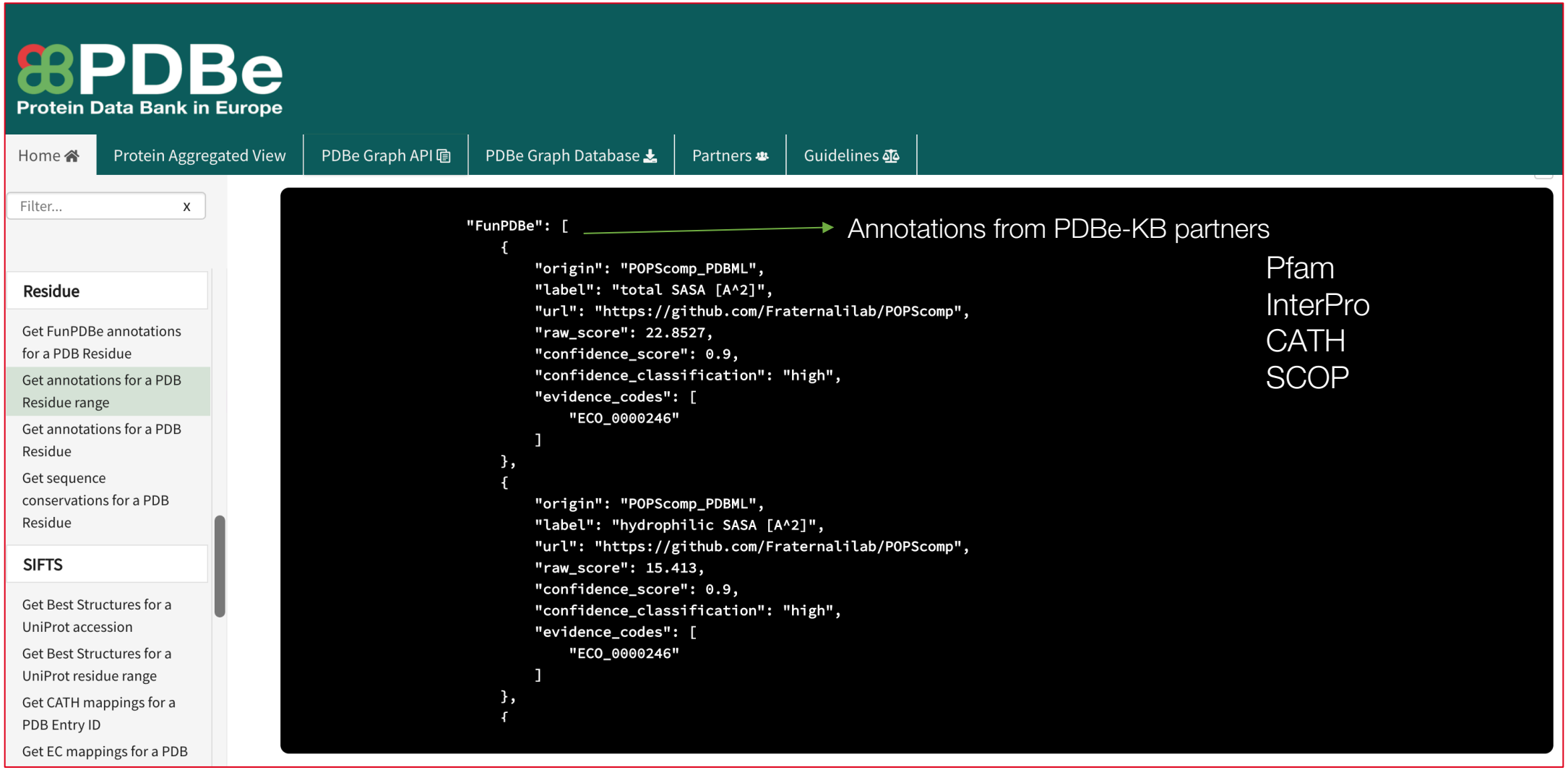
API Documentation – Residue annotations



API Documentation – Residue annotations



PDBe.org/ aggregated-api

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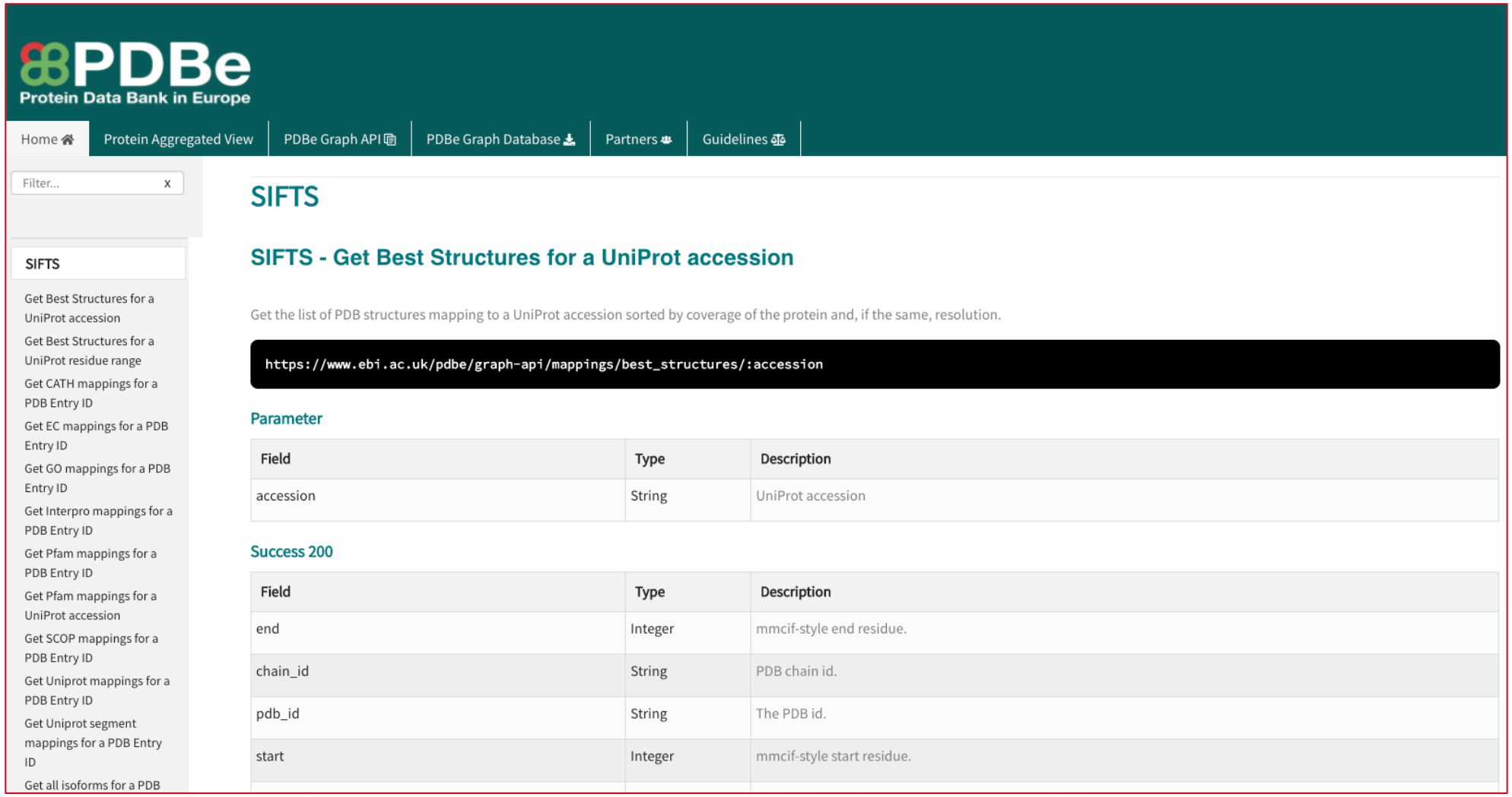
API Documentation – SIFTS



PDBe.org/ aggregated-api

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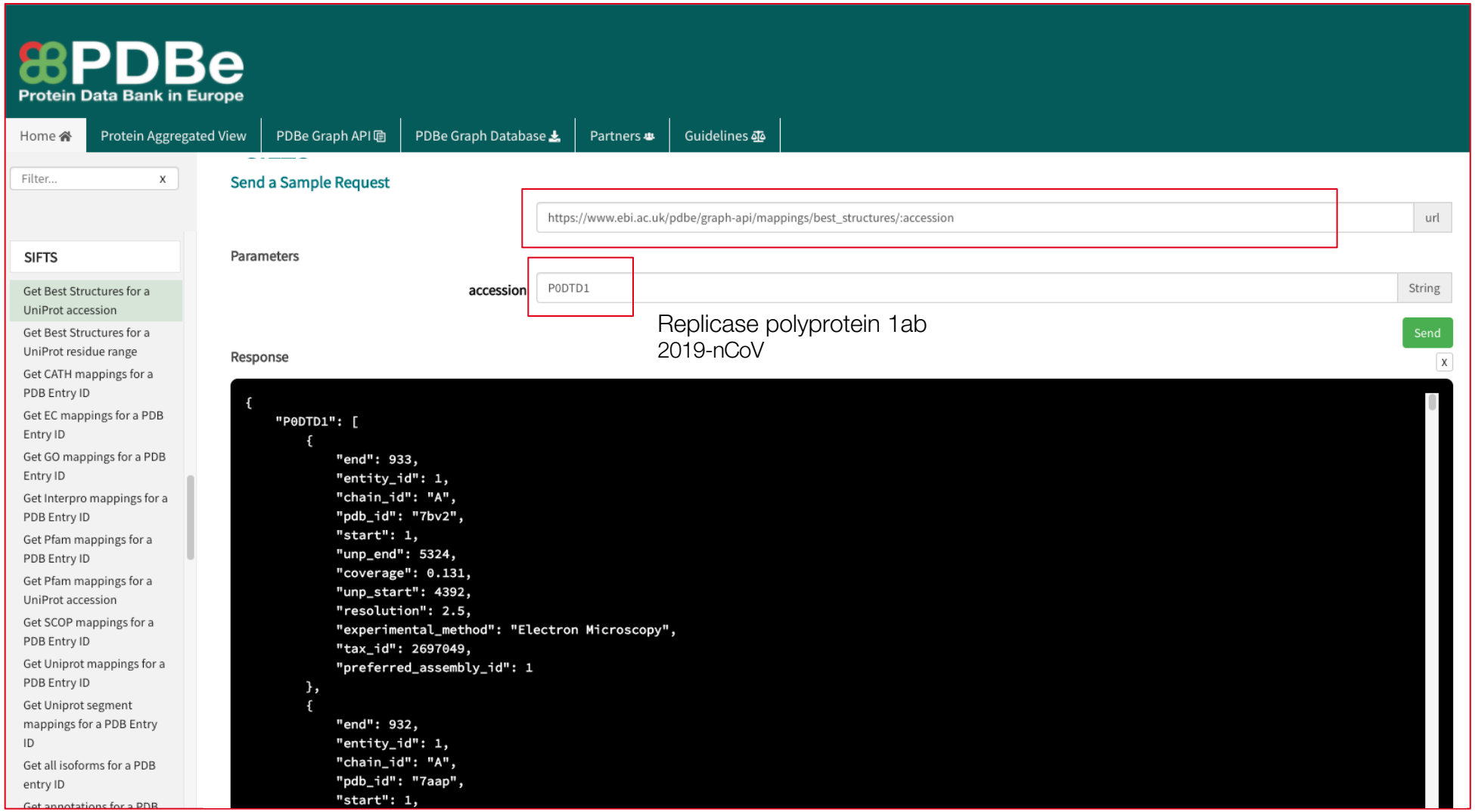
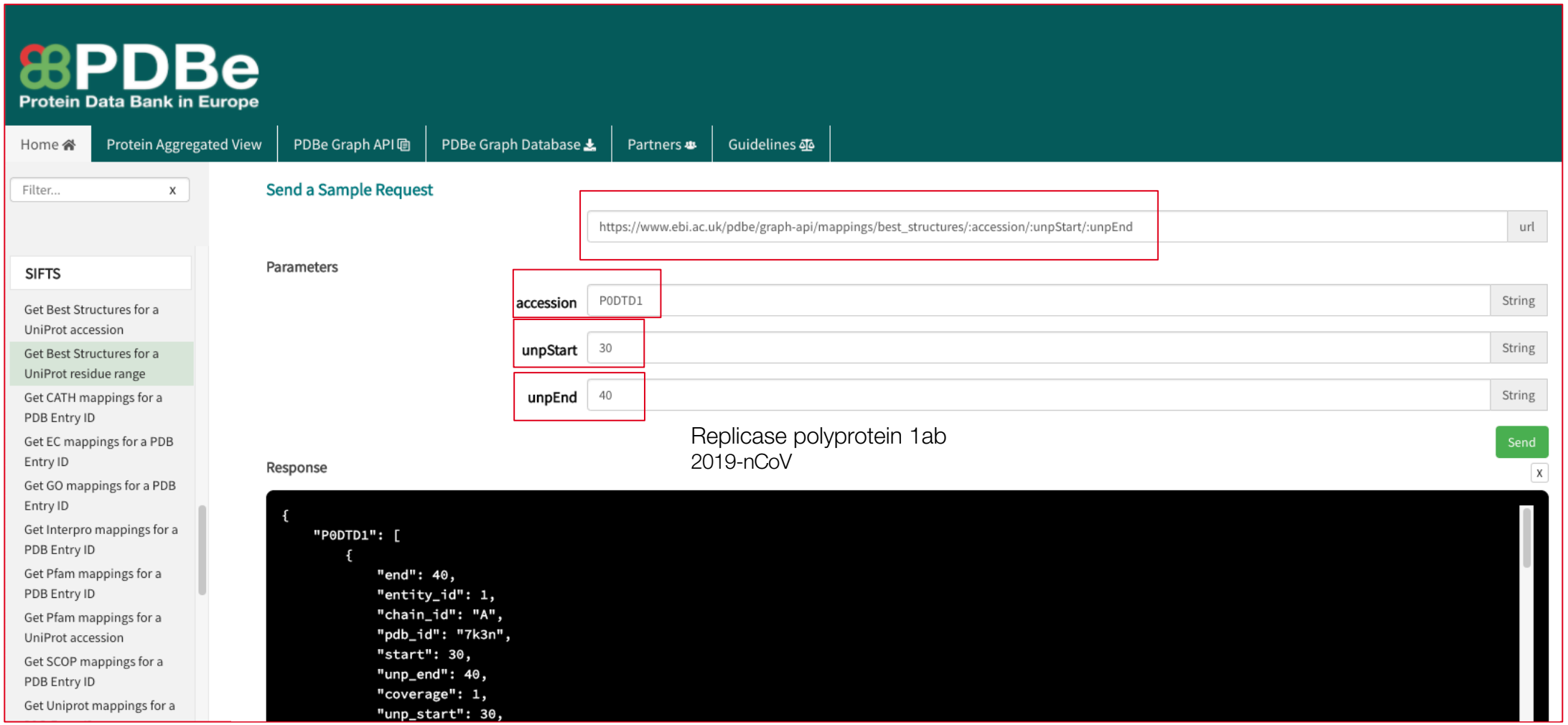
API Documentation – SIFTS



PDBe.org/ aggregated-api

EMBL-EBI

API Documentation – SIFTS



PDBe.org/ aggregated-api

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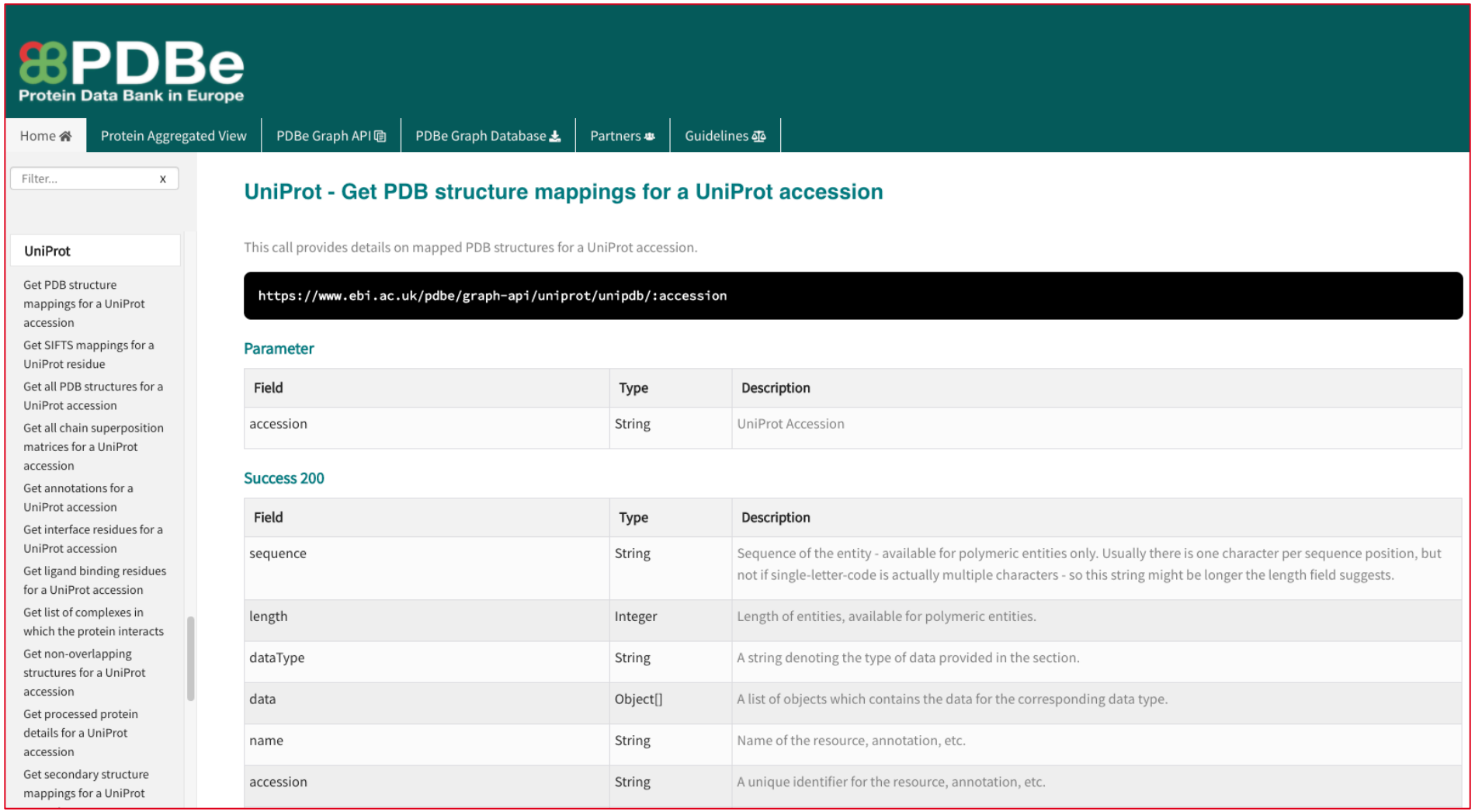
API Documentation – UniProt



PDBe.org/ aggregated-api

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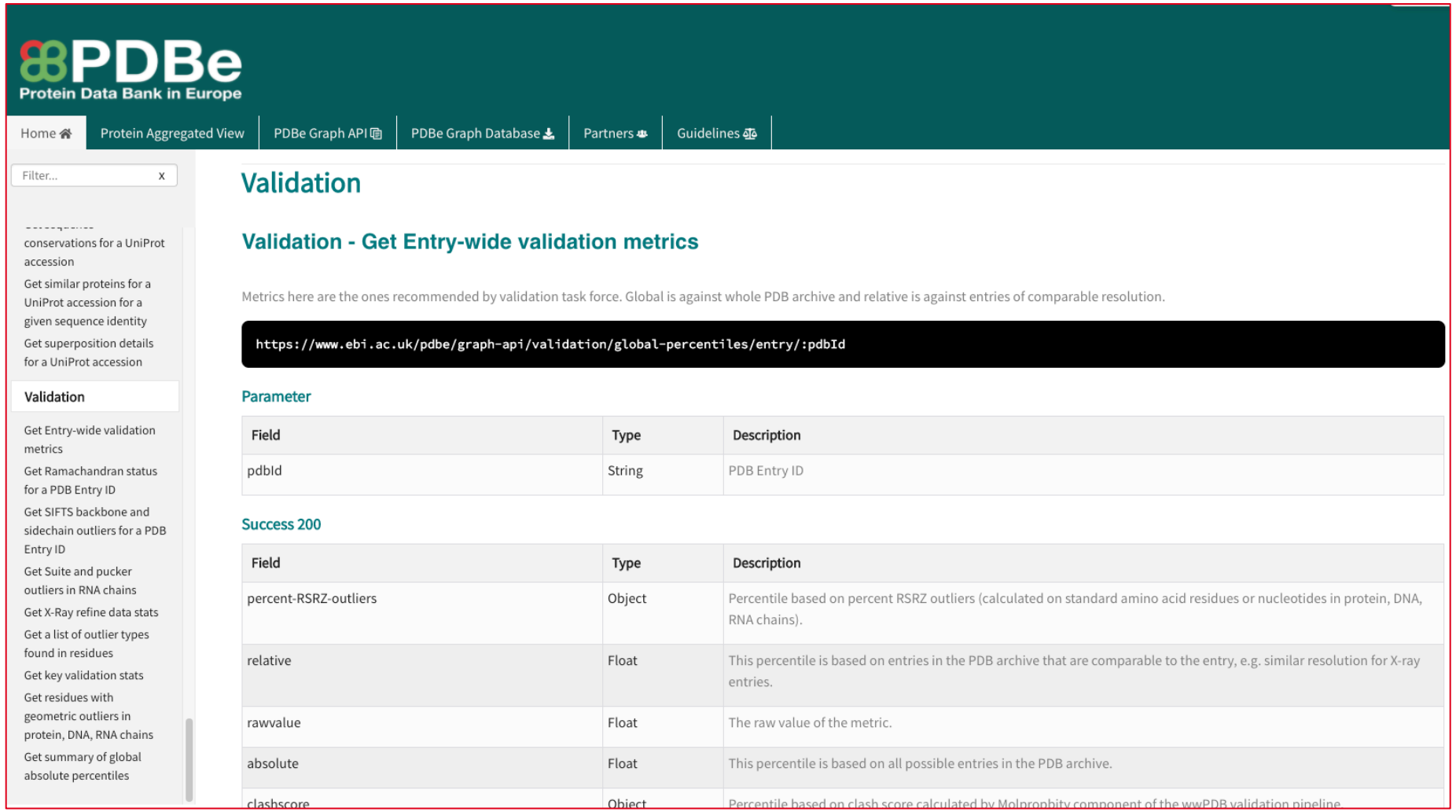
API Documentation – Validation



PDBe.org/ aggregated-api

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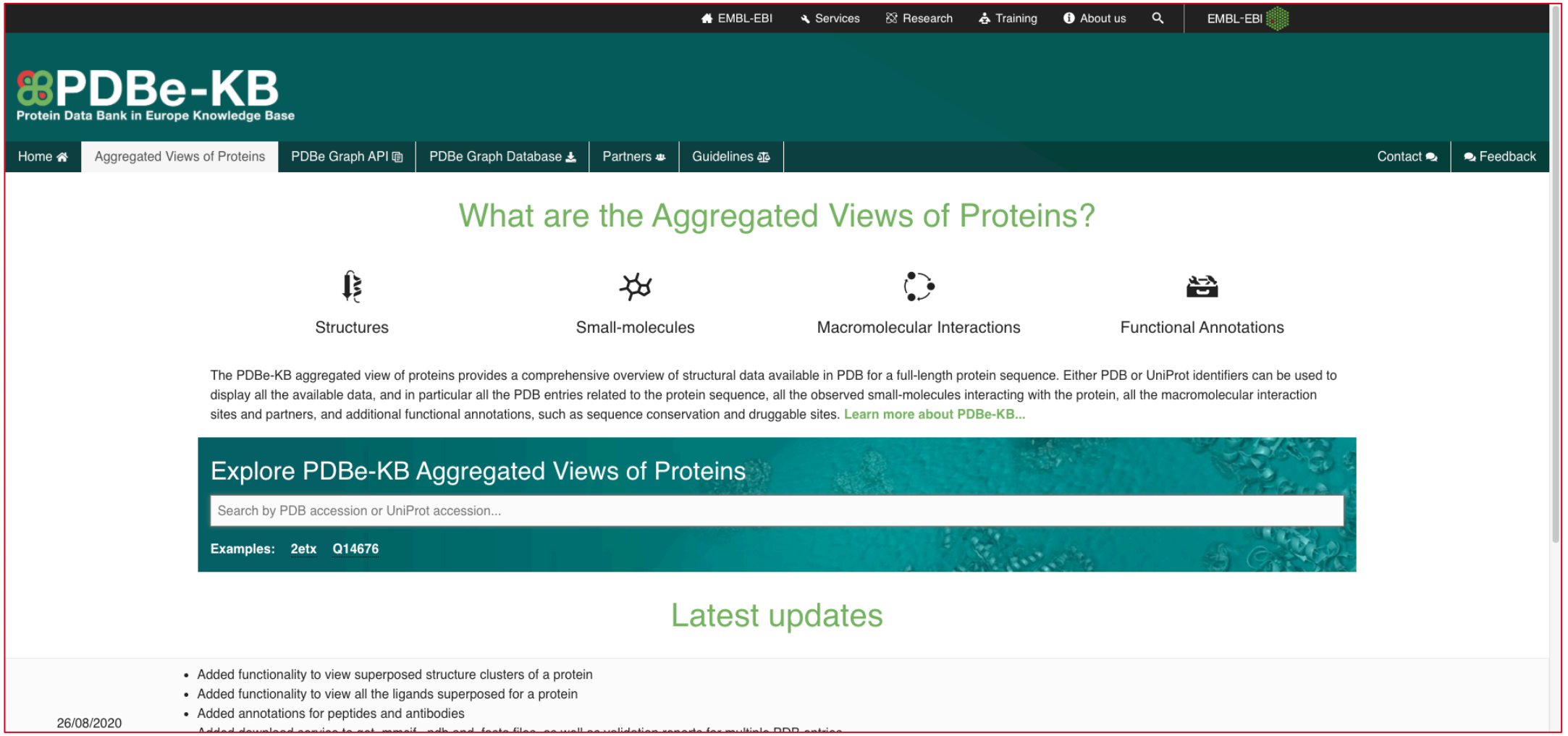
Where do we use it?

Aggregated views of proteins



pdbe-kb.org/protein

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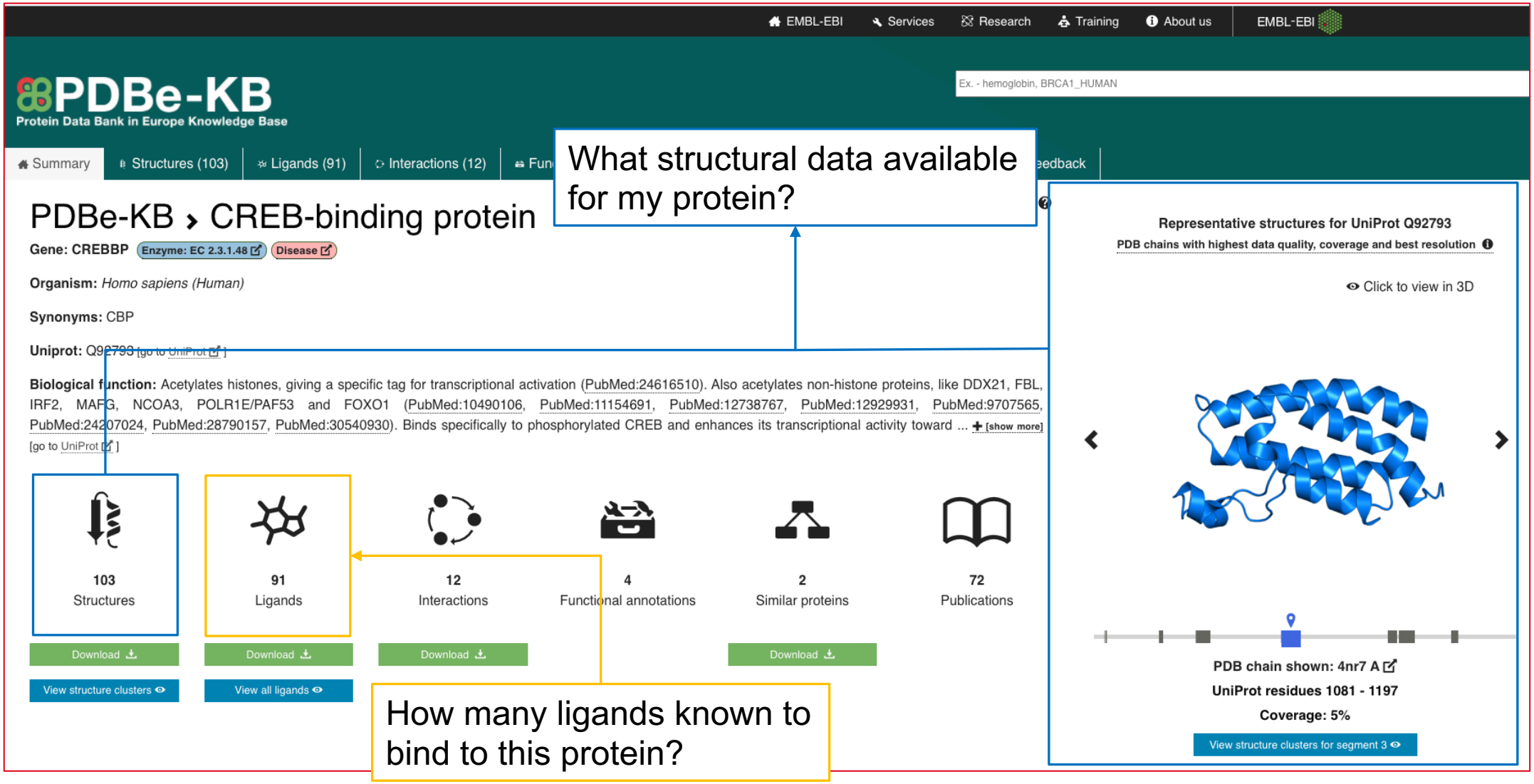
Aggregated views of proteins



CREB-binding protein, structures available in PDB

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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.

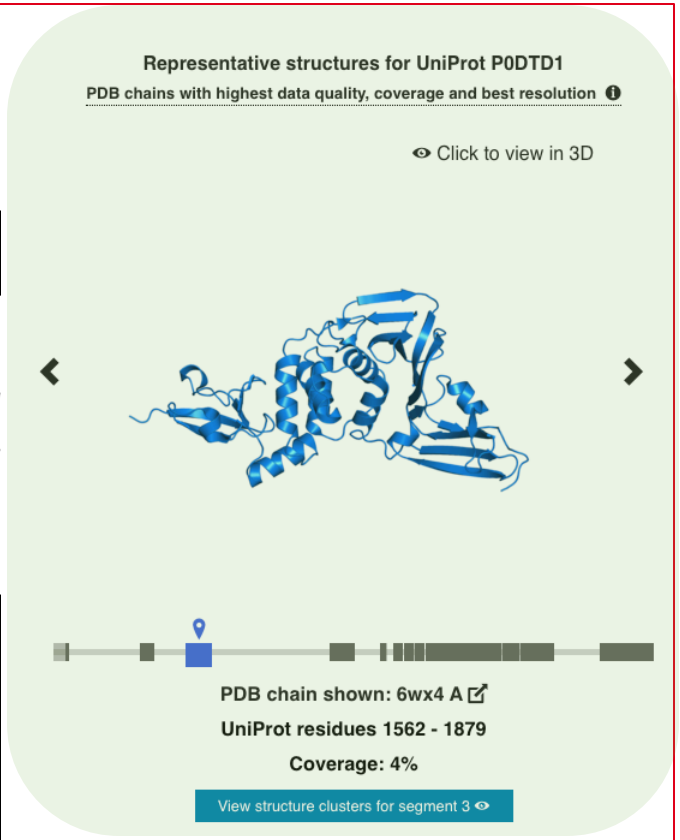
```
https://www.ebi.ac.uk/pdbe/graph-api/uniprot/best_non_overlapping_structures/:accession
```

Parameters

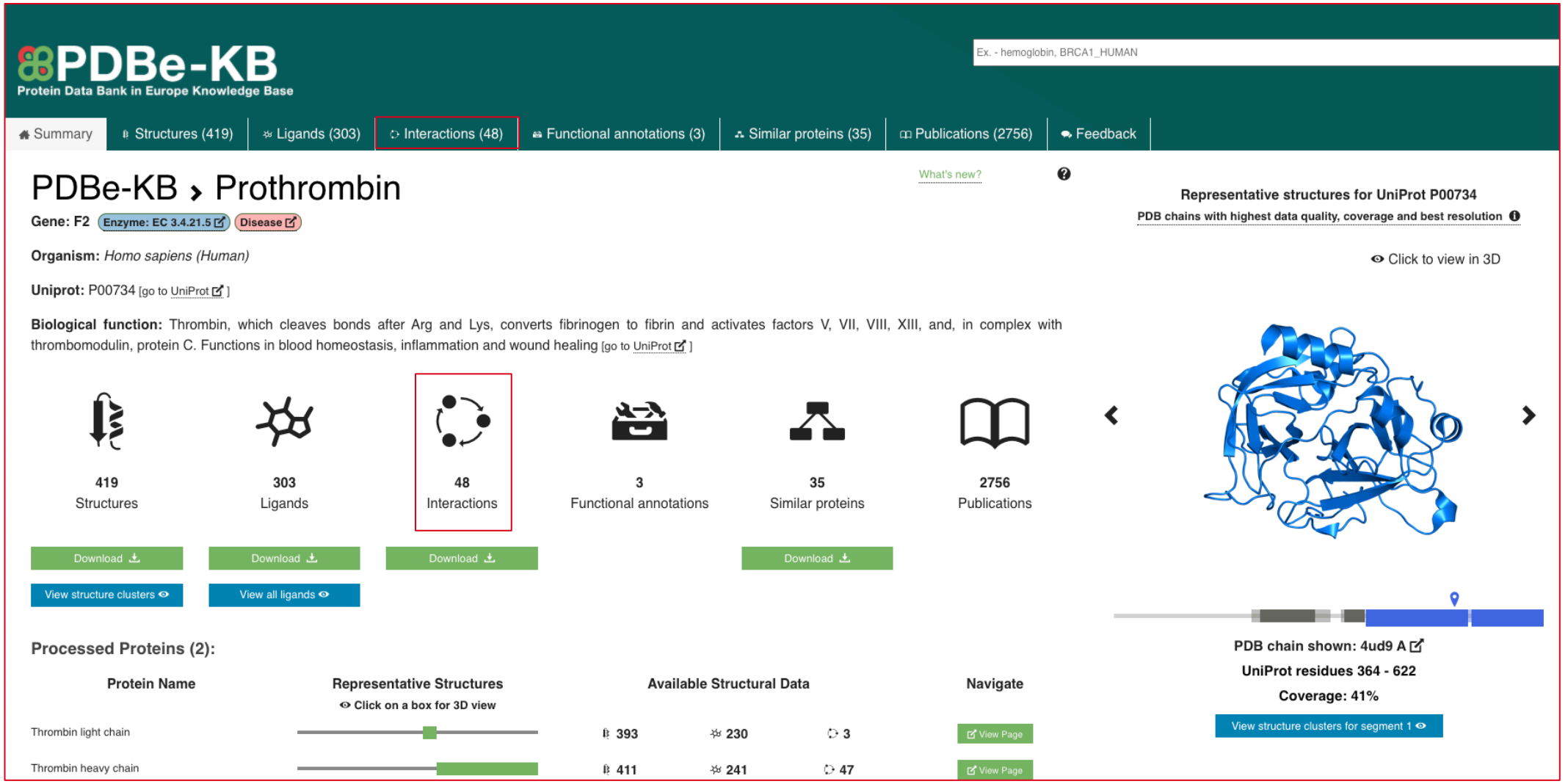
accession P0DTD1

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": [
                {
```

Interface residues



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

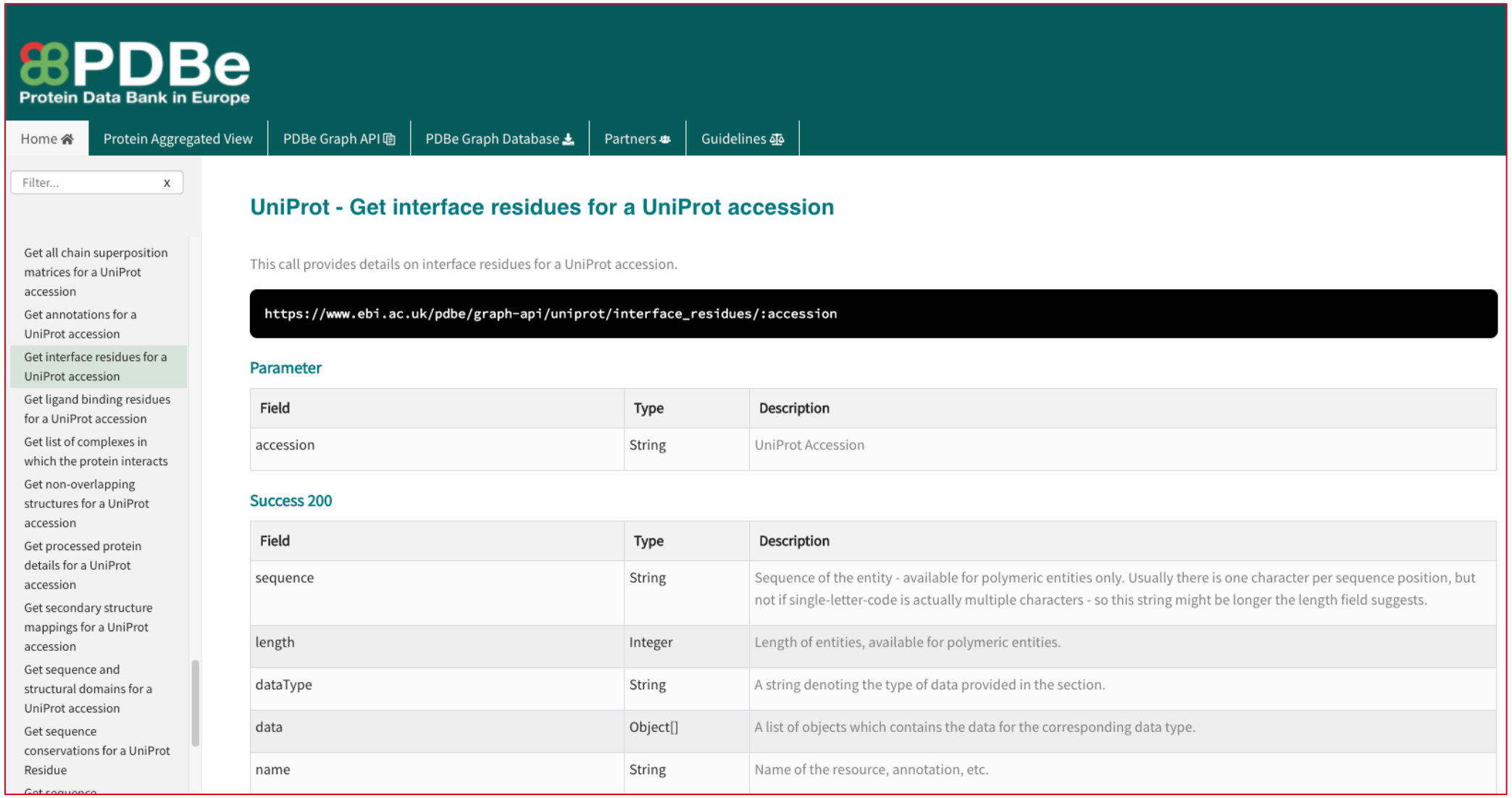
EMBL-EBI

Interface residues

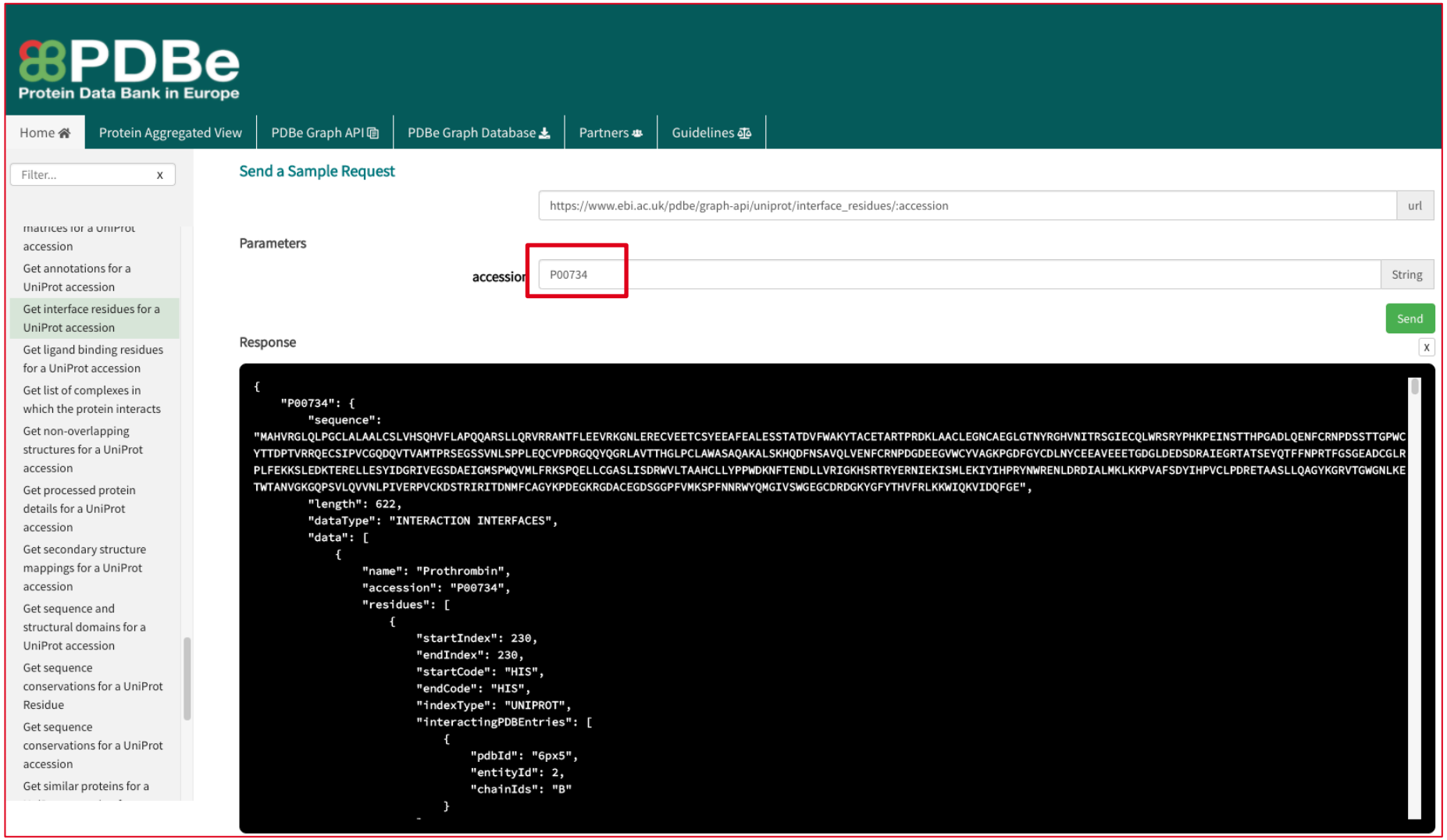
Thrombin (pdbe-kb.org/protein/P00734)

EMBL-EBI

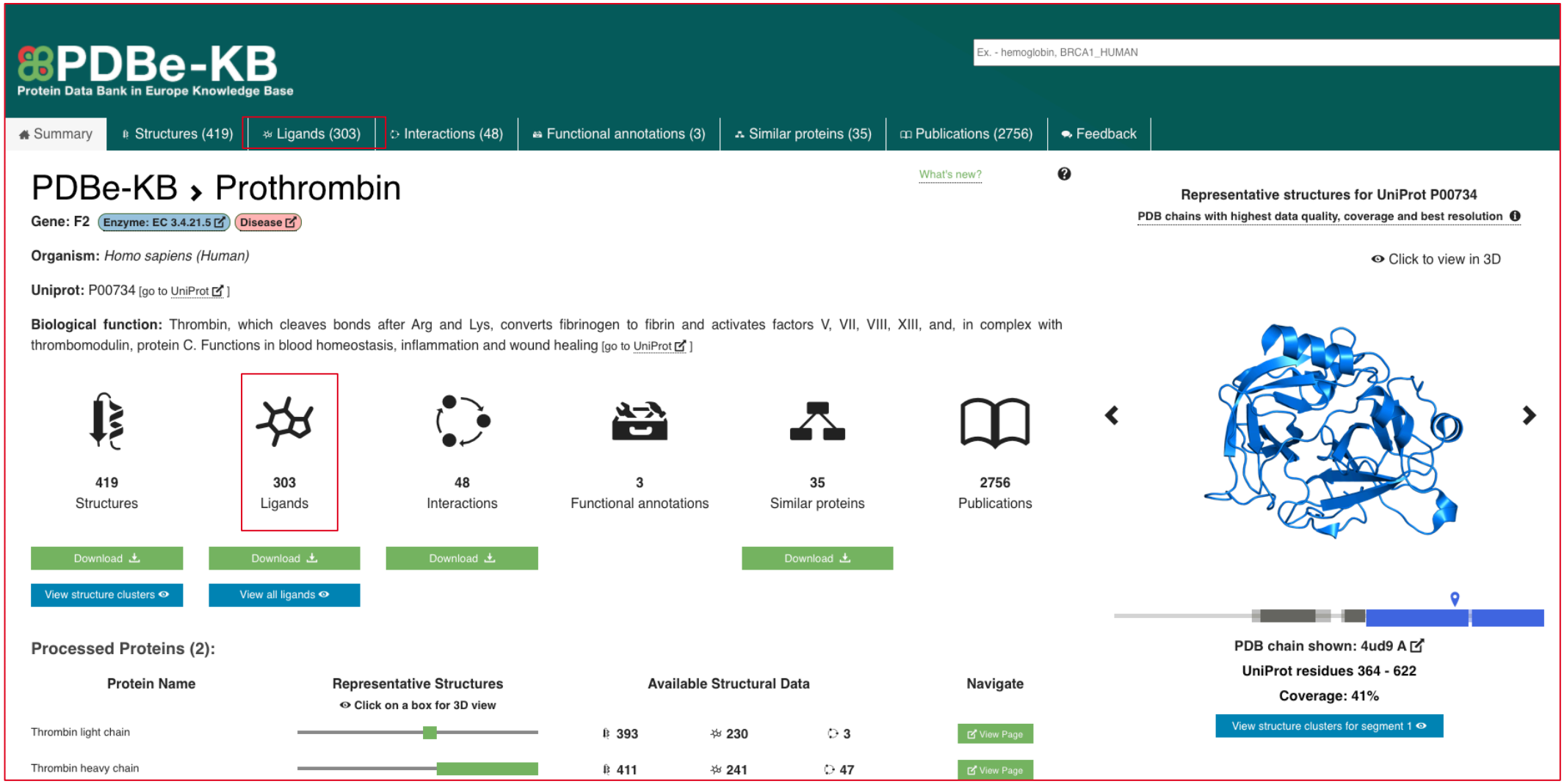
Interface residues



Interface residues



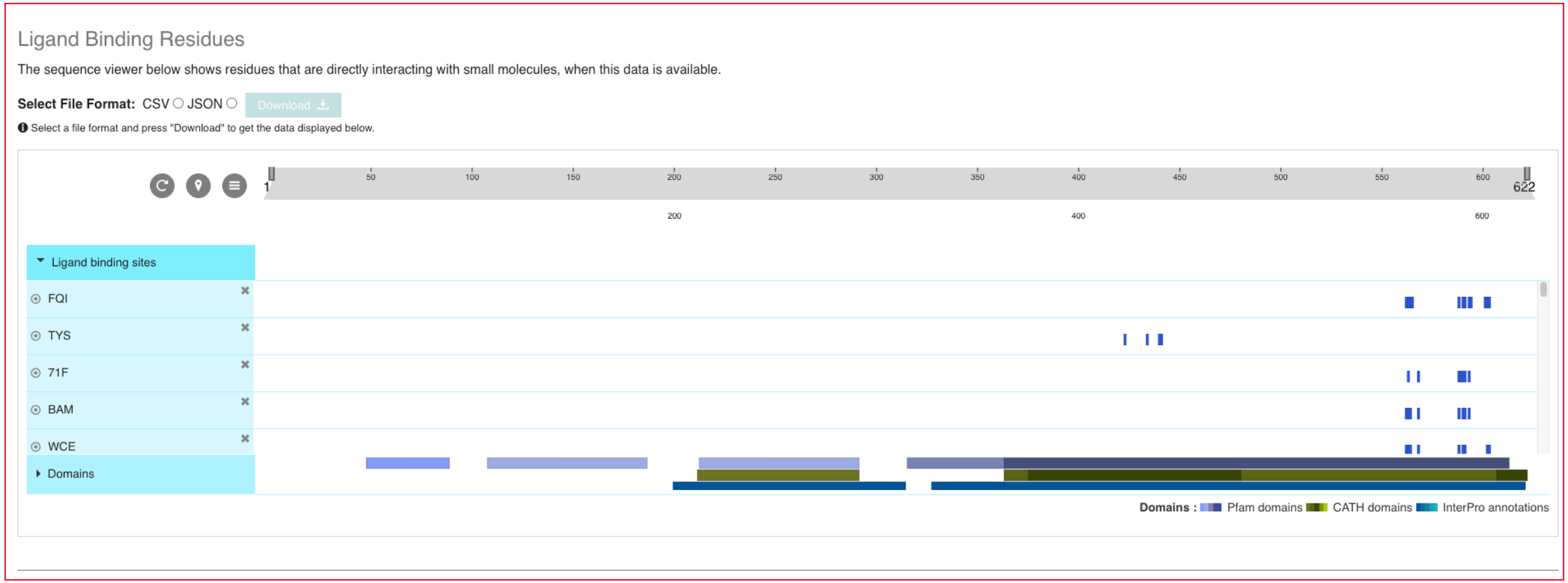
Ligand binding residues



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

EMBL-EBI

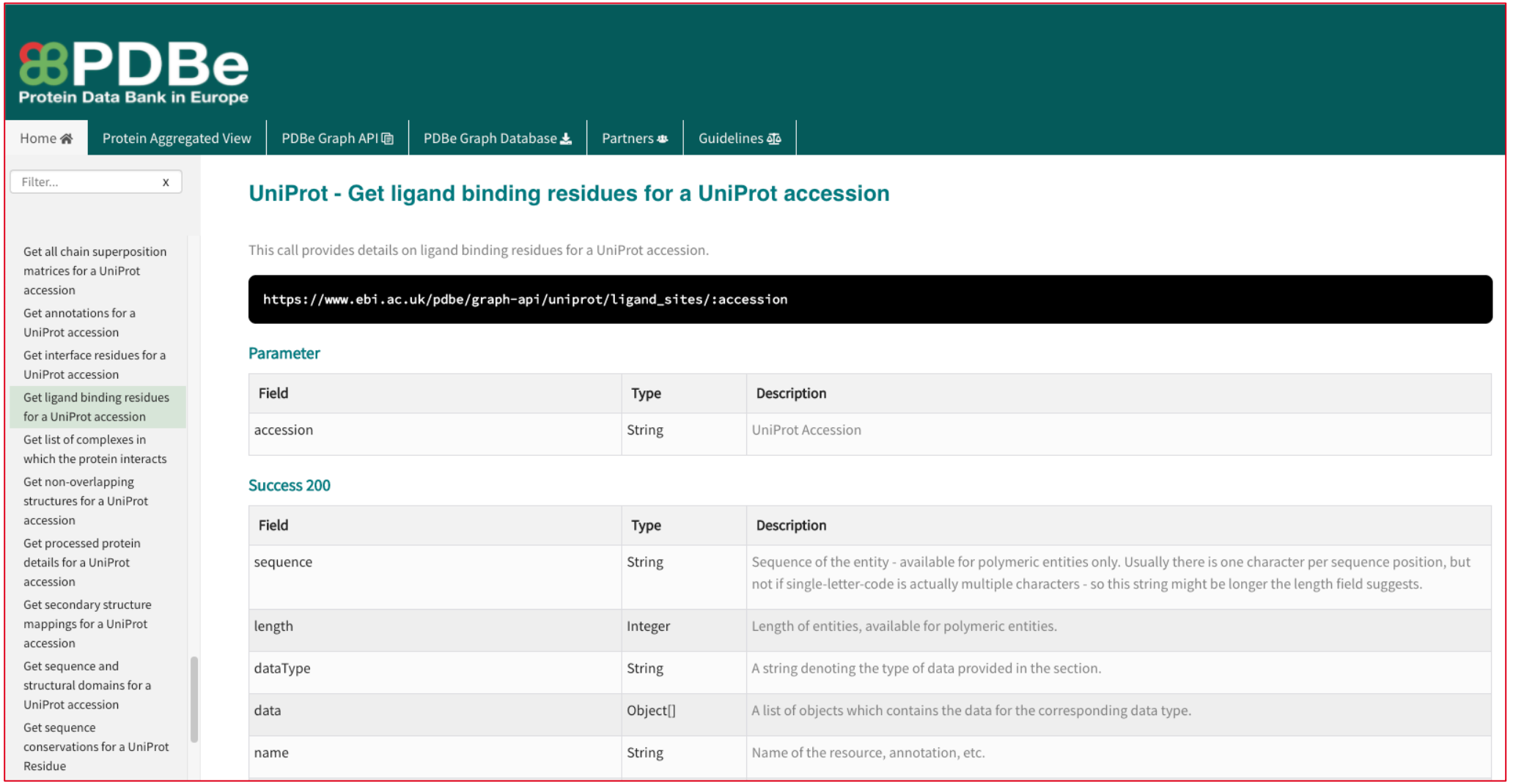
Ligand binding residues



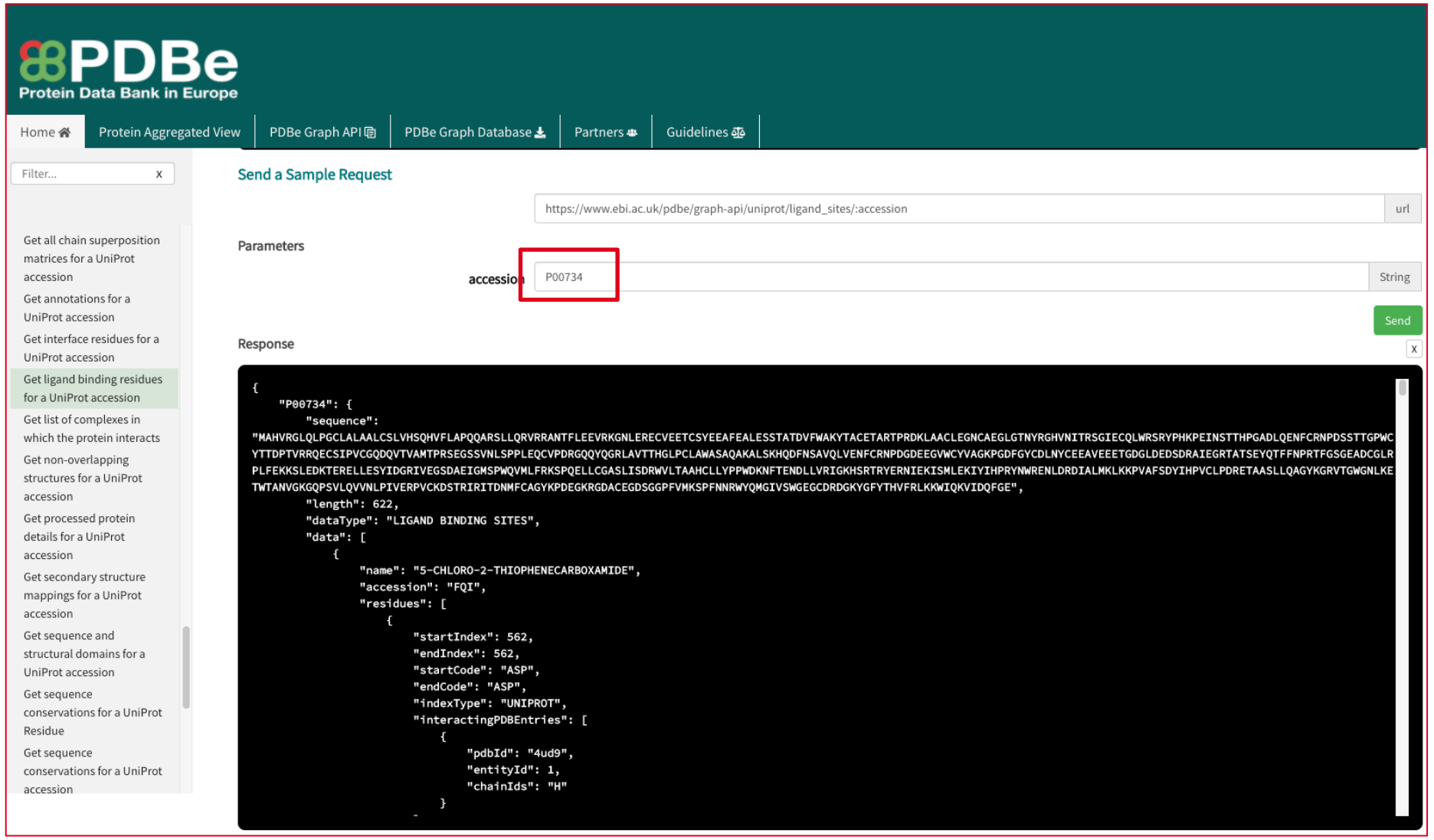
Thrombin (pdbe-kb.org/protein/P00734)

EMBL-EBI

Ligand binding residues



Ligand binding residues



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

Thrombin – interface binding small molecule ligands

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Ligand environment

EMBL-EBI Services Research Training About us

Protein Data Bank in Europe
Bringing Structure to Biology

Search
Examples: hemoglobin, BRCA1_HUMAN Advanced search
Feedback

PDBe › 4r7i

X-ray diffraction
2.75Å resolution

Crystal structure of FMS kinase domain with a small molecular inhibitor, GLEEVEC

Source organism: *Homo sapiens*

Primary publication:

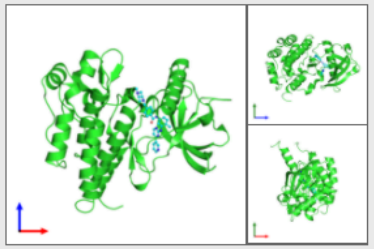
Structure-Guided Blockade of CSF1R Kinase in Tenosynovial Giant-Cell Tumor.

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

Released: 12 Aug 2015
DOI: 10.2210/pdb4r7i/pdb

Model geometry
Fit model/data



Function and Biology

Details

Reaction catalysed:

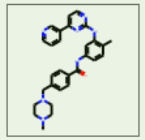
```
ATP + a [protein]-L-tyrosine = ADP + a [protein]-L-
tyrosine phosphate
```

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

Quick links

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

View
Downloads
3D Visualisation

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

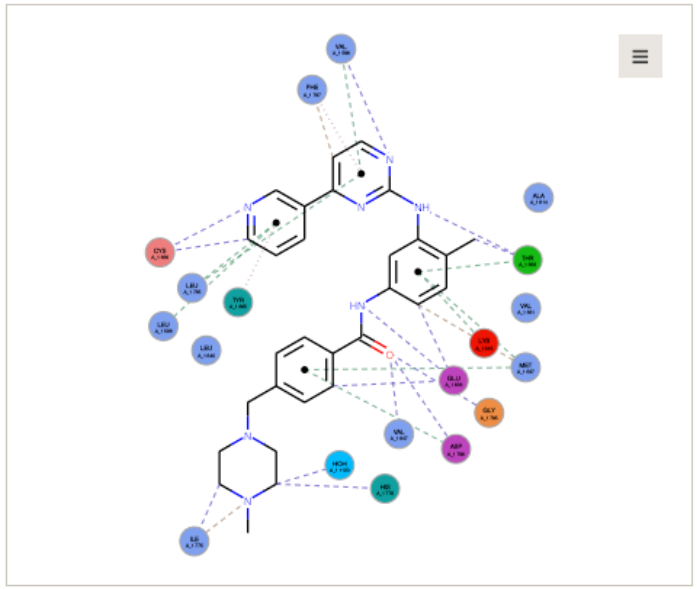
Model Geometry

FMS Kinase domain with Gleevec (PDB 4r7i)

EMBL-EBI

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

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

Parameters

pdbId	4r7i	String
chain	A_1	String
seqId	1001	Integer

Send

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,
```


FMS Kinase domain with Gleevec (PDB 4r7i)

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Use case

Accessible residues for a PDB structure

Send a Sample Request

https://www.ebi.ac.uk/pdbe/graph-api/pdb/funpdbe_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,
```


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/funpdbe_annotation/:origin/:pdbId
```

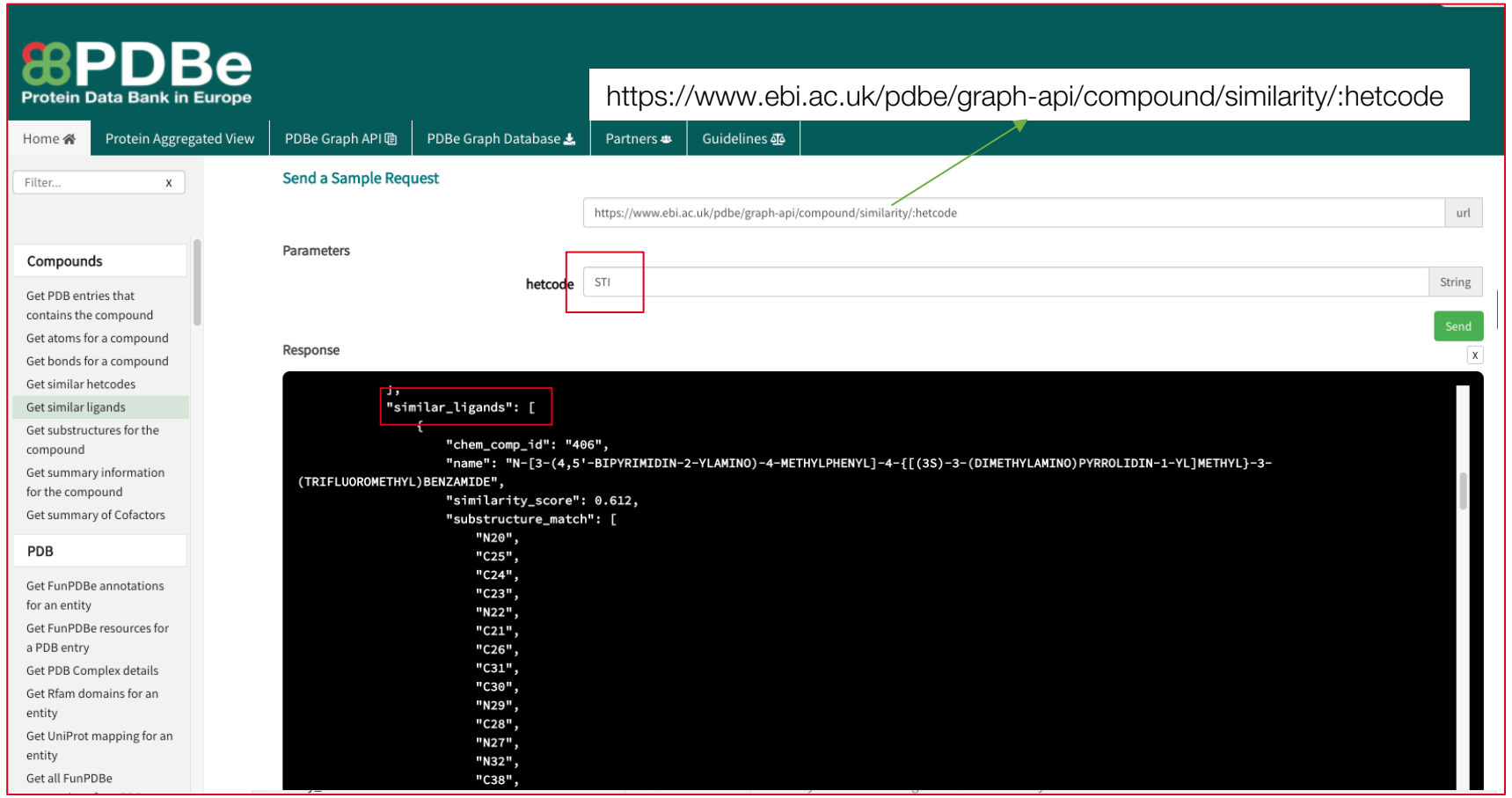
Parameter

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", "ProKinO"
pdbId	String	PDB Entry ID

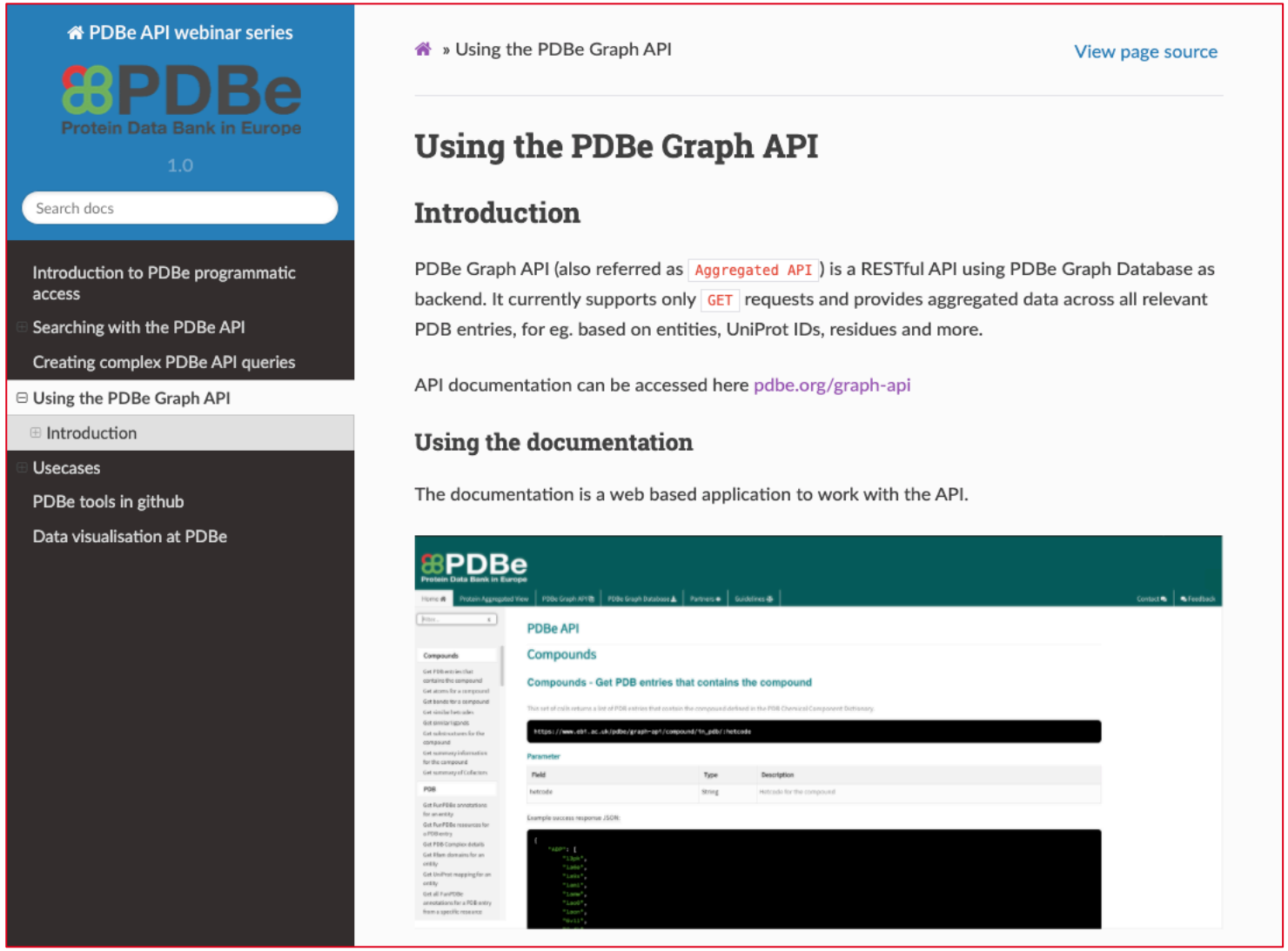
label = ASA_alone
raw_score > 0

Use case

Ligands similar to drug Imatinib (STI)



Teaching resources



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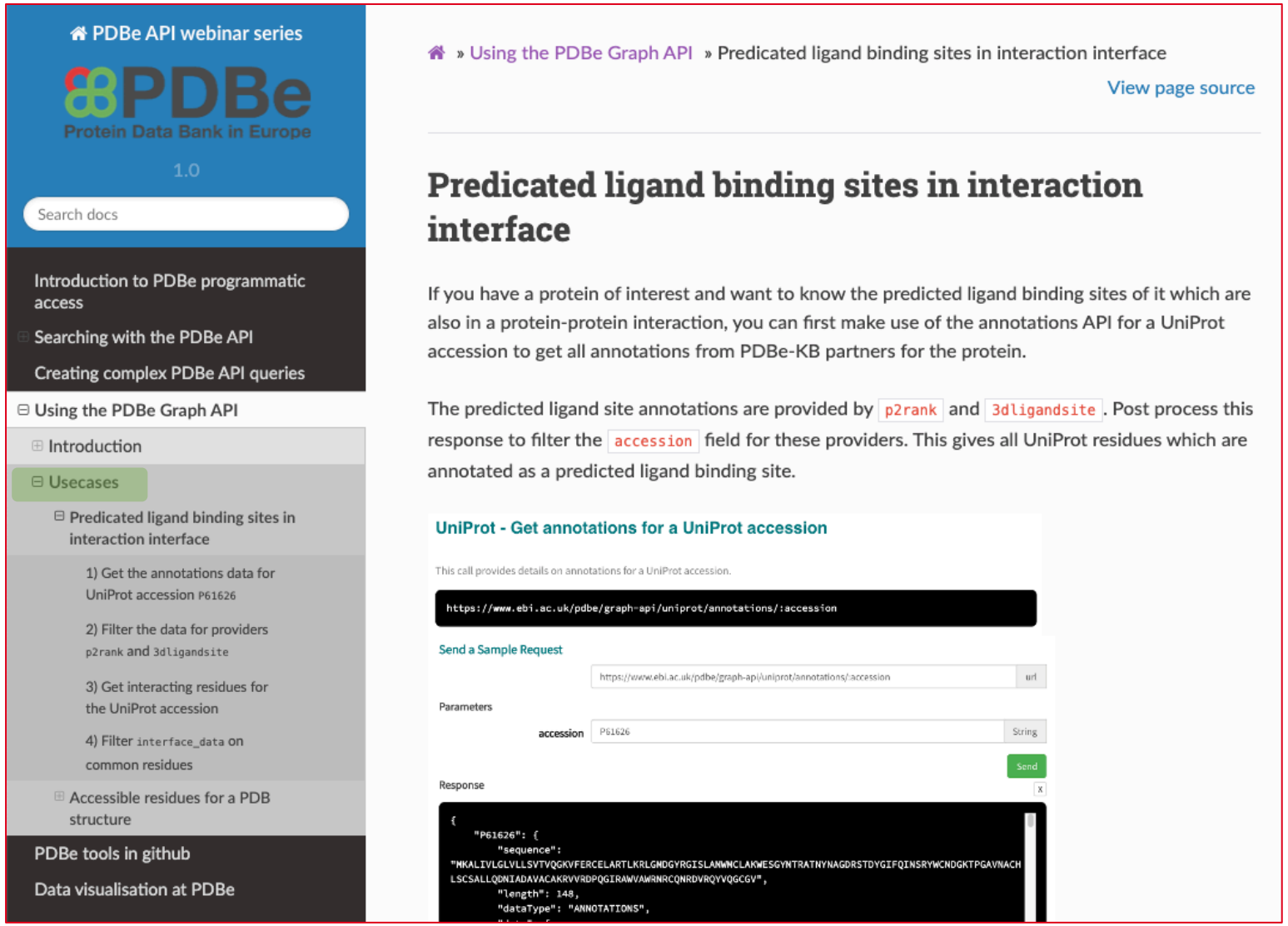
Teaching resources – worked out examples

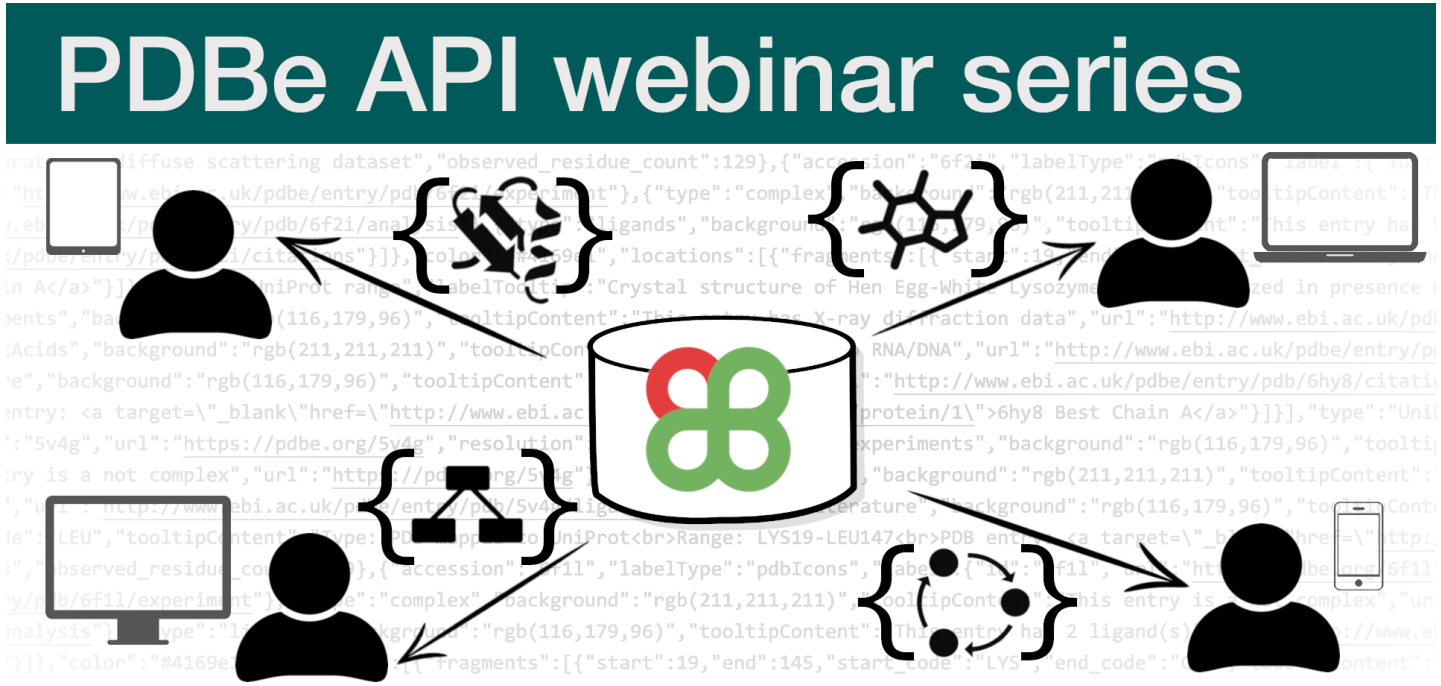


PDBe API webinar series

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!!!



Thank you for your attention!
Any questions?

PDBe.org/graph-api

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