

Recent updates to the PDBe Knowledge Base (PDBe-KB)

Protein Data Bank in Europe - Knowledge Base

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Bioinformatician

CCP4 Virtual Study Weekend
7th January 2021

Overview

- Brief introduction to PDBe-KB
- PDBe-KB aggregated views of proteins
- Major new features in 2020
 - Covid-19 data portal (<https://www.ebi.ac.uk/pdbe/covid-19>)
 - Structures superposition
 - Batch download
 - “Processed proteins”
 - Similar proteins

A macromolecular structure is but one piece of the puzzle

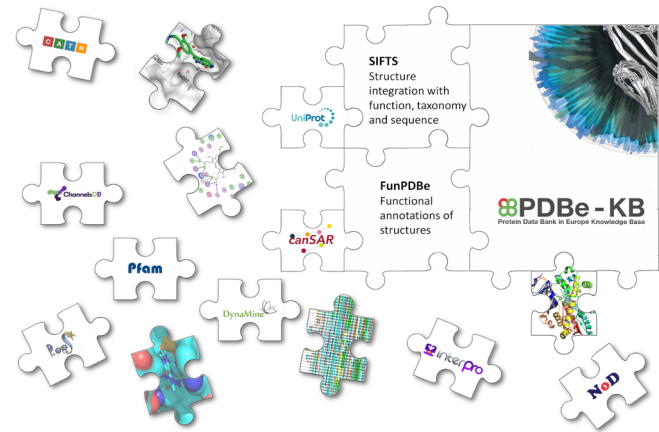
“Coordinates by themselves just specify shape and are not necessarily of intrinsic biological value, unless they can be related to other information”

Integrative database analysis in structural genomics, Mark Gerstein, Nature Structural Biology 7, 960 , 2000

Protein Data Bank in Europe Knowledge Base (<https://pdbe-kb.org>)

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

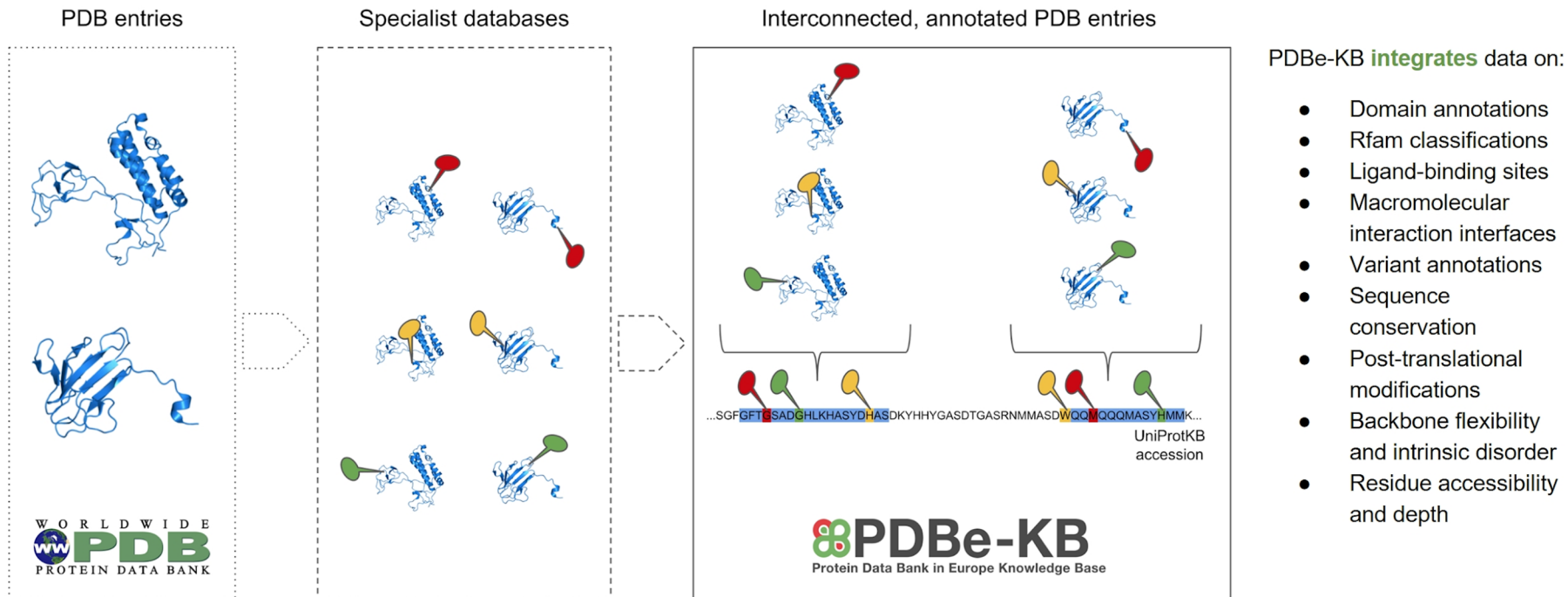
- Create data standards
- Create data access mechanisms
- Reduce fragmentation



PDBe-KB: a community-driven resource for structural and functional annotations, Nucl.Acids Res. 2019 Oct

<https://doi.org/10.1093/nar/gkz853>

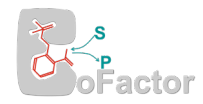
Integrating annotations from specialist data resources



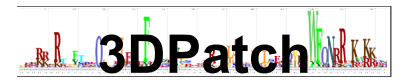
EMBL-EBI 



M-CSA



Arpeggio



NoD



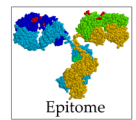
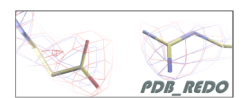
14-3-3-Pred



AKID



Phyre2



3DLigandSite

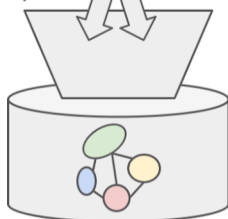


ProKinO



Simplified infrastructure overview

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

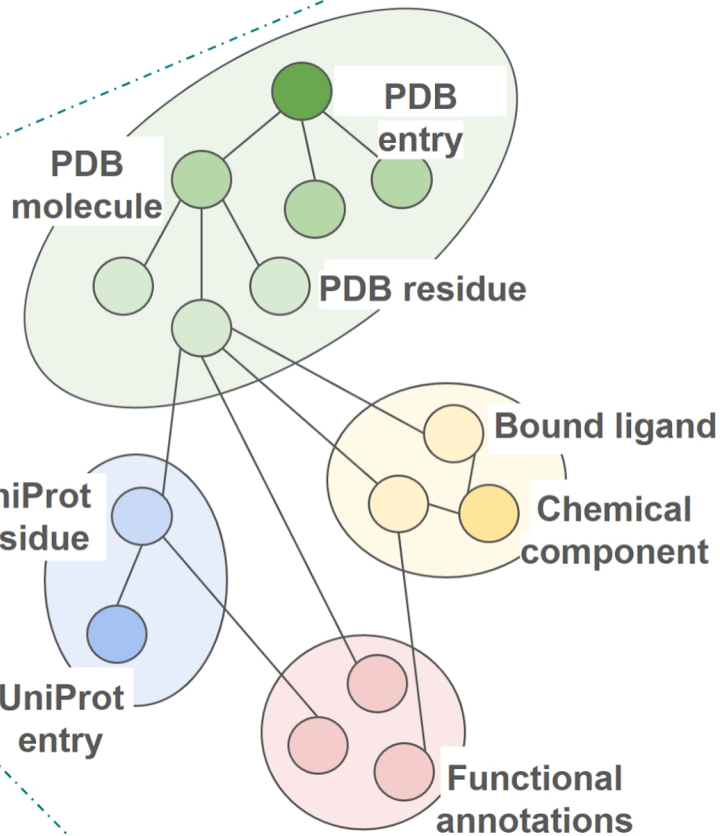


PDBe Graph Database

Programmatic Access



PDBe-KB pages



Aggregated view of proteins

Accessing the aggregated views of proteins

The protein-centric PDBe-KB pages can be accessed by:

1. From the PDBe-KB protein aggregated views landing page
<https://pdbe.kb.org/proteins/>
2. Using a PDB or UniProt identifier
e.g. <https://pdbe.kb.org/protein/2etx>
e.g. <https://pdbe.kb.org/protein/Q92793>
3. From PDBe entry pages / search
4. UniProt entry pages

3D structure databases

SMR ⁱ	<input type="text" value="P08684"/>
ModBase ⁱ	<input type="text" value="Search..."/>
PDBe-KB ⁱ	<input type="text" value="Search..."/>

Structure analysis [Details](#)

Assemblies monomeric ([preferred](#))
composition: homo tetramer
Entry contents: 1 distinct polypeptide molecule

Macromolecule:
Cytochrome P450 3A4

[Molecule details >](#)

Chain: A
Length: 486 amino acids
Theoretical weight: 55,59 kDa
Source organism: *Homo sapiens*
Expression system: *Escherichia coli*

UniProt:
◦ Canonical: [P08684](#) (Residues: 22-503; Coverage: 96%)

Gene names: CYP3A3, CYP3A4
Sequence domains: [Cytochrome P450](#)
Structure domains: [Cytochrome P450](#)

Live demo

Summary

PDBe-KB > Replicase polyprotein 1ab

[What's new?](#) ?

Gene: rep [Enzyme: EC 2.7.7.48](#)

Organism: *Severe acute respiratory syndrome coronavirus 2 (2019-nCoV)*

Uniprot: P0DTD1 [\[go to UniProt\]](#)

Biological function: Methyltransferase that mediates mRNA cap 2'-O-ribose methylation to the 5'-cap structure of viral mRNAs. N7-methyl guanosine cap is a prerequisite for binding of nsp16. Therefore plays an essential role in viral mRNAs cap methylation which is essential to evade immune system [\[go to UniProt\]](#)

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

[Click to view in 3D](#)



545
Structures

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[View structure clusters](#)



423
Ligands

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[View all ligands](#)



10
Interactions

[Download](#)



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Functional
annotations

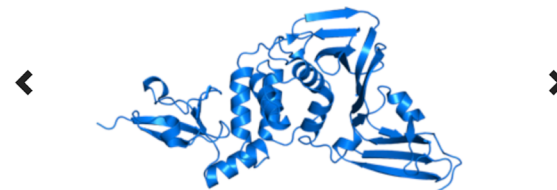


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Similar proteins

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PDB chain shown: [6wx4 A](#)

UniProt residues 1562 - 1879

Coverage: 4%

[View structure clusters for segment 5](#)

PDBe-KB > Replicase polyprotein 1ab

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Processed Proteins (15):

Protein Name

Representative Structures

Available Structural Data

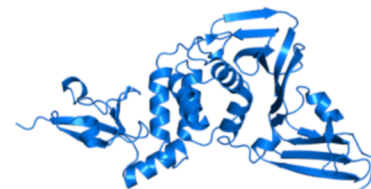
Navigate

Click on a box for 3D view

[What's new?](#)

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

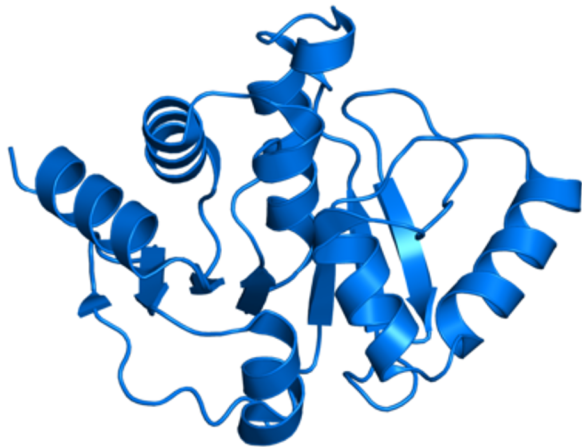
Coverage: 4%

[View structure clusters for segment 5](#)

Representative structures for UniProt P0DTD1

PDB chains with highest coverage and resolution ⓘ

👁 Click to view in 3D

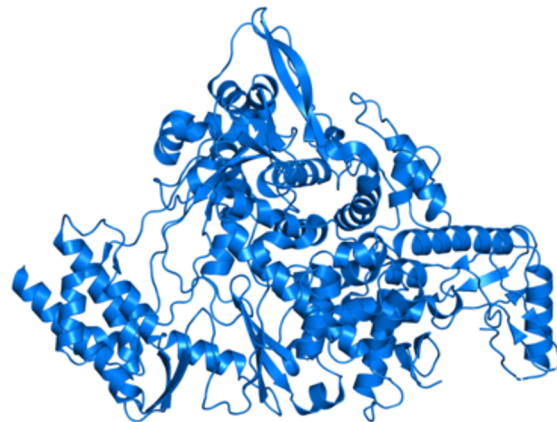


PDB chain shown: [6wen A](#) ⓘ
UniProt residues 1024 - 1192
Coverage: 2%

Representative structures for UniProt P0DTD1

PDB chains with highest coverage and resolution ⓘ

👁 Click to view in 3D



PDB chain shown: [6m71 A](#) ⓘ
UniProt residues 4393 - 5324
Coverage: 12%

Select PDB entry from dropdown: PDB 6w9c chain B assembly 1



6w9c

Source

Source	Assembly
Asm. Id	1 (Preferred)

Back Apply

Annotations

Validation report Show

Map

Display Hide

Map settings

+	2Fo-Fc σ		1.5
+	Fo-Fc(+ve) σ		3
+	Fo-Fc(-ve) σ		-3

Entry 6w9c

View Around Interaction

View Properties

Back Nothing to Update

3D Labels

Display Show

Visual settings

Polymer Hide

Polymer Properties

Het Groups Hide

Het Groups Properties

Map Streaming enabled, click on a residue or an atom to view the data.

NEW FEATURE

Processed proteins



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Processed Proteins (15):

Protein Name	Representative Structures Click on a box for 3D view	Available Structural Data			Navigate
Host translation inhibitor nsp1		16	5	3	View Page
Non-structural protein 2		0	0	0	
Non-structural protein 3		171	0	4	View Page
Non-structural protein 4		1	0	0	View Page

Show more items

NEW FEATURE

Structure download

PDBe-KB > Replicase polyprotein 1ab

[What's new?](#) ?

Gene: rep [Enzyme: EC 2.7.7.48](#)

Organism: *Severe acute respiratory syndrome coronavirus 2 (2019-nCoV)*

Uniprot: P0DTD1 [\[go to UniProt\]](#)

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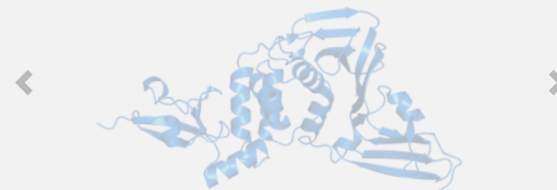
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PDB chain shown: 6wx4 A [!](#)

UniProt residues 1562 - 1879

Coverage: 4%

[View structure clusters for segment 5](#)

PDBe-KB > Replicase polyprotein 1ab

Gene: rep [Enzyme: EC 2.7.7.48](#)

Organism: *Severe acute respiratory syndrome coronavirus 2 (2019-nCoV)*

Uniprot: P0DTD1 [\[go to UniProt\]](#)

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Download data of 545 PDB entries mapped to P0DTD1

Structure:

- Updated mmCIF file
- Archive mmCIF file
- PDB file

Sequence:

- Combined FASTA
- Individual FASTA files

Other:

- Validation data

Download

Cancel

Download

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[view structure clusters](#)

[view all ligands](#)

PDB chain shown: 6wx4 A [\[external link\]](#)

UniProt residues 1562 - 1879

Coverage: 4%

[View structure clusters for segment 5](#)

PDBe File Download service 1.2 OAS3

</pdbe/download/openapi.json>

PDBe download service API entry point

This API allows for a batch download of arbitrary subsets of the PDB data.

Servers

▾

Macromolecular data ▾

GET </pdb/entry/updated> Updated mmCIF files download

POST </pdb/entry/updated> Updated mmCIF files download

GET </pdb/entry/archive> Archive coordinate files download

NEW FEATURE

Structures superposition

Superposition

- We have implemented a new process that calculates superposition matrices for individual proteins in the whole PDB archive
- The process uses GESAMT to align PDB chains mapped to UniProt segments
- Clusters are generated based on the alignments
- The matrix files and the superposition clusters are accessible via API
- **The clusters do not necessarily correspond to biological functions.**



PDBe-KB > Replicase polyprotein 1ab

[What's new?](#) ?

Gene: rep [Enzyme: EC 2.7.7.48](#)

Organism: *Severe acute respiratory syndrome coronavirus 2 (2019-nCoV)*

Uniprot: P0DTD1 [\[go to UniProt\]](#)

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[Click to view in 3D](#)



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Structures



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Ligands



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Interactions



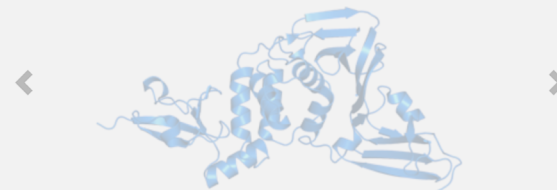
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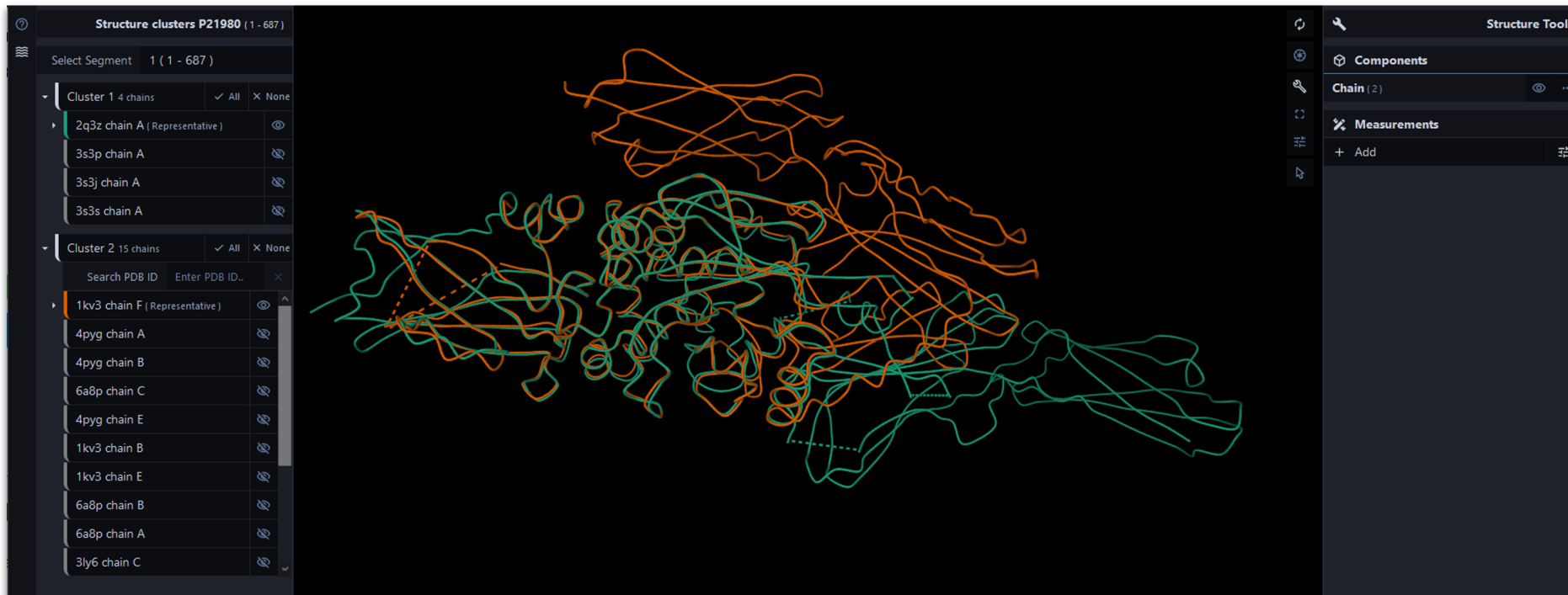
PDB chain shown: 6wx4 A [!](#)

UniProt residues 1562 - 1879

Coverage: 4%

[View structure clusters for segment 5](#)

Protein-glutamine gamma-glutamyltransferase 2



Protein-glutamine gamma-glutamyltransferase 2

The screenshot displays the PDB-KE server interface for protein structure P21980. The central visualization shows a protein structure with a central pink ligand. The interface is divided into several panels:

- Structure clusters P21980 (1 - 687):** A list of structure clusters. Cluster 1 contains 4 chains (2q3z A, 3s3p A, 3s3j A, 3s3s A). Cluster 2 contains 15 chains (1kv3 B, 1kv3 E, 6a8p B, 6a8p A, 3ly6 C, 3ly6 B, 1kv3 A, 1kv3 D, 3ly6 A, 1kv3 C).
- Structure Tools:** A sidebar on the right containing a search icon, a refresh icon, and a list of components. The components list includes Chain (2), Ligand (5) (SO4, GOL, GDP, GTP, ATP), and Measurements.

Cluster	Chain ID	Residues	Notes
Cluster 1 (4 chains)	2q3z A	(SO4)	Representative
	3s3p A	(SO4)	
	3s3j A	(SO4, GOL)	
	3s3s A	(SO4)	
Cluster 2 (15 chains)	1kv3 B	(GDP)	
	1kv3 E	(GDP)	
	6a8p B	(GTP)	
	6a8p A	(GTP)	
	3ly6 C	(ATP)	
	3ly6 B	(ATP)	
	1kv3 A	(GDP)	
	1kv3 D	(GDP)	
	3ly6 A	(ATP)	
	1kv3 C	(GDP)	

3C-like proteinase

The screenshot displays the PDB-KE interface for protein cluster PRO_0000449623. The central 3D view shows a protein structure with multiple chains colored in cyan, orange, and magenta. The left sidebar lists structure clusters and their members:

- Cluster 1** (5 chains):
 - 6xhm B (V2M) (Representative)
 - 6xbg B (GOL, NA)
 - 6xmk B (QYS, PG4)
 - 7jkv B (V7G, 1PE)
 - 7d1m B (K36)
- Cluster 2** (1 chain):
 - 7kvg B (Representative)
- Cluster 3** (279 chains):
 - 6xhm A (V2M + 1) (Representative)
 - 7cwc A (No Ligand found)
 - 6zru A (DMS, U5G)
 - 5re8 A (DMS, T0V)
 - 6y2g A (GLY, O6K)
 - 5rgp A (DMS, U1M)
 - 5rf1 A (DMS, T5G)
 - 6xkf B (EDO)
 - 7k6e A (DMS, SV6)
 - 7d3i A (GQU, TRS)

The right sidebar, titled "Structure Tools", shows the "Components" panel with the following data:

Component	Count	Visibility
Chain	3	Visible
Ligand	200	Visible
V2M	2	Visible
EDO	9	Visible
GOL	10	Visible
NA	5	Visible
QYS	2	Visible
PG4	1	Visible
V7G	3	Visible
1PE	1	Visible
K36	9	Visible
DMS	180	Visible
U5G	9	Visible
T0V	1	Visible
GLY	2	Visible
O6K	3	Visible
U1M	1	Visible
T5G	1	Visible
CL	28	Visible
SV6	5	Visible
GQU	1	Visible

Structures and domains

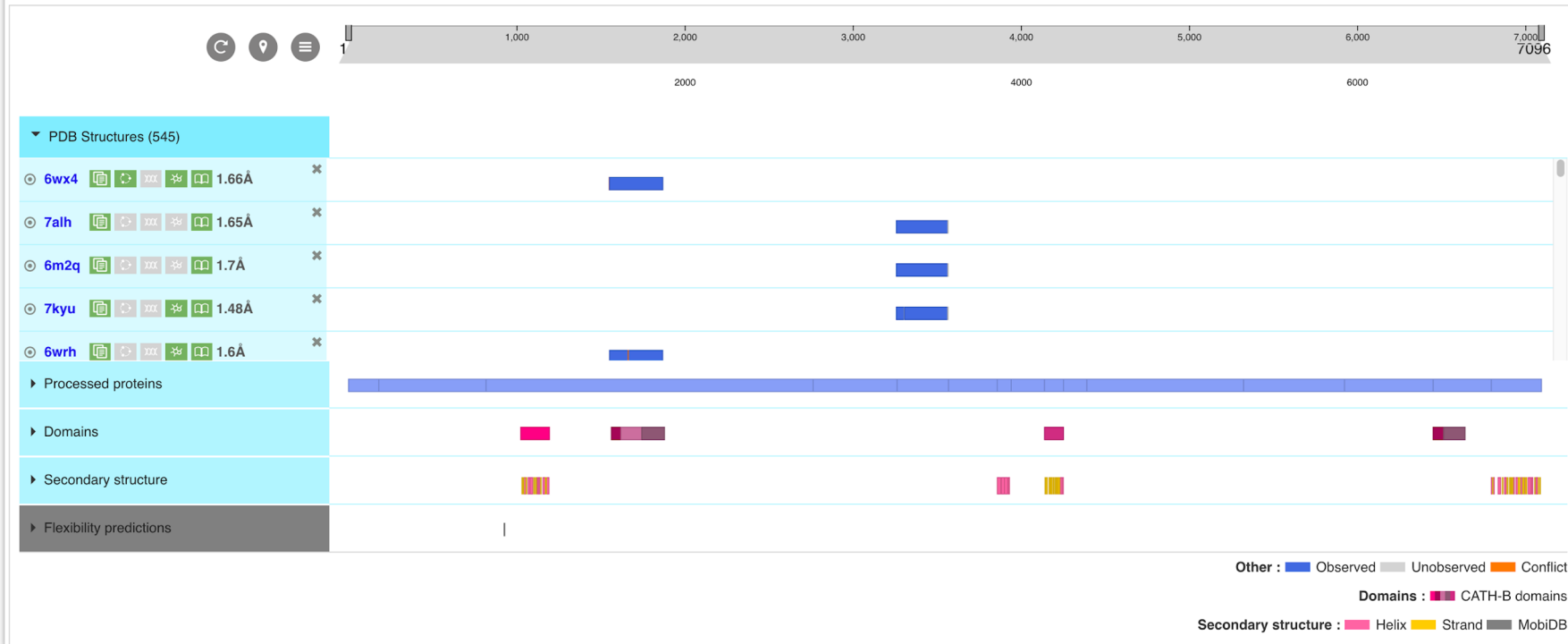
Structures and Domains



The visualisation below shows information on domains (Pfam, CATH and SCOP), protein structures covering various regions of the sequence and known secondary structural elements content of the protein.

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

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



Ligands

Ligands and Environments

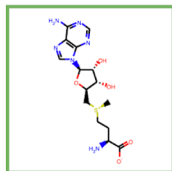


All Ligands (430)

This section, by default, shows ligands observed directly bound to the protein of interest, if such ligands are available. Click on the checkbox to see every ligand from all PDB entries (some may not directly interact with the protein). If there are no directly interacting ligands, all ligands will be shown by default. Click on the images to see the related PDB entries. For ligand binding residues, see the section below.

Search:

Search by molecule name, code or PDB id.

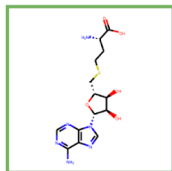


3D view

SAM

cofactor-like

Found in 13 entries

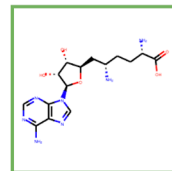


3D view

SAH

cofactor-like

Found in 6 entries

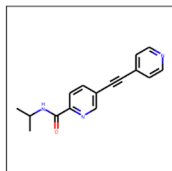


3D view

SFG

cofactor-like

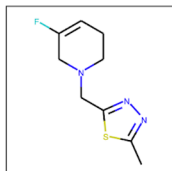
Found in 2 entries



3D view

S8B

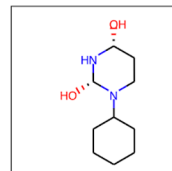
Found in 1 entry



3D view

UOM

Found in 1 entry



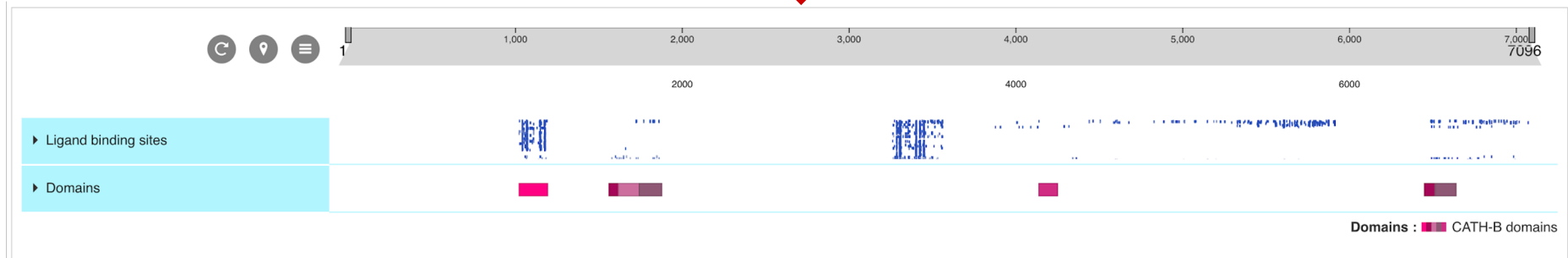
3D view

X1Y

Found in 1 entry



+ Show all items



Macromolecules

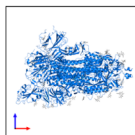
Macromolecular Interactions

Interaction Partners (9)

This section shows macromolecules observed together with the protein of interest in PDB entries. Click on the images to see the related PDB entries. The interaction partner is colored blue.

Search:

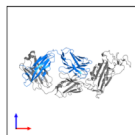
Search by molecule name, code or PDB id.



3D view

P0DTC2 (self) ⓘ

Found in 104 entries

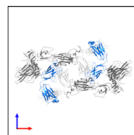


3D view

IG-heavy chain ⓘ

antibody

Found in 55 entries

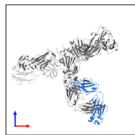


3D view

IG-light kappa chain ⓘ

antibody

Found in 39 entries



3D view

IG-light lambda chain ⓘ

antibody

Found in 8 entries



Show all items

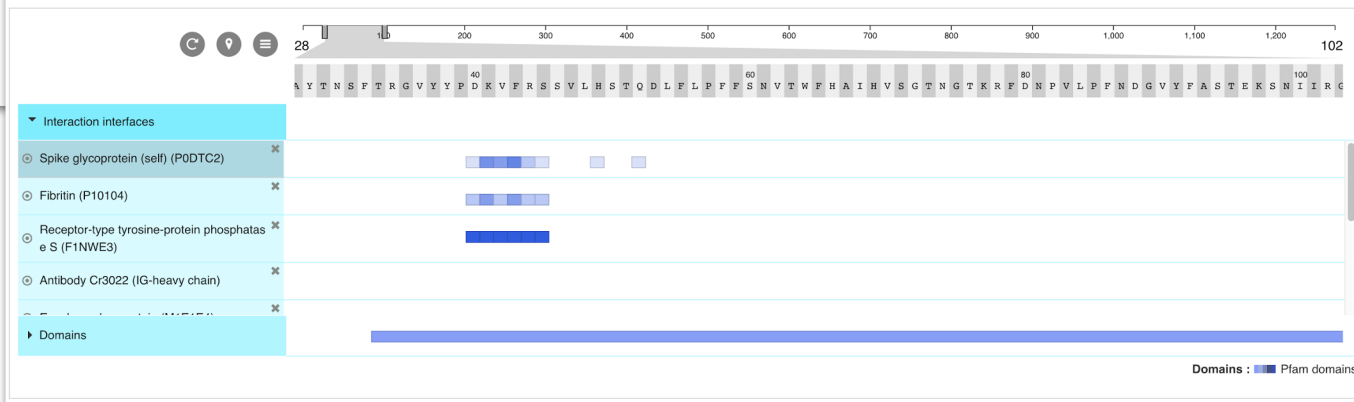
NEW FEATURE

Interface Residues

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

Select File Format: CSV JSON

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



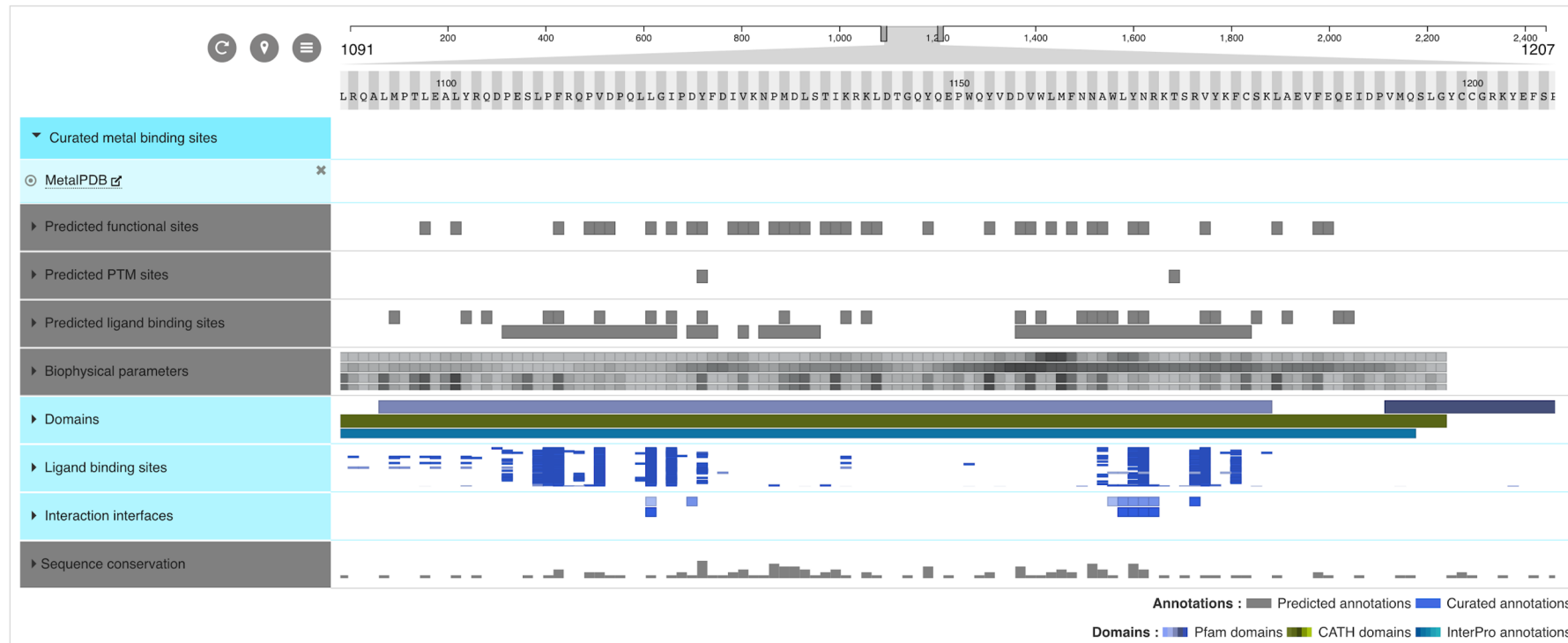
Additional annotations

Additional Functional Annotations

Additional residue-level functional annotations available for the PDB entries related to this protein are displayed below. The majority of the annotations are contributed by collaborators of PDBe-KB. ([Find out more about PDBe-KB partners](#)).

Select File Format: CSV JSON

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



Sequence conservation



Amino acid probabilities

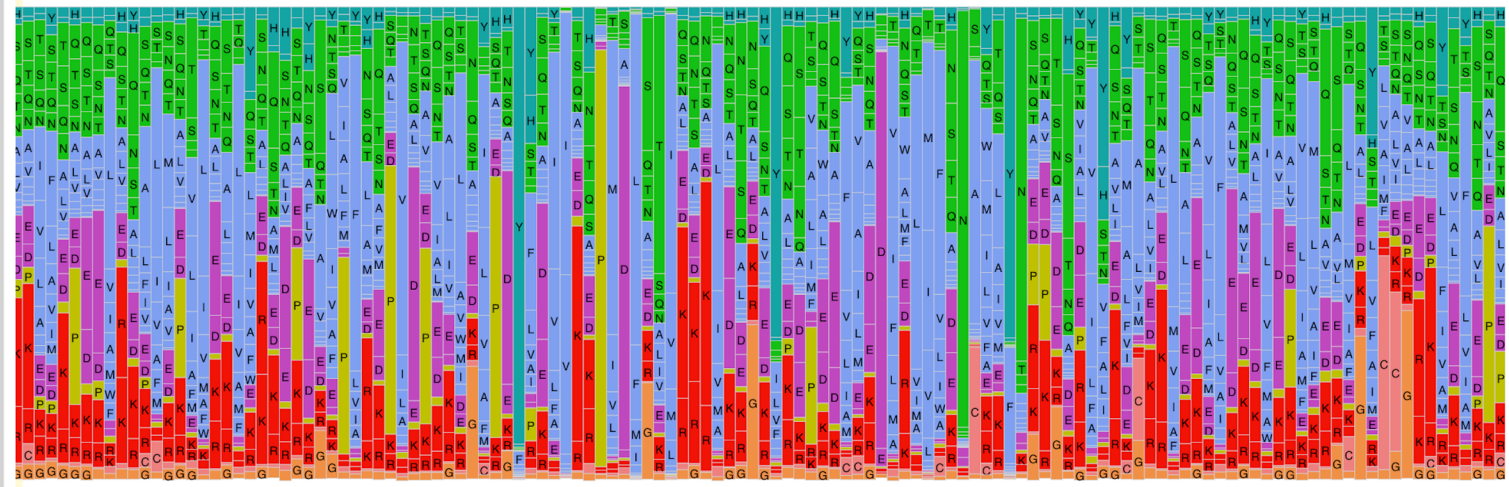
Data displayed by

Probability

Property

Amino acid properties

- Aromatic
- Polar
- Hydrophobic
- Negative charge
- Proline
- Positive charge
- Cysteine
- Glycine



Annotations : Predicted annotations Curated annotations

Domains : Pfam domains CATH domains InterPro annotations

NEW FEATURE

Similar proteins

Similar Proteins (2128)

Proteins with 90% or greater sequence identity to **P0DTC2**

Search:

Search by species, taxonomy id or protein name.








Select File Format: CSV JSON



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

Similar Proteins with highly identical PDB sequences to P0DTC2 (20)

PDB entries with more than 90% sequence identity to the protein of interest.

Protein Name (UniProt ID)	Species	Segments Mapped to PDB <small>Click on a box for 3D view</small>	Navigate
Receptor-type tyrosine-protein phosphatase S (F1NWE3)	<i>Gallus gallus</i>		<input type="button" value="View Page"/>
Envelope glycoprotein (M1E1E4)	<i>Human immunodeficiency virus 1</i>		<input type="button" value="View Page"/>
Spike glycoprotein (P59594)	<i>Severe acute respiratory syndrome-related coronavirus</i>		<input type="button" value="View Page"/>
Surface glycoprotein (A0A6N1WIU8)	<i>Severe acute respiratory syndrome coronavirus 2</i>		<input type="button" value="View Page"/>
Surface glycoprotein (A0A6N1NAV4)	<i>Severe acute respiratory syndrome coronavirus 2</i>		<input type="button" value="View Page"/>
Fibrin (P10104)	<i>Escherichia virus T4</i>		<input type="button" value="View Page"/>
Spike glycoprotein (A0A6B9WHD3)	<i>Bat coronavirus RaTG13</i>		<input type="button" value="View Page"/>

Publications

Publications



Primary PDB publications, reviews associated with PDB entries and UniProt publications are listed below. Click on the plus signs to expand the publication lists.

Search:

Search by keyword in the title or by PDB id or PubMed id.

PDB publications (77)

Go to page: [1](#) [2](#) [3](#) [4](#)

Select File Format: CSV BibTeX

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

D614G mutation alters SARS-CoV-2 spike conformational dynamics and protease cleavage susceptibility at the S1/S2 junction.

Gobeil S, Janowska K, McDowell S, Mansouri K, Parks R et al.

bioRxiv (2020)

PMID: [33052347](#)

doi: [10.1101/2020.10.11.335299](#)

Related PDB entries: [7kdl](#) [7kdj](#) [7kdk](#) [7kdh](#) [7kdi](#) [7kea](#) [7kdg](#) [7kec](#) [7keb](#) [7ke9](#) [7ke8](#) [7ke4](#) [7ke7](#) [7ke6](#)

A neutralizing human antibody binds to the N-terminal domain of the Spike protein of SARS-CoV-2.

Chi X, Yan R, Zhang J, Zhang G, Zhang Y et al.

Science (2020)

PMID: [32571838](#)

doi: [10.1126/science.abc6952](#)

Related PDB entries: [7c2l](#)

A pH-dependent switch mediates conformational masking of SARS-CoV-2 spike.

PDB-related reviews (182)

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Insights into the Recent 2019 Novel Coronavirus (SARS-CoV-2) in Light of Past Human Coronavirus Outbreaks.

PMID: [32143502](#)

Related PDB entries: [6vsvb](#)

Should COVID-19 Concern Nephrologists? Why and to What Extent? The Emerging Impasse of Angiotensin Blockade.

PMID: [32203970](#)

Related PDB entries: [6m17](#)

One size does not fit all - Patterns of vulnerability and resilience in the COVID-19 pandemic and why heterogeneity of disease matters.

PMID: [32205119](#)

Related PDB entries: [6vsvb](#)

Elevated Plasmin(ogen) as a Common Risk Factor for COVID-19 Susceptibility.

PMID: [32216698](#)

Related PDB entries: [6vxx](#) [6vsvb](#) [6vyb](#)

UniProt publications (20)

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A new coronavirus associated with human respiratory disease in China.

Wu F., Zhao S., Yu B., Chen Y.M., Wang W. et al.

Nature 265-269 (2020)

PMID: [32015508](#)

SARS-CoV-2 cell entry depends on ACE2 and TMPRSS2 and is blocked by a clinically proven protease inhibitor.

Hoffmann M., Kleine-Weber H., Schroeder S., Krueger N., Herrler T. et al.

Cell 1-10 (2020)

PMID: [32142651](#)

Structural basis for the recognition of the SARS-CoV-2 by full-length human ACE2.

Yan R., Zhang Y., Li Y., Xia L., Guo Y. et al.

Science - (2020)

PMID: [32132184](#)

A multibasic cleavage site in the Spike protein of SARS-CoV-2 is essential for infection of human lung cells.

Data availability

- Aggregated views: <https://pdbe.kb.org/proteins>
- Graph database: <https://pdbe.kb.org/graph-download>
- REST API: <http://pdbe.org/aggregated-api>
- Download service API: <https://www.ebi.ac.uk/pdbe/download/docs>
- Visualization components: <https://www.ebi.ac.uk/p1dbe/pdb-component-library>
- API webinars: https://bit.ly/PDBe_API_webinars

 **PDBe-KB**

Protein Data Bank in Europe - Knowledge Base

COVID-19 Data Portal

[PDBe.org/covid19](https://pdbe.org/covid19)

































PDBe-KB COVID-19 Data Portal

An unprecedented number of scientific efforts are taking place worldwide in order to help combat the new coronavirus epidemic (COVID-19). One of the biggest challenges in this fast-moving situation is to share data and findings in a coordinated way, in order to understand the disease and to develop treatments and vaccines.

To support research efforts to understand more about the SARS-CoV-2 virus and the structures of its proteins, we have created dedicated PDBe-KB pages to highlight important structural features from released PDB entries. These pages include all **observed ligand binding sites and protein-protein interaction residues**, to help researchers easily identify important structural features to support the development of treatments and vaccines.

The pages available are listed below, with links to the relevant PDBe-KB protein pages:

PDBe-KB page	Data Summary															
<p>PODTD1 - Replicase polyprotein 1ab</p> <p>The orf1ab polyprotein is a multifunctional protein involved in the transcription and replication of viral RNAs. It contains the proteinases responsible for the cleavages of the polyprotein.</p>	<table><tbody><tr><td></td><td></td><td></td><td></td><td></td></tr><tr><td>545</td><td>423</td><td>10</td><td>0</td><td>12</td></tr><tr><td>Structures</td><td>Ligands</td><td>Interactions</td><td>Functional Annotations</td><td>Similar Proteins</td></tr></tbody></table>						545	423	10	0	12	Structures	Ligands	Interactions	Functional Annotations	Similar Proteins
																
545	423	10	0	12												
Structures	Ligands	Interactions	Functional Annotations	Similar Proteins												
<p>PRO_0000449619 - Host translation Inhibitor nsp1 (nsp1)</p> <p>Inhibits host translation by interacting with the 40S ribosomal subunit. The nsp1-40S ribosome complex further induces an endonucleolytic cleavage near the 5'UTR of host mRNAs, targeting them for degradation. Viral mRNAs are not susceptible to nsp1-mediated endonucleolytic RNA cleavage thanks to the presence of a 5'-end leader sequence and are therefore protected from degradation. By suppressing host gene expression, nsp1 facilitates efficient viral gene expression in infected cells and evasion from host immune response.</p>	<table><tbody><tr><td></td><td></td><td></td><td></td><td></td></tr><tr><td>16</td><td>5</td><td>3</td><td>1</td><td>0</td></tr><tr><td>Structures</td><td>Ligands</td><td>Interactions</td><td>Functional Annotations</td><td>Similar Proteins</td></tr></tbody></table>						16	5	3	1	0	Structures	Ligands	Interactions	Functional Annotations	Similar Proteins
																
16	5	3	1	0												
Structures	Ligands	Interactions	Functional Annotations	Similar Proteins												

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Questions and discussion



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