

PDBj provides a featured content webpage that is focused on novel coronavirus infectious disease (COVID-19).



COVID-19 featured content was released

<https://pdbj.org/featured/covid-19>

COVID-19 featured content

This page is also available in: [日本語](#) [简体中文](#) [繁體中文](#) [한국어](#)

The recent outbreak of the Novel Coronavirus disease (COVID-19) is a serious threat to people all over the world. In order to understand and develop an effective drug against the virus (Severe Acute Respiratory Syndrome Coronavirus 2; SARS-CoV-2), structural work on the related proteins has already started and the resultant entries are accumulating in the PDB. PDBj provides a portal page for the COVID-19 related entries for our users. New entries will be added simultaneously with the public release from thewwPDB.

An explanation article covering one of the proteins of this virus is available on the "Molecules of the Month" page below:

- 242: Coronavirus Protease
- 246: SARS-CoV-2 Spike

The tab "All entries" contains all PDB IDs, in case you want to check all independent entries, including group depositions by the same authors. The "Repr. entries" tab contains only representative PDB entries with the highest resolution, excluding duplicate entries with 100% amino acid sequence identity, even if they contain a different ligand. Finally, the "New entries" tab contains the latest entries released this week.

Created: 2020-03-11 (last edited: 6 days ago)

All entries (328) Repr. entries (125) Latest entries (3)

7COM **CRYSTAL STRUCTURE OF THE SARS-COV-2 MAIN PROTEASE IN COMPLEX WITH BOCEPREVIR (SPACE GROUP P212121)**

Descriptor: main protease, boceprevir (bound form)

Authors: Zeng, F., Qian, J.K., Wang, Y.F., Li, Y.S., Yao, R., Liu, J.M., Zhou, Y.L., Chen, P., Yang, S.Y., Lei, J.

Deposit date: 2020-08-04

Release date: 2020-08-04

Method: X-RAY DIFFRACTION (2.25 Å)

Cite: Crystal structure of the SARS-CoV-2 main protease in complex with Boceprevir (space group P212121) To Be Published

6X79 **REFUSION SARS-COV-2 S ECTODOMAIN TRIMER COVALENTLY STABILIZED IN THE CLOSED CONFORMATION**

Protein structural information solved by researchers around the world must be deposited in the database in advance via one of the sites in Japan, the US, or Europe. For the structures of SARS-CoV-2, The wwPDB member directly contacts the depositor of SARS-CoV-2 structures and recommends their immediate release even if the paper is not published in order to promote drug development research.

In addition, PDBj is collaborating with other data centers in Europe and the US to collate protein structures of the new coronavirus and release the data precisely. All data from Japan, the US, and Europe are released every Wednesday. We provide the COVID-19 featured page that only collects SARS-CoV-2. In this list structures from similar viruses such as SARS and MERS have already been filtered.

On this page, we also provide links to the related explanation articles of "Molecule of the Month".

COVID-19 featured page at HOMCOS

<http://homcos.pdbj.org/?LANG=en>

HOMCOS is a database that provides templates for searching and modeling complexes of 3D structures. Considering the emergence of the pandemic, we have now introduced a featured content page that includes information on COVID-19 related proteins and chemical components. The page summarizes structural information about closely related proteins and similar chemical components as well as the structures that have already been solved. The page is updated weekly to reflect the latest PDB data. We encourage the utilization of this information in order to accelerate structural biology research on coronaviruses.

HOMCOS
3D structures of Coronavirus SARS-CoV-2 proteins and related drugs in HOMCOS server

Last Update: 20200727. Data for updating PDB: 20200715

- We summarize 3D structures of proteins in Coronavirus SARS-CoV-2 that causes coronavirus disease 2019 (COVID-19) in a following table.
- We provide analysis [Searching Contact Molecules with Query Protein](#) of HOMCOS for each protein of the virus. Monomers and bound 3D structures of the virus proteins and their homologs are summarized. Found 3D structures can be used for templates of homology modeling. Details of the usage are explained in [DataHELP.aspx](#).
- For large proteins with > 1000 amino acids, making the analysis page will take more than 10 seconds. Please wait for a while.

Proteins in UniProt

AC	ID	length (amino acids)	Short name	Full name
P08212	NS3	38		
P08213	NS4A	275		Protein 3a; Accessory protein 3a;Protein 3a
P08214	NS4B	419	NC_Protein N1	Nucleoprotein 1; Nucleocapsid protein 1
P08215	NS5	91	NS5	Non-structural protein 5; Accessory protein 5

Reported Efficient Drugs

- 3D bound protein structures with compounds reported as [candidate drugs](#) for Coronavirus SARS-CoV-2 are summarized in a following table.
- We provide analysis [Searching Contact Molecules with Query Compound](#) of HOMCOS for each compound. Bound protein 3D structures with the compound and its analogues are summarized.

REGID	Structure	NAME	OTHER NAME	EFFICACY
004523		301302 Ciclesonide (JANUSAN/INQ; Alvecco (TN); Omicron (TN); Zileton (TN))	Alvecco (TN); Omicron (TN); Zileton (TN)	Antiasthmatic; Anti-inflammatory; Bronchodilator; Respiratory support
004543		301425 Lopinavir (IANUS/UP/INQ)		

COVID-19 related data deposition in BSM-Arc

<https://bsma.pdbj.org/featured/covid-19>

BSM-Arc (Biological Structure Model Archive) is a database of molecular structures derived by molecular dynamics and homology modeling. In principle, BSM-Arc only accepts peer-reviewed published research data. However, considering the urgency of research on new coronaviruses, we have decided to make the pre-peer-reviewed data available in the RTPI (Research Topics of Paramount Importance) category. We have already accepted and released two sets of data containing 38 atomic coordinates (as of 6th July 2020).

BSM-Arc

Welcome to BSM-Arc: The Biological Structure Model Archive (BSMA or BSM-Arc for short) top page.

We welcome depositions of raw data and supplementary information corresponding to published, peer-reviewed papers.

If you have any questions, please contact us. Please note that this archive is still under development and thus we appreciate any feedback you might have.

2020-07-08 (last updated: 2020-07-08)

Hot Structural News on COVID-19

Help Menu

- How to use BSM-Arc
- How to submit a new entry
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- How to cite
- How to use the BSM-Arc API
- How to use the BSM-Arc database

Latest entries

- Exhaustive search of the configurational space of Hsp90 with its inhibitor by McMD based dynamic docking**
Gen'lan Bando, Masayo Inoue, Kengo Shimizu, Yoshiko Okano, Takanori Kitama
Deposition date: 2019-12-12
Modification date: 2020-04-09
Release date: 2020-04-09
- Knowledge-based structural models of SARS-CoV-2 proteins and their complex with potential drugs**
Atsushi Hagiwara, Clara Shioyama, Mitsuru Saito, Naoki Masuhiro, Shiroki Ota, Shigetaka Kanaya, Tsuyoshi Shira
Deposition date: 2020-05-18
Modification date: 2020-05-11
Release date: 2020-05-19
- Mutual population-hBFT driven antibody-peptide binding elucidated by molecular dynamics simulations**
Ryohei Saito, Ryohei Kikuchi, Naoki Masuhiro, Shiroki Ota
Deposition date: 2019-10-02
Modification date: 2020-05-29
Release date: 2020-05-29
- A novel rare variant R292H in RTN4R affects growth cone formation and possibly contributes to schizophrenia susceptibility**
Mitsuru Saito, Ryohei Kikuchi, Naoki Masuhiro, Shiroki Ota, Shigetaka Kanaya, Tsuyoshi Shira, Takahiro Otsu, Naoki Masuhiro, Yota Ueno, Takahiro Otsu, Naoki Masuhiro, Shiroki Ota, Shigetaka Kanaya, Tsuyoshi Shira, Takahiro Otsu, Naoki Masuhiro, Yota Ueno, Takahiro Otsu, Naoki Masuhiro, Shiroki Ota, Shigetaka Kanaya, Tsuyoshi Shira
Deposition date: 2019-12-20
Modification date: 2020-05-29

EMPIAR-PDBj accepts HDD for submission

<https://empiar.pdbj.org/>

EMPIAR is a database for raw 2D electron microscopy images, and PDBj has established its mirror site EMPIAR-PDBj. To assist data submission from Asian EM researchers, we accept hard disc drives by postal mail or courier service. We have seen a large number of SARS-CoV-2 structures, such as spike protein and RNA polymerase, being determined rapidly and deposited into EMD and PDB. Eight SARS-CoV-2 entries have been registered in EMPIAR (as of 31st July 2020). We are now appealing to researchers for the rapid deposition of raw 2D data to EMPIAR.

The screenshot shows the EMPIAR website interface. At the top, there's a search bar with 'SARS-CoV-2' entered. Below the search bar, there's a table of search results. The table has columns for Dataset, Title, Authors, Related EMD/PDB entries, Size, and Resolution. Three entries are visible:

Dataset	Title	Authors	Related EMD/PDB entries	Size	Resolution
EMPIAR-10469	Single particle cryo EM dataset of SARS-CoV-2 spike protein in unclassifiable form, which generated a 2.8 Å reconstruction of the closed state. (9x10 multi-frame micrographs composed of 30 frames each in HRC format)	Wrobel AG, Benton DJ, Nans A, Rosenthal PJ, Gumbart JC	[PubMed: 32647363] [DOI: 10.1038/s41594-020-0968-7]	2.4 GB	
EMPIAR-10453	Cryo electron tomography - 0R-series of SARS-CoV-2 (246 0R series in HRC format)	Tarsovalá B, Szlora M, Schürmann C, Hagen W, Weick S, Blanc TEC, von Bülow S, Gächter M, Bagdas K, Hörner C, von Langermann G, Högberg M, Schwarz A, Corvino R, Müllerbach HD, Hummer G, Lasker JC, Beck M	[DOI: 10.1101/2020.06.26.172476]	469.1 GB	
EMPIAR-10441	Tetrameric SARS-CoV-2 ORF3a in a lipid nanodisc (79x2 multi-frame micrographs composed of 50 frames each in TFF format)	Kern EM, Sorani B, Hoel CM, Sridharan S, Kemis JR, Toso DB, Brohawn SG	[PubMed: 32627916] [DOI: 10.1101/2020.06.17.150554]	EMD-22138 4.8 GB	6.5

COVID-19 featured page at PDBj-BMRB

<https://bmrdep.pdbj.org/>

The screenshot shows the PDBj-BMRB website. At the top, there's a navigation bar with 'Deposition', 'Search', 'Archives', 'Mirrors', 'Language', and 'About'. Below the navigation bar, there's a search bar with 'Everything' selected. The main content area features a banner for 'COVID-19/SARS-CoV-2 featured content'. Below the banner, there's a search bar with a search button. At the bottom, there's a footer with information about the PDBj-BMRB group in Osaka University.

BMRB is a database of NMR experimental information about biological macromolecules. The PDBj-BMRB Group has set up a special page on SARS-CoV-2. Moreover, we also provide search examples using our original BMRB/PDB/EMDB/UniProt cross-database search function as well as new coronavirus entries deposited in BMRB.

COVID-19 featured page at the EM Navigator

<https://pdbj.org/emnavi/covid19.php>

"EM Navigator" is a web service that enables users to browse the data in EMD, the database of 3D electron density maps obtained by electron microscopy. In addition, in this service, we provide a featured page that collects data related to SARS-CoV-2.

The screenshot shows the EM Navigator website. At the top, there's a navigation bar with 'Browse 3DEM data' and 'Submit'. Below the navigation bar, there's a search bar with 'Keywords / EMD-ID / PDB-ID'. The main content area features a 'Recently released data' section. Below this section, there's a grid of search results showing various 3D electron density maps. The grid is organized into rows and columns, with each cell containing a small image of a density map and its corresponding ID number. At the bottom, there's a pagination bar with 'Pages: 1 2 3 < Previous > Next'.

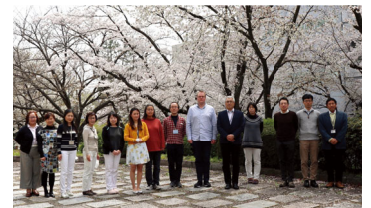
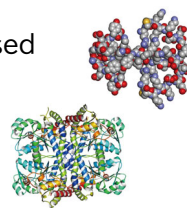
PDBj 20 Year Anniversary

Protein Data Bank Japan (PDBj) celebrated its 20 year anniversary in July 2020. With the support of JST-BIRD (at that time), the biocuration of the first PDB entry was completed on July 6th, 2000. With the help of the RCSB PDB, the number of data processed in PDBj improved from only 157 in 2000 to 376 in 2001 and 602 in 2002. In 2003, together with the RCSB PDB and PDBe, we founded wwPDB, which has grown to become responsible for the single global archives. Since then, the amount of deposited data from China has increased rapidly and, since 2016, we are now responsible for Asia and the Middle East. During this period, we have managed secondary databases such as eF-site and ProMode, introducing new formats such as PDBMLplus and RDF, and developing related tools such as Molmil and MagRO. This is the result of continuous support from depositors, users, the Ministry of Education, Culture, Sports, Science and Technology, JST, AMED, and other related organizations. PDBj will continue to work hard as an information hub for the Protein Data Bank in Asia and the Middle East, and we ask for your continuous support.

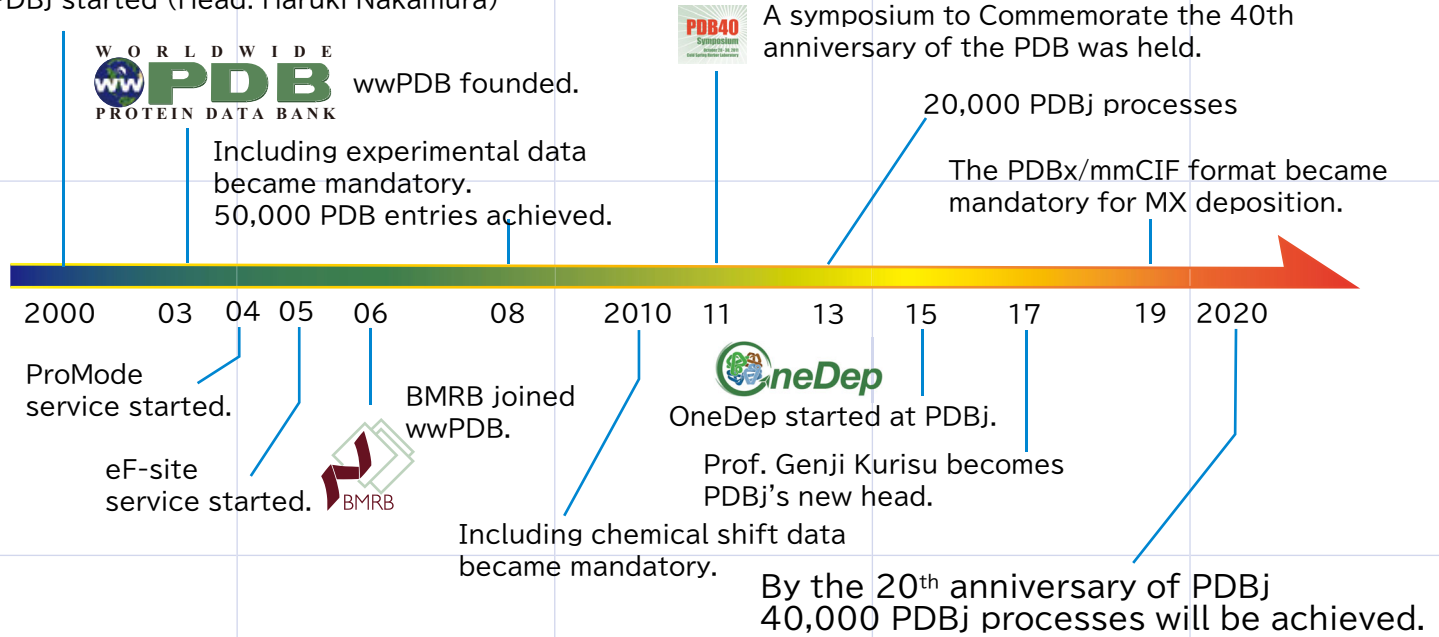


The first NMR structure processed by PDBj is 1EJQ (syndecan)

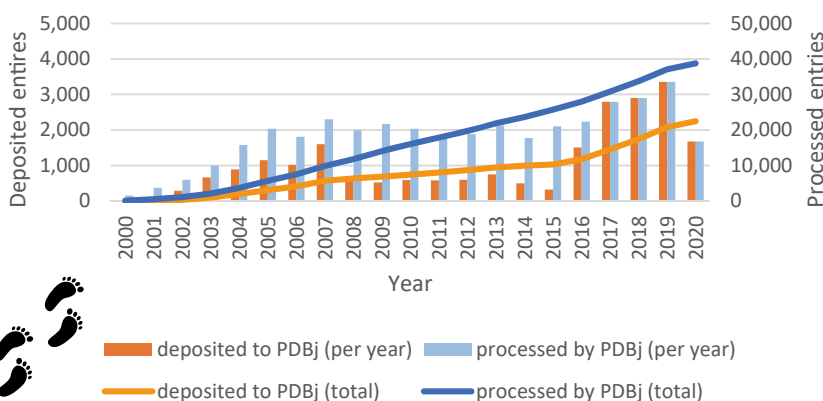
The first structure processed by PDBj is 1GC0 (methionine gamma lyase)



PDBj started (Head: Haruki Nakamura)



Deposited/Processed entries by PDBj (~2020-04-03)



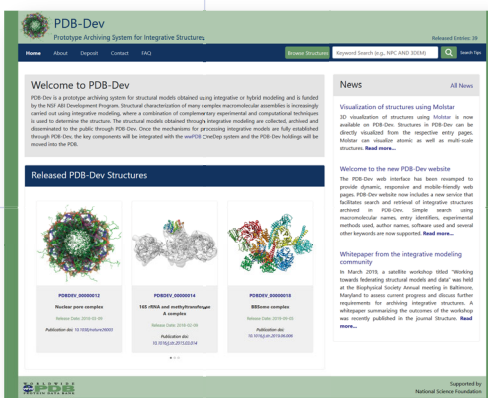
No.1

PDBj has an annotator that has processed the most number of entries in wwPDB. She has already processed more than 9,800 entries and will achieve 10,000 soon. Wow!

Award

1 An Updated PDB-Dev Website

PDB accepts structures determined by these three methods: crystal analysis, NMR, and electron microscopy. For the structures solved by combining various experimental techniques such as cross-linking mass spectrometry, 2D electron microscopy, FRET, and SAXS, we recommend depositing in Pyour data DB-Dev (<http://pdb-dev.wwpdb.org/>). The web site has been updated and has an enhanced search function. We encourage its use when academic journals request that you publish your data. <https://pdbj.org/news/20200410>



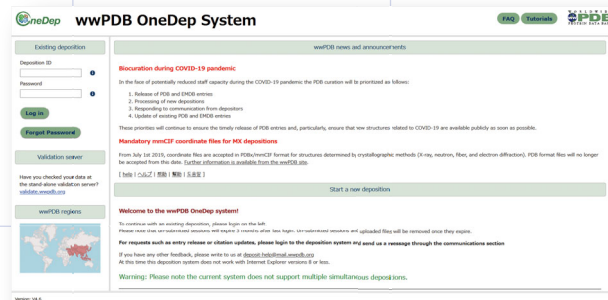
2 Advance Release of Metadata in EMDB Terminated

Since April 15th, 2020, we ceased publishing metadata before the release of primary map data. This change brings the management policy of EMDB in line with that of wwPDB. <https://pdbj.org/news/20200408>



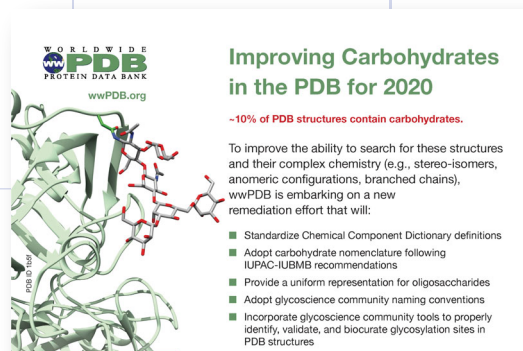
3 Improve Previously-Released Coordinates

Coordinates deposited before August 2019 via the previous PDB deposition system (ADIT, Autodep, etc.) can be updated without changing PDBIDs via the current PDB deposition system (OneDep). <https://pdbj.org/news/20200219>



4 Improving Carbohydrates in the PDB

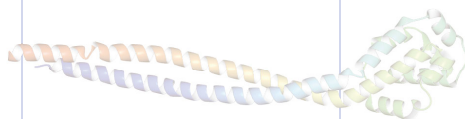
We have improved the representation of carbohydrates in PDB by adopting the nomenclature recommended by IUPAC-IUBMB, the names used in the glycoscience community, and expression that uniquely identifies the structure of oligosaccharides. <https://pdbj.org/news/20200226>



5 Unified Format of NMR Data Deposition

We have now extended the functions of the OneDep deposition system to enable the NMR structures with a single NEF or NMR-STAR file. This makes it easier to store, distribute, and reuse the NMR data. <https://pdbj.org/news/20200115>





PDBj has been awarding PDBj Poster Awards since 2018 for outstanding student presentations at conferences in Asia and the Middle East, where PDBj is responsible for data deposition. At the 16th Asian Crystallographic Association (AsCA2019) held at Singapore National University from December 17th to 20th 2019, we awarded the 2nd PDBj Poster Prize.

The winner was Mr. Prashant Kumar Singh (All India Institute of Medical Sciences, India). The title of his poster presentation is "Structural basis of activation of mammalian heme peroxidases." We presented him with the award certificate and the book "Integrative Structural Biology with Hybrid Methods (Editors: Haruki Nakamura, Gerard Kleywegt, Stephen K. Burley, John L. Markley)" edited by PIs of wwPDB.

The winner was announced by the selection committee appointed by the executive board of AsCA 2019. We would like to thank the local executive board and the selection committee for their support.



We opened a donation window at the Osaka University Foundation in order to enhance and improve public relations activities that cannot be paid for by research funds from public institutions.

For more information, please visit our website.
<https://pdbj.org/info/donation?lang=en>



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