

Archiving Electron Microscopy Data – EMDB and EMPIAR



Jack Turner

EMDB

Outline of session



Introduction to EMDB and EMPIAR



Websites and Validation



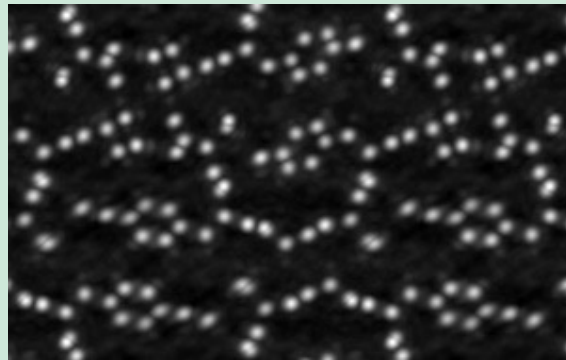
Deposition

The Electron Microscopy Data Bank - EMDB

- Established in 2002 at EMBL-EBI
- wwPDB Partner
- Electron microscopy volume maps and Tomograms
- All data is freely and openly available under a CC0 license

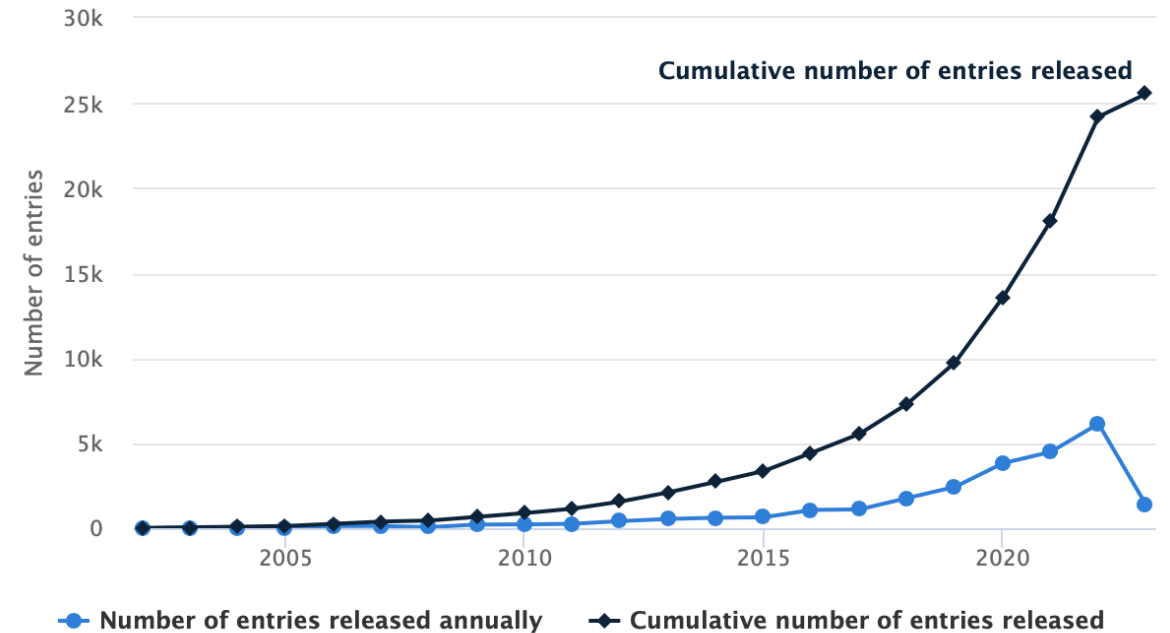


EMD-15182



EMD-0698

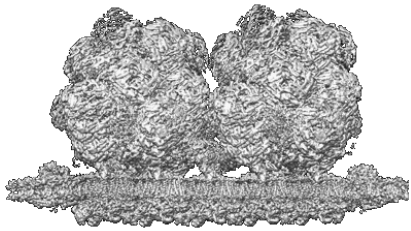
EMDB entries released per year and cumulatively



EMDB - Methodologies

Single Particle

Double-PBS-PSII-PSI-LHCs megacomplex

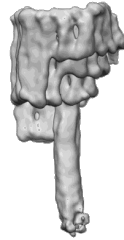


EMD-33658

Author List:
You X, Zhang X,
Cheng J, Xiao YN,
Sun S, Sui SF

Subtomogram Averaging

DNA Origami Signpost



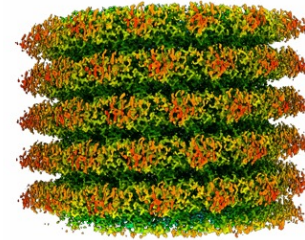
EMD-12188

Author List: silvester
E, Vollmer B, Prazak V,
Vasishtan D, Machala EA,
Whittle C, Black S, Bath J,
Turberfield AJ, Gruenewald
K, Baker LA

[1]

Helical Reconstruction

Tobacco Mosaic Virus

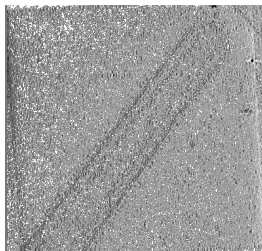


EMD-16572

Author List:
Bhella D, Love AJ,
Streetley J,
Taliensky M,
McGeachy K,
Bukharova T

Tomography

Syncytial Virus Filamentous Virion



EMD-13856

Author List:
Conley MJ ,
Vijayakrishnan S ,
Bhella D

[2]

Electron Crystallography

Metarhodopsin I



EMD-1079

Author List:
Ruprecht JJ,
Mielke T, Vogel
R, Villa C,
Schertler GFX

[3]

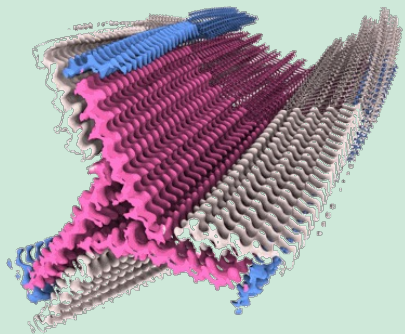
[1] Silvester, E., Vollmer, B., Pražák, V., Vasishtan, D., Machala, E. A., Whittle, C., Black, S., Bath, J., Turberfield, A. J., Grünewald, K., & Baker, L. A. (2021). DNA origami signposts for identifying proteins on cell membranes by electron cryotomography. *Cell*, 184(4), 1110-1121. e16. <https://doi.org/https://doi.org/10.1016/j.cell.2021.01.033>

[2] The EMBO Journal (2022) 41: e109728 <https://doi.org/10.15252/embj.2021109728>

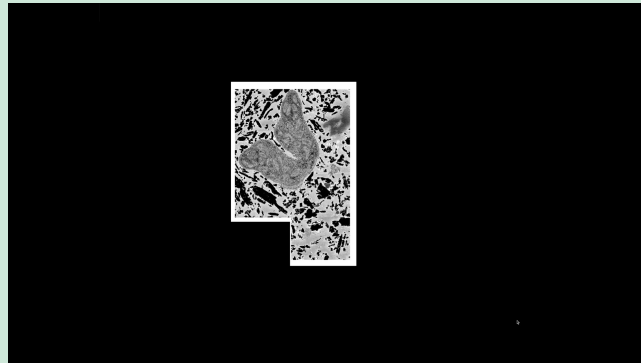
[3] Ruprecht, J.J., Mielke, T., Vogel, R., Villa, C. and Schertler, G.F. (2004), Electron crystallography reveals the structure of metarhodopsin I. *The EMBO Journal*, 23: 3609-3620. <https://doi.org/10.1038/sj.emboj.7600374>

Electron Microscopy Public Image Archive - EMPIAR

- Raw imaging data used to produce maps found in the EMDB
- Volume EM techniques and X-ray tomography and microscopy
- All data is freely and openly available under a CC0 license

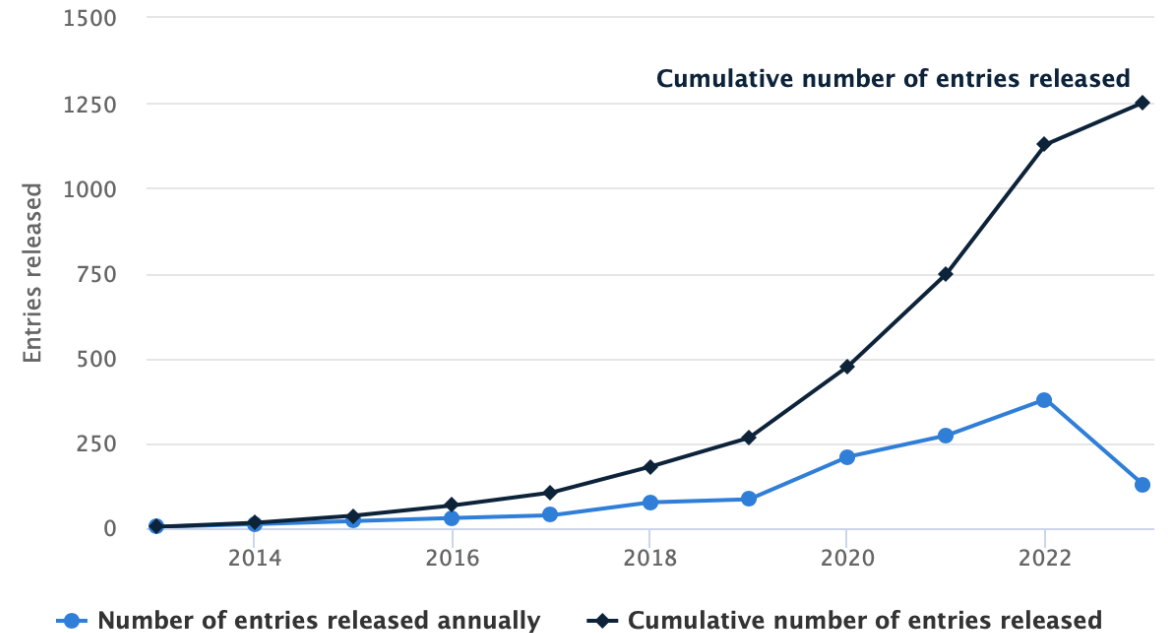


EMPIAR-11278/EMD-14167



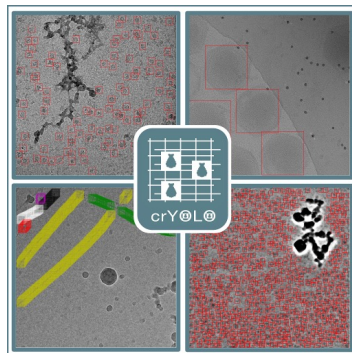
EMPIAR-10310

EMPIAR entries released per year and cumulatively



EMPIAR & EMDB – Data Re-use – Machine Learning

- **DeepEMhancer:** Sanchez-Garcia, R., Gomez-Blanco, J., Cuervo, A. et al. DeepEMhancer: a deep learning solution for cryo-EM volume post-processing. *Commun Biol* 4, 874 (2021). <https://doi.org/10.1038/s42003-021-02399-1>
- **Deep Consensus:** Sanchez-Garcia, R., Segura, J., Maluenda, D., Carazo, J. M. & Sorzano, C. O. S. (2018). *IUCrJ* 5, 854-865.
- **DRPnet:** Nguyen, N.P., Ersoy, I., Gotberg, J. et al. DRPnet: automated particle picking in cryo-electron micrographs using deep regression. *BMC Bioinformatics* 22, 55 (2021). <https://doi.org/10.1186/s12859-020-03948-x>
- **crYOLO:** Wagner, T., Merino, F., Stabrin, M. et al. SPHIRE-crYOLO is a fast and accurate fully automated particle picker for cryo-EM. *Commun Biol* 2, 218 (2019). <https://doi.org/10.1038/s42003-019-0437-z>
- **WARP:** Tegunov, D., Cramer, P. Real-time cryo-electron microscopy data preprocessing with Warp. *Nat Methods* 16, 1146–1152 (2019). <https://doi.org/10.1038/s41592-019-0580-y>
- **M:** Tegunov, D., Xue, L., Dienemann, C. et al. Multi-particle cryo-EM refinement with M visualizes ribosome-antibiotic complex at 3.5 Å in cells. *Nat Methods* 18, 186–193 (2021). <https://doi.org/10.1038/s41592-020-01054-7>

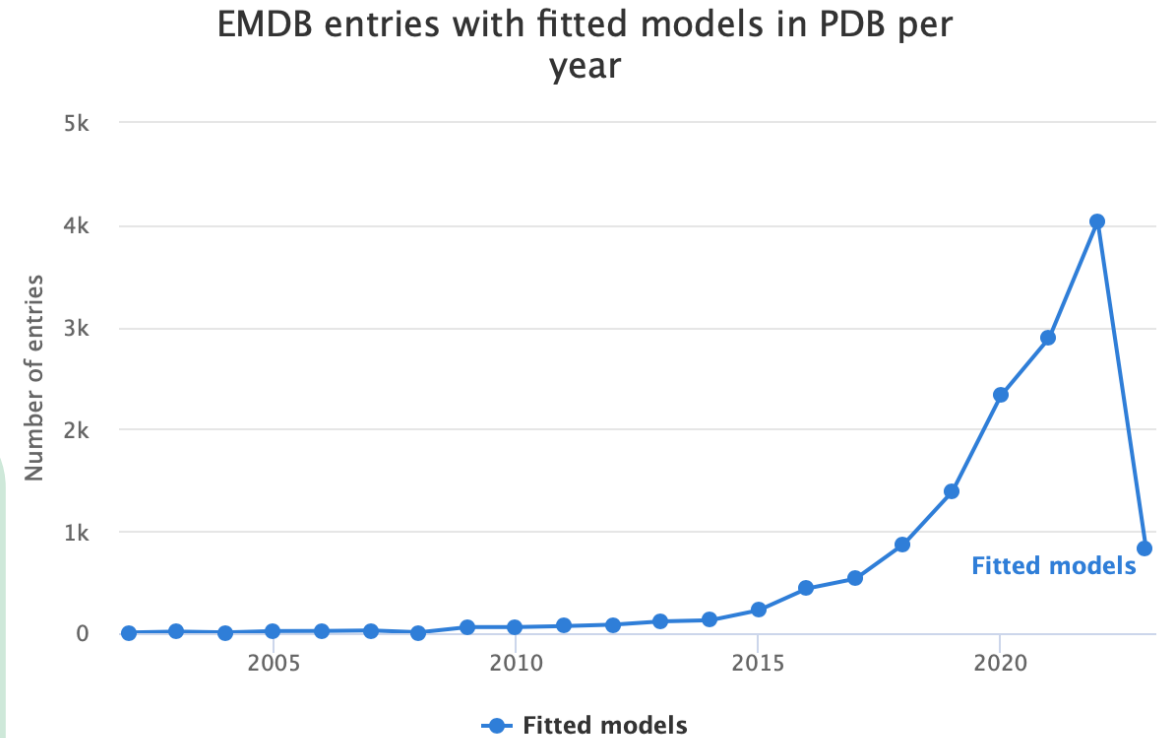
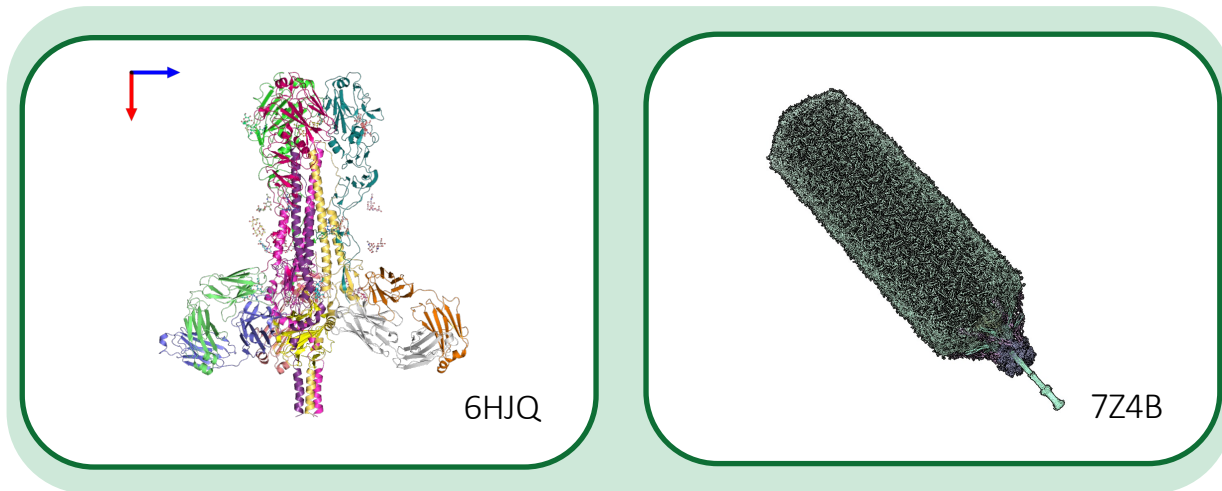


EMPIAR & EMDB – Data Re-use

- **Relion 4:** Dari Kimanius, Liyi Dong, Grigory Sharov, Takanori Nakane, Sjors H. W. Scheres; New tools for automated cryo-EM single-particle analysis in RELION-4.0. *Biochem J* 22 December 2021; 478 (24): 4169–4185. doi: <https://doi.org/10.1042/BCJ20210708>
- **Relion with DeepEMhancer and SIDESPLITTER:** Ramirez-Aportela, E., Carazo, J. M. & Sorzano, C. O. S. (2022). *IUCrJ* 9, 632-638. <https://doi.org/10.1107/S2052252522006959>
- **CISTEM:** Timothy Grant, Alexis Rohou, Nikolaus Grigorieff (2018) cisTEM, user-friendly software for single-particle image processing *eLife* 7:e35383 <https://doi.org/10.7554/eLife.35383>
- **Cryoem-cloud-tools:** Cianfrocco MA, Lahiri I, DiMaio F, Leschziner AE. cryoem-cloud-tools: A software platform to deploy and manage cryo-EM jobs in the cloud. *J Struct Biol.* 2018 Sep;203(3):230-235. doi: 10.1016/j.jsb.2018.05.014. Epub 2018 Jun 1. PMID: 29864529; PMCID: PMC6091888.
- **cryoSPARC:** Punjani, A., Rubinstein, J., Fleet, D. et al. cryoSPARC: algorithms for rapid unsupervised cryo-EM structure determination. *Nat Methods* 14, 290–296 (2017). <https://doi.org/10.1038/nmeth.4169>

Protein Data Bank - PDB

- Archiving Coordinate models from EM, X-ray and NMR
- All data is freely and openly available under a CC0 license



~14,000 entries

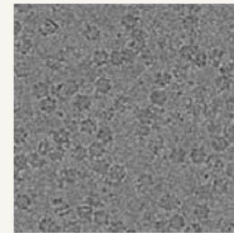
EMDB, EMPIAR & PDB Summary

- Archive the full electron microscopy (EM) processing workflow
- EMPIAR – Supporting development of software and scientists
- EMDb – Refined EM structures and tomograms
- PDB - Coordinate models from X-ray, EM and NMR

MODELLING IN ICE

In cryo-electron microscopy (cryo-EM), thousands of raw EM images are collected and computationally analysed to build up a density map that reflects the shape of the protein.

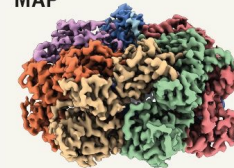
RAW IMAGE



Where to share data

Electron Microscopy Public Image Archive (EMPIAR)

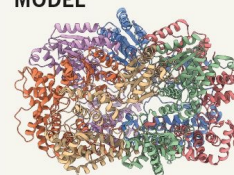
MAP



Electron Microscopy Data Bank (EMDB)

This map is then combined with the known protein sequence to create a final model showing the placement of atomic groups.

MODEL



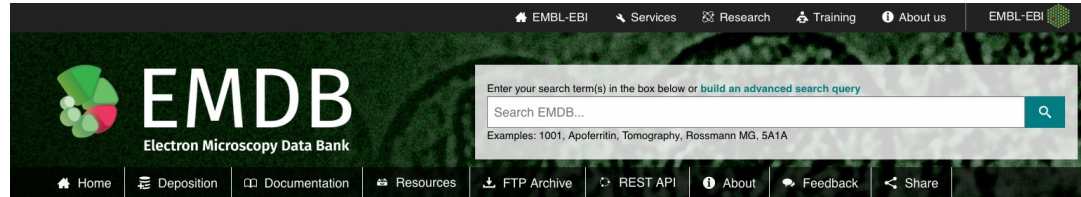
Protein Data Bank (PDB)

©nature

Introduction to EMDB Website and Validation



The EMDB website – Homepage



EMBL-EBI Services Research Training About us EMBL-EBI

EMDB

Electron Microscopy Data Bank

Enter your search term(s) in the box below or [build an advanced search query](#)

Examples: 1001, Apoferritin, Tomography, Rossmann MG, 5A1A

Home Deposition Documentation Resources FTP Archive REST API About Feedback Share

EMDB (the Electron Microscopy Data Bank) is a public repository for electron cryo-microscopy maps and tomograms of macromolecular complexes and subcellular structures. It covers a variety of techniques, including single-particle analysis, electron tomography, sub-tomogram averaging, fibre diffraction and electron crystallography. [More...](#)

As of 16 March 2022, EMDB contains 19125 entries ([latest entries](#), [trends](#)).

EMDB News

- wwPDB is switching to version 3 of the EMDB data model. From 9 February 2022 the old data model (v1.9.6) will no longer be supported. Read the [wwPDB announcement](#) for more details.
- In July 2021, the EMDB website moved to a new location. [What do I need to know?](#)



Browse EMDB EMDB statistics SARS-CoV-2 entries Deposit data

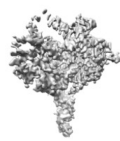
Explore EMDB

Select a graph from the pull-down menu. Click on any element of a graph to see the corresponding list of EMDB entries.

Quick Links

- EMDB Policies
- Talks & Tutorials
- Validation Analysis
- EMDB Citations
- EMPIAR
- PDBe
- Biolmage Archive
- EMDataResource
- EM Navigator
- 3D EM History


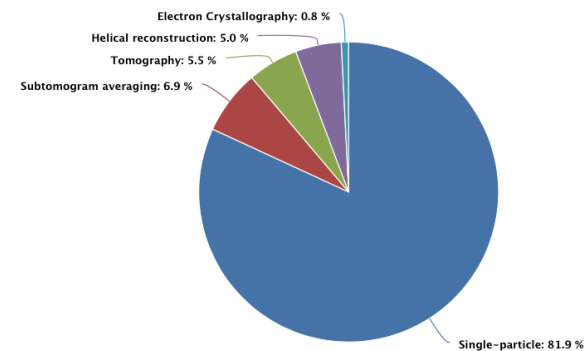
Recent Entries (Show all)



EMD-32390 [1/95]
PimCasX-sgRNAv1-dsDNA ternary complex at its loading state

Explore EMDB


Select a graph from the pull-down menu. Click on any element of a graph to see the corresponding list of EMDB entries.



EMD-32390 [1/95]
PimCasX-sgRNAv1-dsDNA ternary complex at its loading state

[View Entry](#)

Tweets by @EMDB_EMPIAR



EMDB - EMPIAR @EBI @EMDB_EMPIAR
Where cryo-EM meets volume
EMDevcell.em.sciencesconf.org

[Embed](#) [View on Twitter](#)

The EMDB website – Statistics

EMDB
Electron Microscopy Data Bank

Enter your search term(s) in the box below or build an advanced search query

Search EMDB...

Examples: 1001, Apolentini, Tomography, Rossmann MG, 5A1A

Home | Deposition | Documentation | Resources | FTP Archive | REST API | About | Feedback | Share

EMDB (the Electron Microscopy Data Bank) is a public repository for electron cryo-microscopy maps and tomograms of macromolecular complexes and subcellular structures. It covers a variety of techniques, including single-particle analysis, electron tomography, sub-tomogram averaging, fibre diffraction and electron crystallography. [More...](#)

As of 09 November 2022, EMDB contains 23271 entries (latest entries, trends).

EMDB News

- 12 October 2022: EMDB Validation Analysis (VA) is officially launched at <https://www.ebi.ac.uk/emdb/va/>. It is available as a local stand-alone package and is coming soon to COP-EM. The tutorial on how to use the VA information is on [EMDB YouTube channel](#). A full description of VA functionality is published in [Acta Crystallographica Section D](#).
- 7 June 2022: EMDB and EMPIAR have launched a dedicated [YouTube channel](#) where you can find talks, tutorials, and much more. Check it out and [let us know](#) what content you would like to see.

Quick links

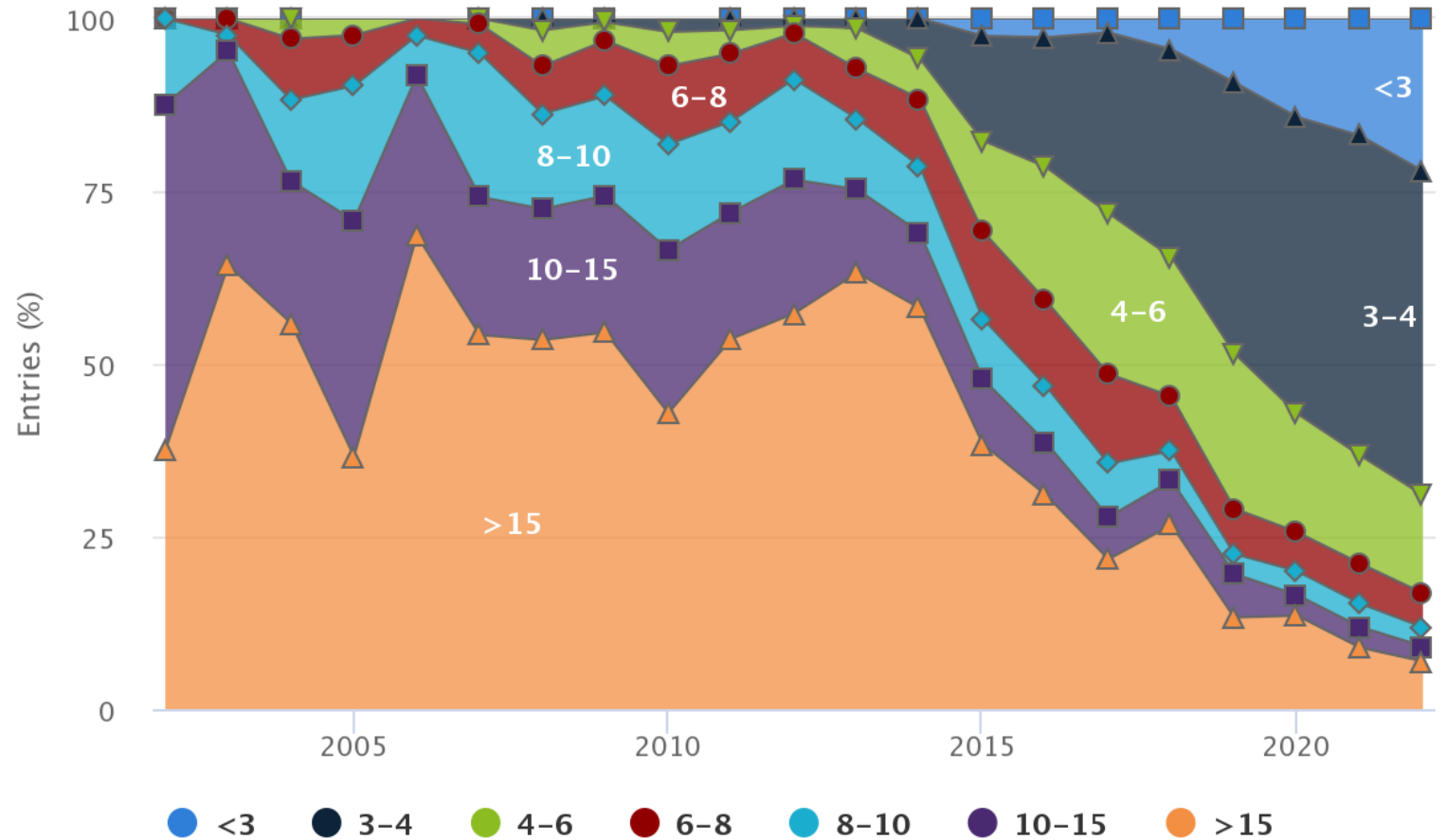
- EMDB Policies
- Talks & Tutorials
- Validation Analysis
- Volume Browser
- EMDB Citations
- EMPIAR
- PDBe
- Biolmage Archive
- EMDataResource
- EM Navigator
- 3D EM History

Recent Entries (Show all)

Browse EMDB | **EMDB statistics** | SARS-CoV-2 entries | Deposit data

EMDB: [ebi.ac.uk/emdb/](https://www.ebi.ac.uk/emdb/)

EMDB entry resolution in shells per year



<https://www.ebi.ac.uk/emdb/>

The EMDB website – Chart Build

Chart builder

Beta version

Archive: EMDB

Chart type: Line

Data X: Year

Initial year: 2002

Final year: 2022

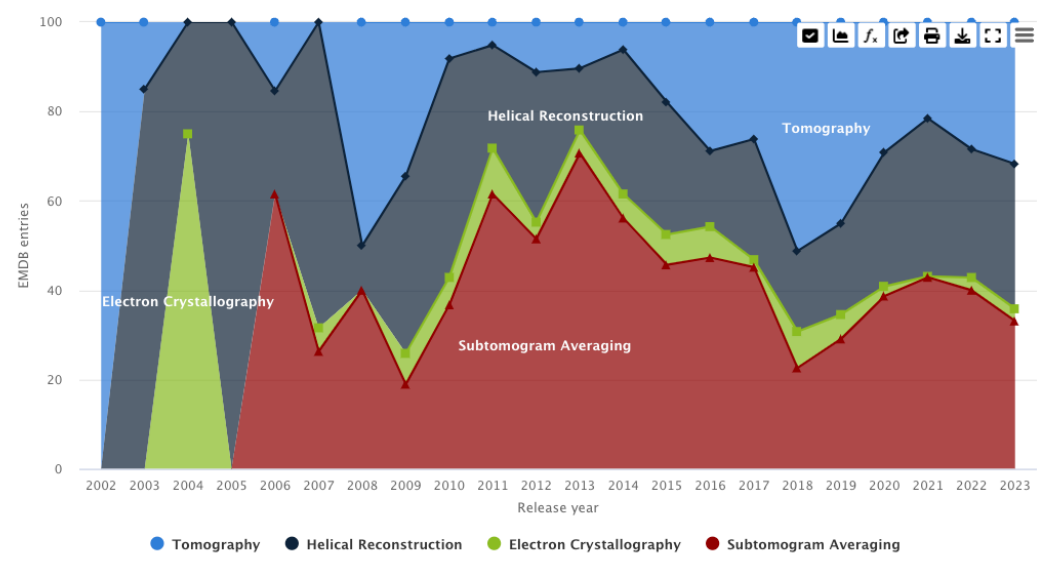
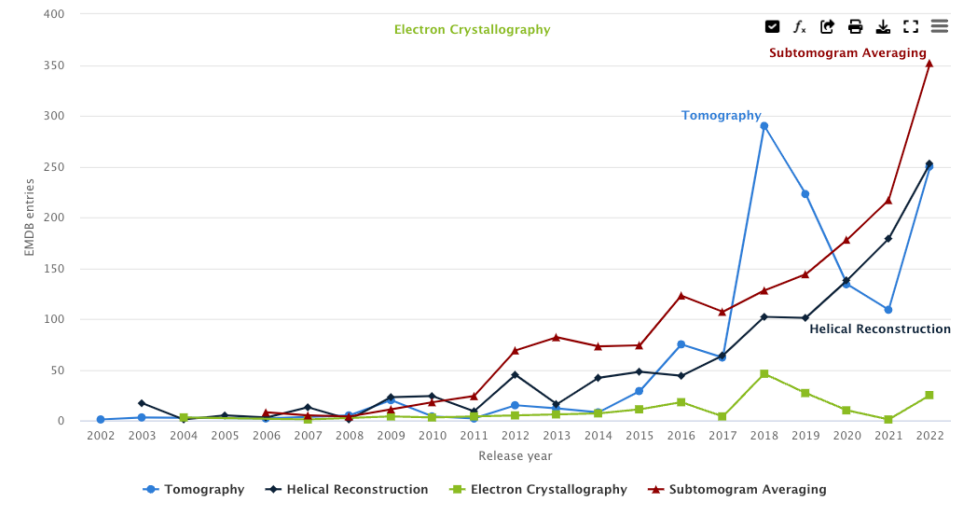
Data Y: EMDB entries

Data series configuration:

Color	Operator	Filter query	Label
Blue	Count (unique)	structure_determination_method:"tomography"	Tomography
Dark Blue	Count (unique)	structure_determination_method:"helical"	Helical Reconstruction
Light Green	Count (unique)	structure_determination_method:"electroncryst"	Electron Crystallography
Dark Red	Count (unique)	structure_determination_method:"subtomogran"	Subtomogram Averaging

Additional options

Generate



The EMDB website – Basic and Advanced Search

The image displays the EMDB website interface. At the top, the EMDB logo is visible. A search bar contains the term 'ribosome'. Below the search bar, there are four columns of search results, each with a 'Show all' link:

- Sample name:** 80S ribosome [86], 70S ribosome [83], Ribosome [72], ribosome [39], Ribosome assembly factor MRT4 [35]
- Organism:** Ribosome display vector pRDV [2]
- Title:** Ensemble cryo-EM uncovers inchworm-like translocation of a viral IRES through the ribosome [11], Ribosome dynamics and tRNA movement as visualized by time-resolved electron cryomicroscopy [11], Ribosome Assembly Factors Prevent Premature Translation Initiation by 40S Assembly Intermediates [7], Stalled E. coli ribosomes (Fo-c SecM nascent chains) and native E. coli membranes containing recombinant YidC [7], Structure of the Ribosome with Elongation Factor G Trapped in the Pre-Translocation State [7]
- Gene Ontology:** structural constituent of ribosome [753], ribosome [732], ribosome biogenesis [431], ribosome binding [353], ribosome assembly [279]
- InterPro:** Ribosome/NADH_DH [26], Ribosome_biogen_GTPase_RsgA [4], Ribosome_recyc_fac [3], Ribosome_recyc_fac_dom [3], Ribosome biogenesis protein Alb1 [2]

Below the search results, there is an 'Image Set' section with the following items:

- 80S ribosome multi-frame micrographs [1]
- Extracted particle images of the 70S ribosome from the human pathogen *Acinetobacter baumannii* in complex with amikacin [1]
- Extracted particle images of the 70S ribosome from the human pathogen *Acinetobacter baumannii* in complex with tigecycline [1]
- Motion-corrected micrographs of the 70S ribosome from the human pathogen *Acinetobacter baumannii* in complex with amikacin [1]
- Motion-corrected micrographs of the 70S ribosome from the human pathogen *Acinetobacter baumannii* in complex with tigecycline [1]

An advanced search dialog box is overlaid on the page, showing the following search criteria:

- Title:** Condition: Contains, Text: ribosomes
- EM method:** Condition: AND, Option: Single-particle
- Field:** (empty)

The dialog box has a 'Search' button at the bottom right.

<https://www.ebi.ac.uk/emdb/>

The EMDB website – Filtering & Statistics

Edit and save complex search queries

Edit your search query here and hit Return to execute it:

HIV-1 AND structure_determination_method:"tomography"

Extensive list of filtering options

Filter By

Current Database

- EMDB [26]

Current status

- REL [26]

Sample type

- Virus [25]
- Sample [14]
- Cellular component [1]

Organism

- Human immunodeficiency virus 1 [24]
- Mus musculus [1]
- Human immunodeficiency virus [1]

EM Method

- Tomography [26]

Model molecular weight

Download

Select database:

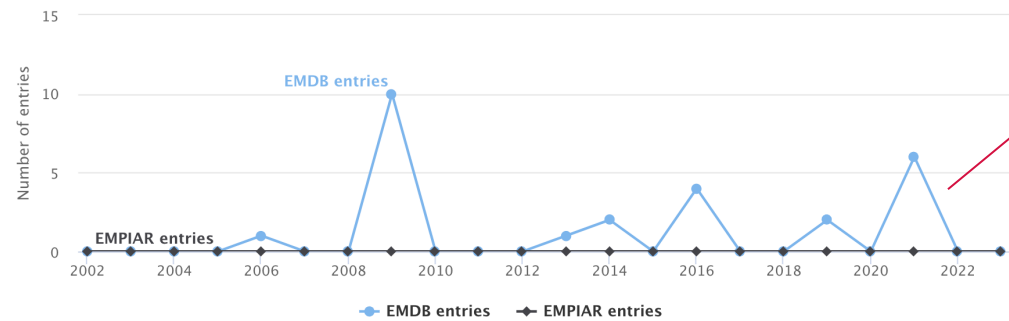
- EMDB [26]

Format: JSON (metada)

Preview first 10

Download

Number of entries released by year



Interactive graph that can be used to filter results

Sort by: Release Date

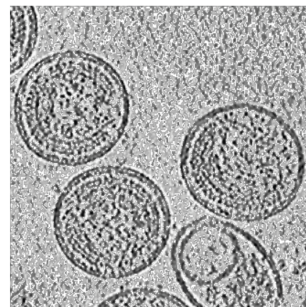
Download

Showing 1 - 10 of 26. Page 1 of 3

Display: 10

Statistics

EMD-13085



Representative cryo-electron tomogram of immature HIV-1 particles

Release date: Aug. 18, 2021

EM Method: Tomography

Qu K, Ke Z, Zila V, Anders-Osswein M, Glass B, Mucksch F, Muller R, Schultz C, Muller B, Krausslich HG, Briggs JAG

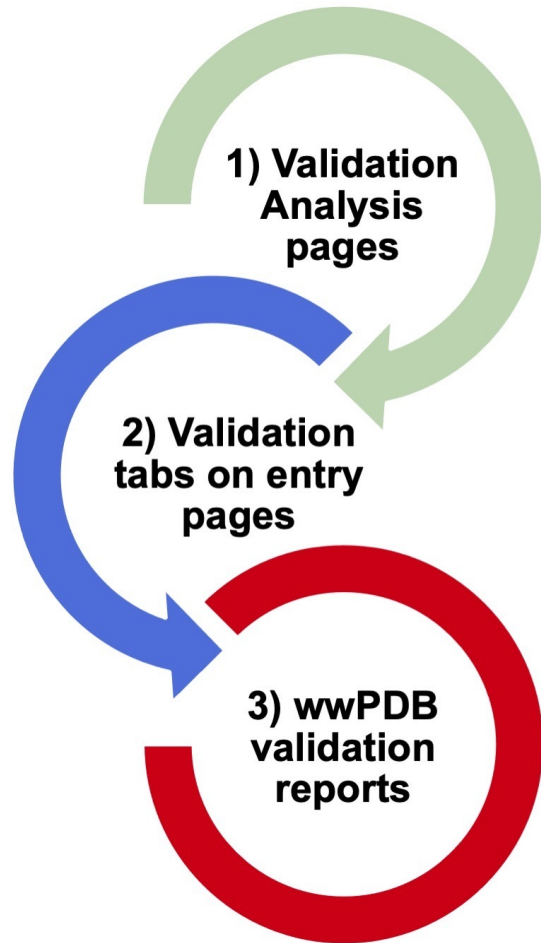
Science (2021) 373 pp. 700-704 [Pubmed: 34353956 DOI: doi:10.1126/science.abe6821]

Sample:

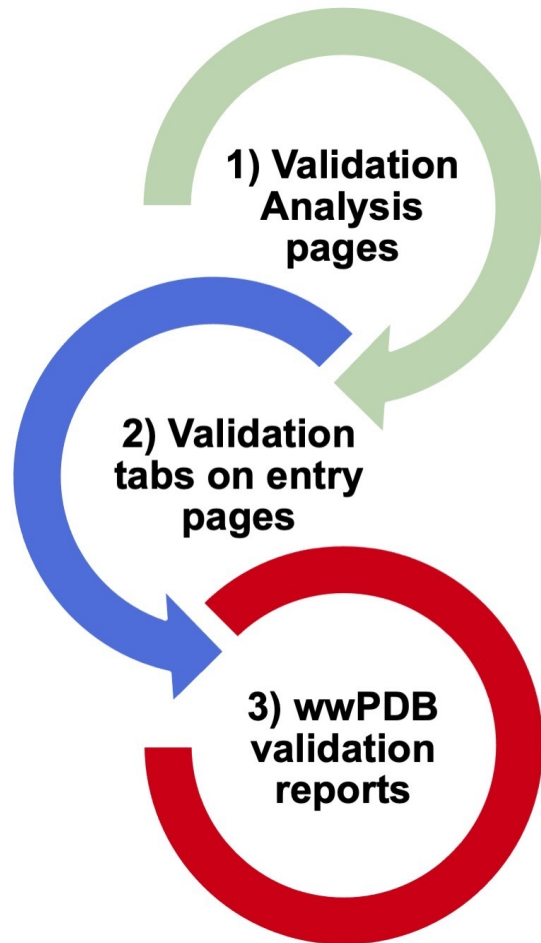
- Human immunodeficiency virus 1 (Virus from Human immunodeficiency virus 1)

<https://www.ebi.ac.uk/emdb/>

EMDB Validation



EMDB Validation



EMD-11145 › Validation analysis

To see the Validation Analysis entry, please enter the EMD (e.g., 8117 or 5ix):

SARS CoV-2 Spike protein, Closed conformation, C3 symmetry

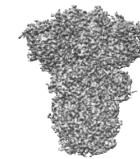
Additional validation information

For more information, please see the wwPDB validation report for this entry with fitted PDB model [6zb5](#).

Resolution:	2.85 Å (FSC 0.143 CUT-OFF, depositor provided)
Method:	Single particle reconstruction
Map released:	2020-09-30
Last modified:	2020-11-18
Sample name:	SARS CoV-2 Spike protein, Closed conformation, C3 symmetry
Organism:	Severe acute respiratory syndrome coronavirus 2
Fitted atomic model:	6zb5

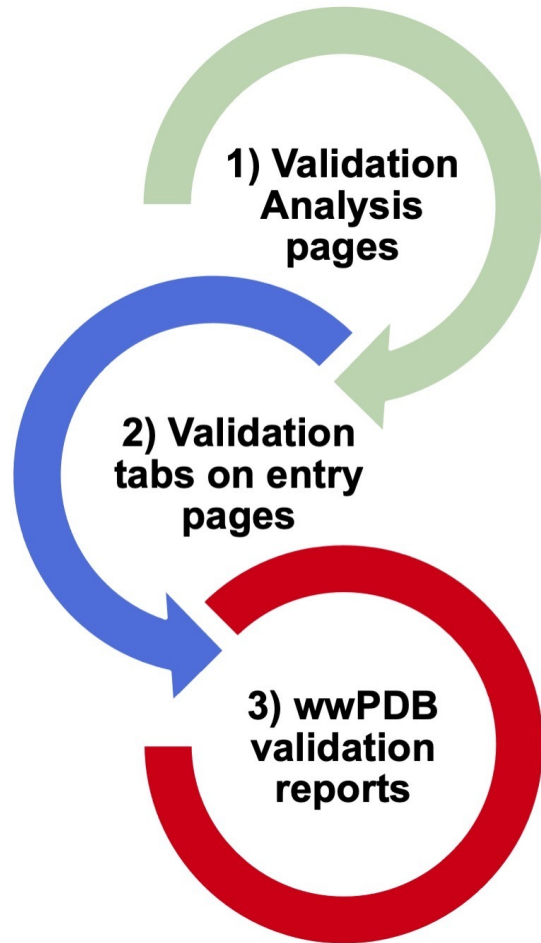
Map parameters

Recommended contour level:	0.006
Number of grid points:	220 × 220 × 220
Voxel size:	1.050 × 1.050 × 1.050 Å
Minimum value:	-0.197
Maximum value:	0.316
Average value:	0.001
Standard deviation:	0.012

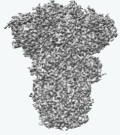


ebi.ac.uk/emdb/va/

EMDB Validation



EMD-11145
Single-particle
2.85 Å



3D View Gallery

Deposition: 07/06/2020
Map released: 30/09/2020
Last modified: 18/11/2020

- Overview
- 3D View
- Sample
- Experiment
- Validation**
- Volume Browser
- Additional data
- Links

EMD-11145

Download ▾

SARS CoV-2 Spike protein, Closed conformation, C3 symmetry

Additional validation information

For more information, please see the wwPDB validation report for this entry with fitted PDB model [6zb5](#). Cryo-EM specialists may also be interested in the more extensive analysis of this entry in the [EMDB Validation Analysis](#) resource.

Resolution: 2.85 Å (FSC 0.143 CUT-OFF, depositor provided)

Method: Single particle reconstruction

Map released: 2020-09-30

Last modified: 2020-11-18

Sample name: SARS CoV-2 Spike protein, Closed conformation, C3 symmetry

Organism: Severe acute respiratory syndrome coronavirus 2

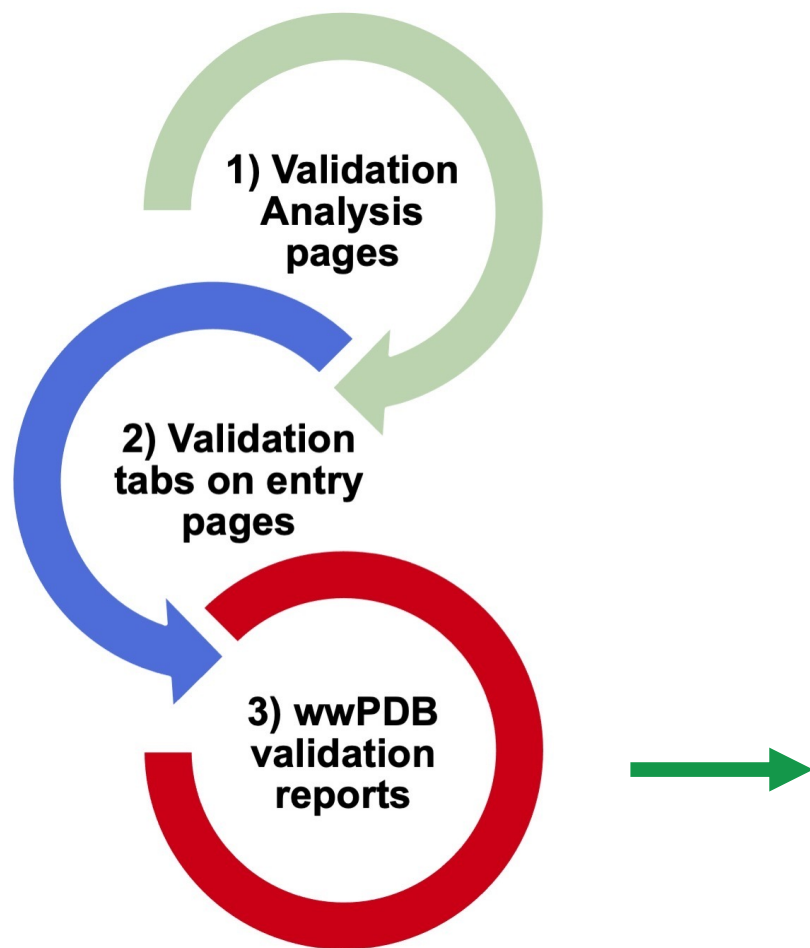
Fitted atomic model: [6zb5](#)

Map parameters

Recommended contour level: 0.006

Number of grid points: 220 × 220 × 220

EMDB Validation



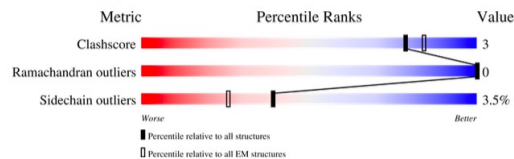
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

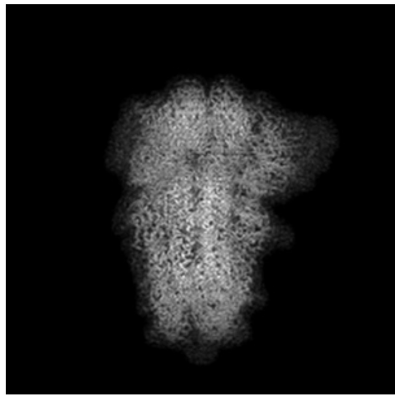
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1259	76% (green), 6% (yellow), 18% (orange), 0% (red), 0% (grey)
1	B	1259	76% (green), 6% (yellow), 18% (orange), 0% (red), 0% (grey)
1	C	1259	76% (green), 6% (yellow), 18% (orange), 0% (red), 0% (grey)
2	D	2	50% (green), 50% (orange), 0% (yellow), 0% (red), 0% (grey)
2	E	2	100% (orange), 0% (yellow), 0% (red), 0% (grey)
2	F	2	100% (yellow), 0% (orange), 0% (red), 0% (grey)

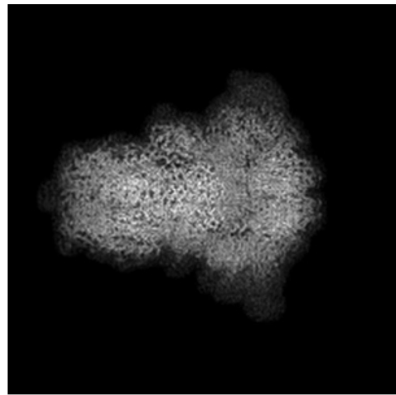
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

EMDB Validation

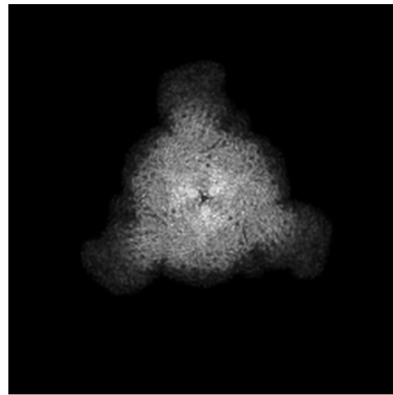
Qualitative



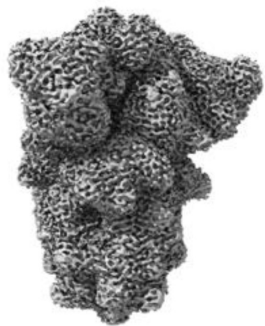
X



Y



Z



X

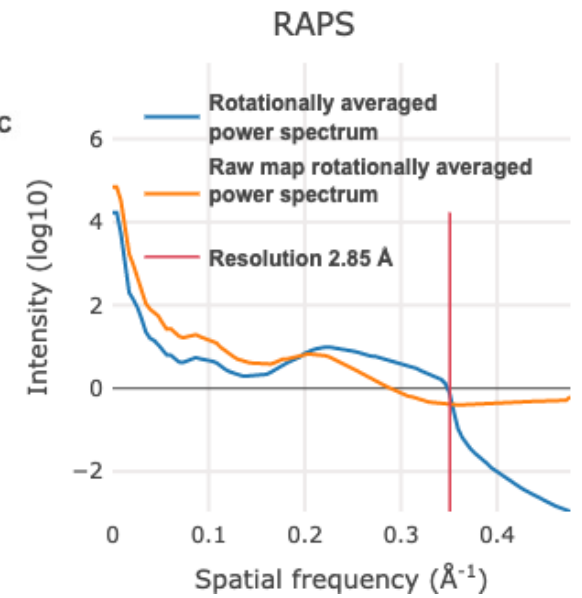
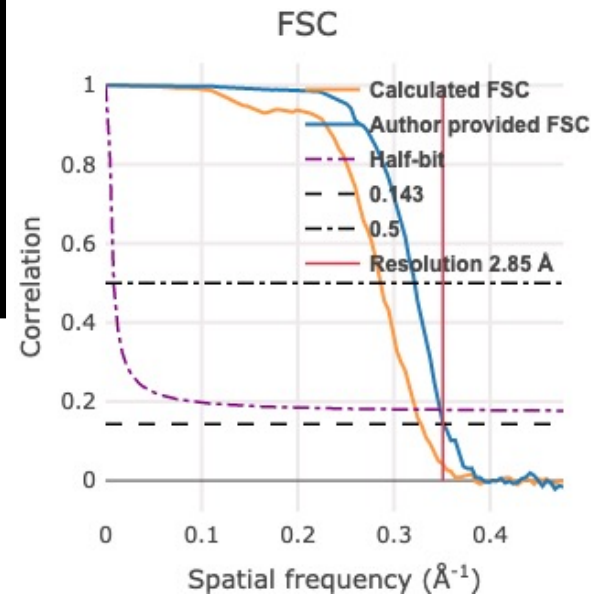


Y



Z

Quantitative



EMD-11145

EMDB Validation - Tomography

Qualitative

Cryo-electron tomogram of *Wolinella* sp. ATCC 33567

Additional validation information

For more information, please see the [WWPDB validation report](#) for this entry.

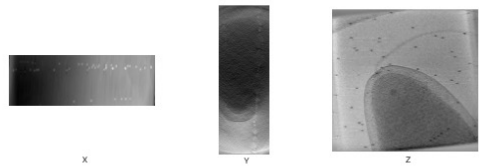
Method: Tomographic reconstruction
 Map released: 2023-04-05
 Last modified: 2023-04-05
 Sample name: *Wolinella* sp. ATCC 33567
 Organism: *Wolinella succinogenes*

Tomogram parameters

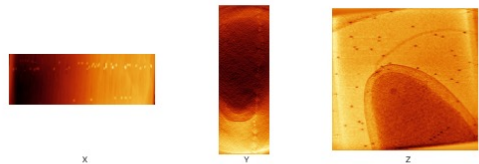
Number of grid points: 960 × 928 × 324
 Voxel size: 8.839 × 8.839 × 8.839 Å
 Minimum value: -128.000
 Maximum value: 127.000
 Average value: 15.010
 Standard deviation: 20.685

Tomogram map analysis

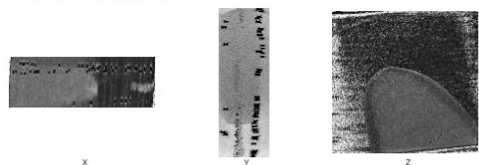
Orthogonal projections



Orthogonal projections (false-colour)



Orthogonal minimum-value projections

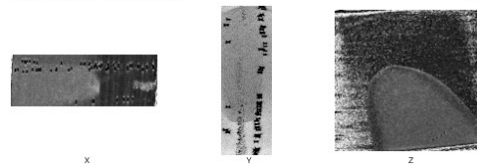


Orthogonal minimum-value projections (false-colour)

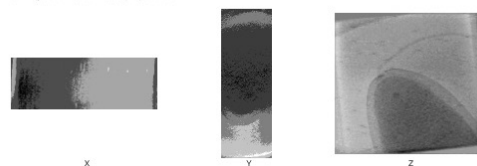


[Navigate](#)
[Top](#)
[Tomog](#)
[Volu](#)

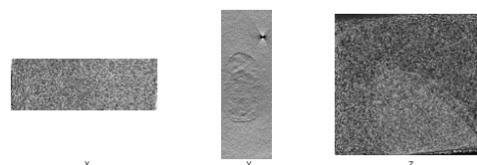
Orthogonal minimum-value projections



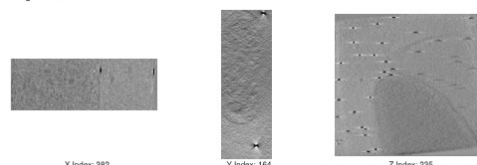
Orthogonal median-value projections



Central slices



Largest variance slices



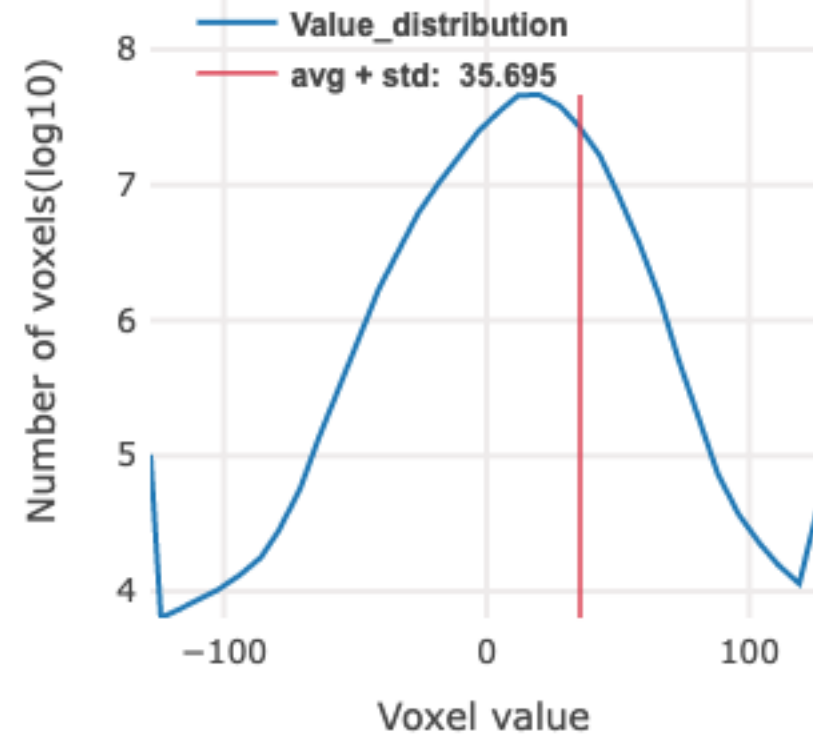
X Index: 382

Y Index: 164

Z Index: 235

Quantitative

Voxel-value distribution (Mode=20)



EMD-15449

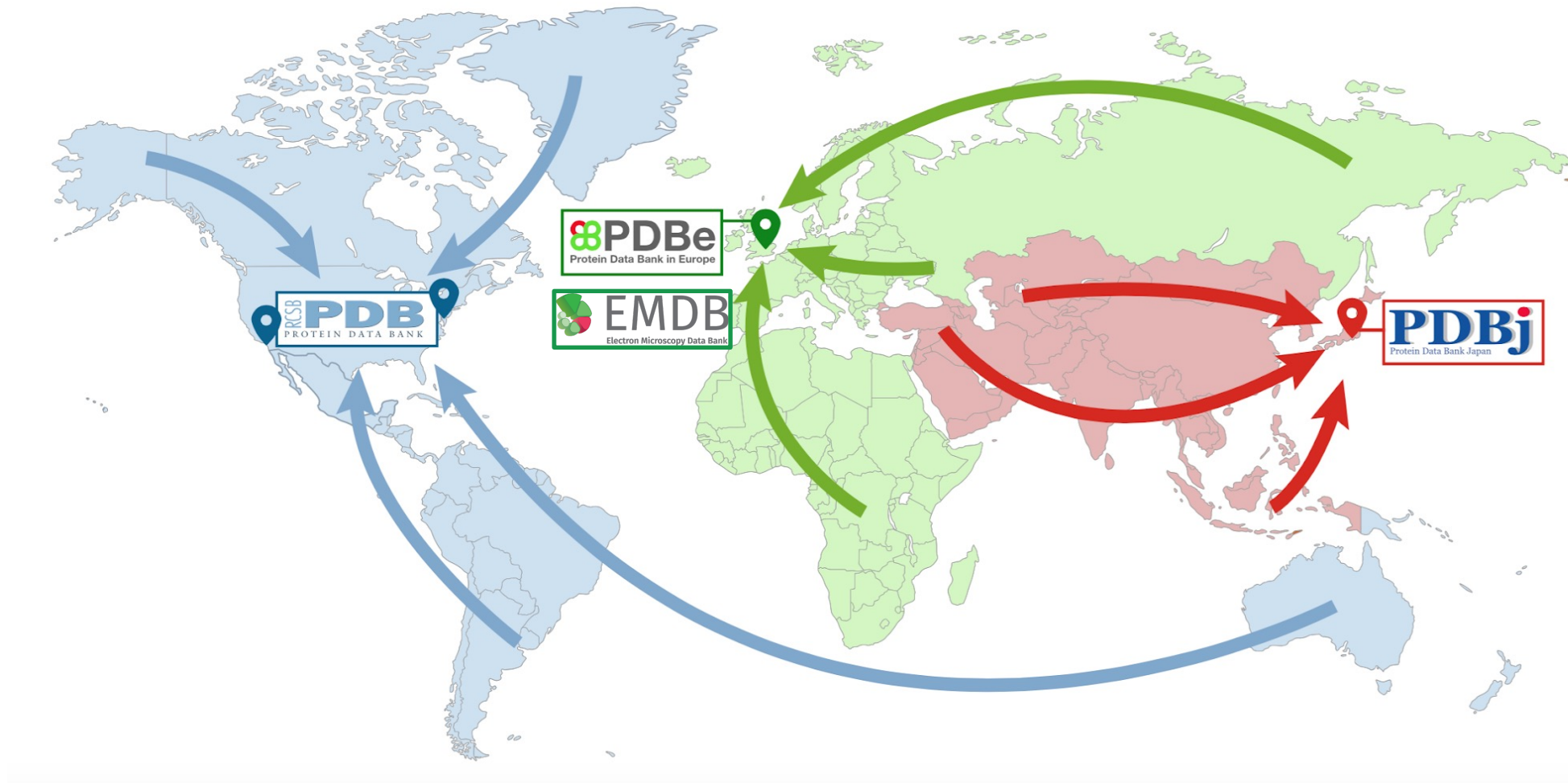
EMDB Validation – Full List

- EM Map view
 - Orthogonal projections x 7
 - Central Slices
 - Largest variance slices
 - Orthogonal surface views
 - EM map with masks
- Volume Graphs
 - Voxel-value distribution
 - Volume estimate
 - RAPs
 - FSC
- Fitted Model Analysis
 - Primary map with model
 - Atom inclusion
 - Map-model FSC
 - Q-score

Deposition

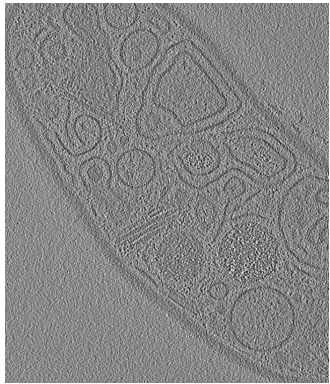


Onedep – A unified deposition system for EM, X-ray and NMR

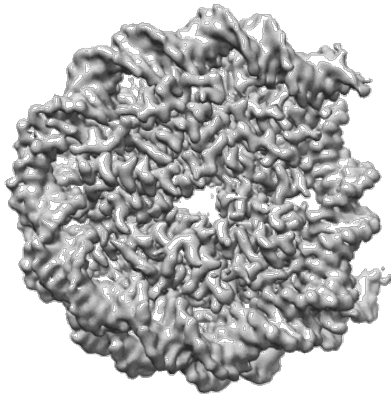


EMDB Deposition - Types

Map Only



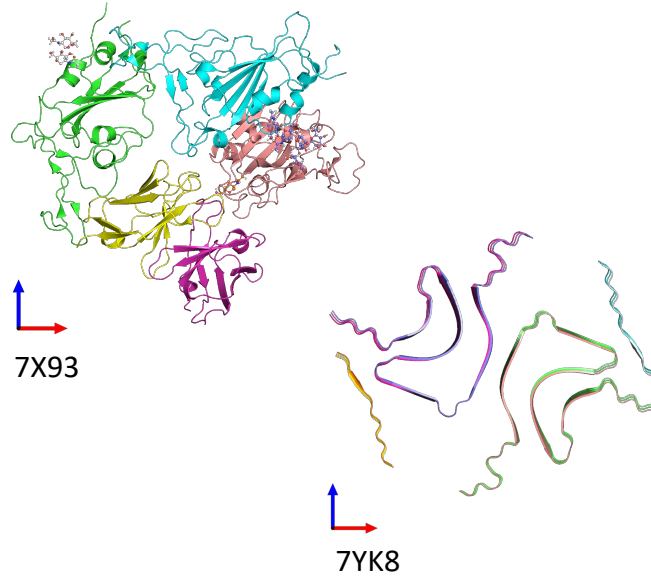
EMD-16202



EMD-29854

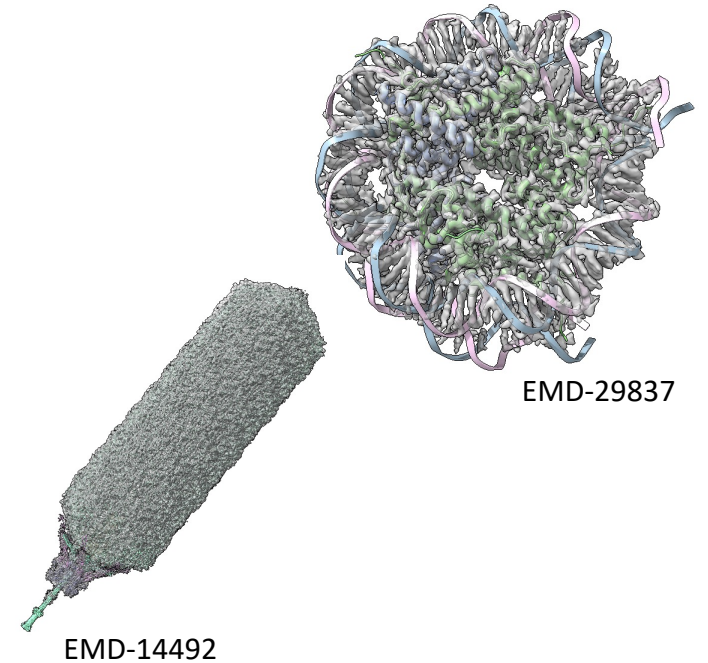
All Methodologies

Model Only



All methodologies
except Tomography

Map + Model



EMD-14492

EMD-29837

All methodologies
except Tomography

Must have associated map!

EMDB Deposition – Brain Page

wwPDB OneDep System

Existing deposition

Deposition ID
Password


Log in
Forgot Password

Sign in with ORCID

Validation server

Have you checked your data at the stand-alone validation server?
validate.wwpdb.org

wwPDB regions



Welcome to the wwPDB OneDep system!

To continue with an existing deposition, please login on the left.
Please note that un-submitted sessions will expire 3 months after last login. Un-submitted sessions and uploaded files will be removed once they expire.

To start a new deposition, please complete the form below. Upon completion, you will be emailed login information specific to your new deposition.

Question about an in-progress deposition? For fastest response, login into your session and select the "Communication" page from the left

For requests such as entry release or citation updates, please login to the deposition system and send us a message through the communications section

If you have any other feedback, please write to us at deposit-help@mail.wwpdb.org
At this time this deposition system does not work with Internet Explorer versions 8 or less.

Warning: Please note that the current system does not support having multiple sessions open at the same time. To switch between existing sessions please

On initiation of a deposition session the wwPDB OneDep system will provide the Corresponding Author with a deposition session password. Responsibility for managing the access information to each deposition is the user's.

Your e-mail address
Password (optional, or we will provide one)
This is a shared "group" password!
(6 to 16 alphanumeric characters)

Country/Region: United States

Reset

Experimental method

- X-Ray Diffraction
- Electron Microscopy
 - Helical
 - Single particle
 - Subtomogram averaging
 - Tomography
- Solution NMR
- Neutron Diffraction
- Electron Crystallography
- Solid-state NMR
- Fiber Diffraction

Are you depositing coordinates with this submission?
 No, experimental data only
 Yes

Has the associated map been deposited previously?
 No
 Yes

Is this a composite map deposition?
 No
 Yes

Requested accession codes
 PDB EMDB BMRB

Please copy this code: 14695

Privacy policy
 Tick to indicate that you have read and accepted the wwPDB policy on personal data privacy, including what data wwPDB collects, how the data is stored and shared. www.wwpdb.org/about/privacy

Start deposition

Experimental method

- X-Ray Diffraction
- Electron Microscopy
 - Helical
 - Single particle
 - Subtomogram averaging
 - Tomography
- Solution NMR
- Neutron Diffraction
- Electron Crystallography
- Solid-state NMR
- Fiber Diffraction

Are you depositing coordinates with this submission?

- No, experimental data only
- Yes

Has the associated map been deposited previously?

- No
- Yes

Is this a composite map deposition?

- No
- Yes

EMDB Deposition - ORCID Login

Existing deposition

Deposition ID




Password



Log in

Forgot Password

 Sign in with ORCID

Deposition list

Depositions available to 0000-0012-3456-789X

Deposition ID	Entry ID	Entry Title	Created	Site	Status	Last login
D_1292111636	7axh	Crystal structure of the hPXR-LBD in complex with alpha-zearalanol	17/03/2023	RCSB	PROC	17/03/2023
D_1292111623	7ax8	Crystal structure of the hPXR-LBD in apo form (P43212 SG)	09/01/2023	PDBe	AUTH	16/03/2023
D_1292100980	6qvt	CMP-Sialic acid bound structure the human ST6Gal1	14/07/2022	PDBj	HPUB	22/09/2022
D_1292100979	6qvs	Unliganded structure of the human wild type ST6Gal1...	04/03/2019	PDBe	REL	15/05/2020
D_1200009063	6fwu	Crystal structure of human wild type B4GalT1 in apo-closed dimeric form	07/03/2018	PDBe	REL	03/02/2019
D_1290050811	4adp	HCV-J6 NS5B POLYMERASE V405I MUTANT	02/01/2012	RCSB	REL	-
D_1290044331	2xi3	HCV-H77 NS5B Polymerase Complexed With GTP	25/06/2010	PDBj	REL	-
D_1290044262	2xhu	HCV-J4 NS5B Polymerase Orthorhombic Crystal Form	21/06/2010	RCSB	REL	-

EMDB Deposition – File Upload Page

Navigation

- ✓ Instructions
- ✓ Communication
- ! File upload

Log out

File upload

Electron microscopy upload information

- Mandatory submission: Map (3D volume) file , Image file(s)
- Strongly recommended: Fourier shell correlation curve (FSC) file(s)
- Optional: Additional map (3D volume) file(s), Mask (3D volume) file(s)
- The above files will be made publicly available upon release of the map

Based on a previous wwPDB deposition

Do you want to import information from a previous wwPDB deposition? Yes No

Previous deposition ID:

Previous deposition password:

What data items would you like to transfer from a previous deposition?

Contact information	<input type="checkbox"/>
Entry authors	<input type="checkbox"/>
Citation information	<input type="checkbox"/>
Grant information	<input type="checkbox"/>
Electron microscopy experimental information	<input type="checkbox"/>

General upload instructions

- Click 'Browse' or 'Choose File' to upload your file. Once the file is uploaded, select the file type from the pull-down list. If you have uploaded more than one file
- After pressing "Continue deposition", you must review the summary page carefully as it will tell you whether your data has been uploaded and interpreted correctly.
- The gzip and bzip2 compression formats are supported for all uploaded files. Archive formats such as tar and windows ZIP archives are not supported.

Map upload instructions

- Uploaded map and masks (CCP4 or MRC map formats only) will be converted to the Electron Microscopy Data Bank map format. For large maps the conversion maybe slow - we appreciate your patience.
- If you wish to upload files larger than 1.5Gb, please try first. If it fails, please contact us through the communication tab to obtain alternate upload options.
- Map must have positive densities (contrast), irrespective to the type of electron microscope images (negative stain, or frozen-hydrated). If the contrast density for the map is found to be negative, a scale factor of (-1) will be applied to map convention recommended by Heymann et al. J. Struct. Biol. 2005 (2):196-207
- Image of your map (500x500 pixel, white background preferred) must be free from copyright restrictions. This image will be displayed on the atlas pages for your entry when the map is released.
- FSC curve files (XML format) can be generated via [this server](#), or using software packages such as EMAN2, RELION or Bsoft. An example of a FSC curve file is available [here](#)

Choose File

⚠ Please provide/select one map file (Spider map format is not allowed). Please provide your half maps. Please provide/select one image of your map.

⚠ Deposition of a FSC file is strongly encouraged.

Based on a previous wwPDB deposition

Do you want to import information from a previous wwPDB deposition? Yes No

Previous deposition ID:

Previous deposition password:

What data items would you like to transfer from a previous deposition?

Contact information

Entry authors

Citation information

Grant information

Electron microscopy experimental information

EMDB Deposition – Deposition Interface

Deposition unlocked

List requirements

All items

Mandatory items

Navigation

- ✓ Instructions
- ✓ Communication
- ! Re-upload files
- ✓ Upload summary
- Admin
 - ✓ Contact information
 - ✓ Grant information
 - ✓ Release status
 - ✓ Entry title & author
 - ✓ Citation information
- Macromolecules
 - ✓ 1) T-complex protein 1 subur
 - ✓ 2) T-complex protein 1 subur
 - ✓ 3) T-complex protein 1 subur
 - ✓ 4) T-complex protein 1 subur
 - ✓ 5) T-complex protein 1 subur
 - ✓ 6) T-complex protein 1 subur
 - ✓ 7) Nanobody Nb18
 - ✓ 8) T-complex protein 1 subur
 - ✓ 9) T-complex protein 1 subur
 - ✓ 10) Actin, cytoplasmic 2
 - ✓ 11) Phosducin-like protein 3
- EM sample
 - ✓ Overall sample description
- EM experiment
 - ✓ Specimen preparation
 - ✓ Microscopy
 - ✓ Image recording
 - ✓ Reconstruction
 - ✓ Fitting interpretation
- ✓ Ligands
- ✓ Assembly
- ✓ Related entries
- ✓ Validation reports
- ✓ Summary & conditions
- Downloads & reports
 - All files
 - Generated mmCif

Log out

Re-upload files

General upload instructions

- Click 'Browse' or 'Choose File' to upload your file. Once the file is uploaded, select the file type from the pull-down list. If you have uploaded more than one file of each type, use the check box to select which file should be used.
- After pressing "Continue deposition", you must review the summary page carefully as it will tell you whether your data has been uploaded and interpreted correctly.
- The gzip and bzip2 compression formats are supported for all uploaded files. Archive formats such as tar and windows ZIP archives are not supported.

Coordinate upload instructions

- Coordinate files should be deposited in mmCIF format.
- Phenix, Refmac and Buster support direct output of mmCIF files (please see www.wwpdb.org/deposition/PDBxDeposit for instructions).
- Please use the latest version of your refinement software to ensure compatibility with the OneDep system.
- If your refinement software does not export mmCIF files we encourage you to use `pdb_extract` to prepare an mmCIF formatted file.
- See www.wwpdb.org/deposition/preparing-pdbx-mmCIF-files for more details.

Map upload instructions

- Uploaded map and masks (CCP4 or MRC map formats only) will be converted to the Electron Microscopy Data Bank map format. For large maps the conversion maybe slow - we appreciate your patience.
- If you wish to upload files larger than 1.5Gb, please try first. If it fails, please contact us through the communication tab to obtain alternate upload options.
- Map must have positive densities (contrast), irrespective to the type of electron microscope images (negative stain, or frozen-hydrated). If the contrast density for the map is found to be negative, a scale factor of (-1) will be applied to make the density positive, following the convention recommended by Heymann et al. J. Struct. Biol. 2005 (2):196-207
- Image of your map (500x500 pixel, white background preferred) must be free from copyright restrictions. This image will be displayed on the atlas pages for your entry when the map is released.
- FSC curve files (XML format) can be generated via [this server](#), or using software packages such as EMAN2, RELION or Bsoft. An example of a FSC curve file is available [here](#)

Choose File

	Converted file name	Author's file name	Upload date/time (UTC)	File size	File type
Previous upload	<input checked="" type="checkbox"/> D_8000211489_em-volume_P1.map.V2	Error retrieving original map name	2022-02-08 11:41	87.81 MB	EM map (MRC/CCP4 format) Pixel spacing (Å)*: <input type="text"/> Contour level*: <input type="text"/> Short description: <div style="border: 1px solid #ccc; height: 40px; width: 100%;"></div>
Previous upload	<input checked="" type="checkbox"/> D_8000211489_img-embd_P1.png.V1	D_1292113241_img-embd-upload_P1.jpg	1970-01-20 00:45	211.41 KB	Entry image for public display Coordinates (mmCIF format)
Previous upload	<input checked="" type="checkbox"/> D_8000211489_model_P1.cif.V12	D_1292113241_model_P1.cif.V17	1970-01-20 00:45	8.95 MB	EM half map (MRC/CCP4 format) Pixel spacing (Å)*: <input type="text"/> Contour level*: <input type="text"/> Short description: <div style="border: 1px solid #ccc; height: 40px; width: 100%;"></div>
Previous upload	<input checked="" type="checkbox"/> D_8000211489_em-half-volume_P2.map.V2	Error retrieving original map name	2022-02-08 11:42	87.81 MB	EM half map (MRC/CCP4 format) Pixel spacing (Å)*: <input type="text"/> Contour level*: <input type="text"/> Short description: <div style="border: 1px solid #ccc; height: 40px; width: 100%;"></div>

EMDB Deposition – Tips & Tricks

- **mmCIF is a metadata file!**
- The provided sequence should be the full sequence in the sample, including any unmodeled regions.
- Half-maps must be unmasked, unfiltered and unsharpened raw maps.
- Defocus values must be in nm and positive values refer to defocus.
- Maps and models should all be present in the same coordinate space and overlay correctly.
- When depositing volume EM data make use of EMPIAR

EMPIAR Deposition

EMPIAR Deposition Step-By-Step

1. Register as a new user on EMPIAR's deposition system
2. Sign-in & Create a New Deposition
3. Complete the Deposition Overview Page
4. Granting rights or transferring ownership of an entry
5. Main EMPIAR Data Upload page
 - a. Globus
 - b. Aspera Command Line
 - c. Aspera Web Interface
6. Complete the Associate image sets with the data page & Submit

EMPIAR Deposition Policies

- EMPIAR is relatively unstructured compared to EMDB
- Policies pages should be visited to understand accepted file types
- Supported Methods (more info on the policies pages):
 - i. EMDB - raw image data relating to structures deposited to the EMDB
 - ii. SBF-SEM - image data collected using serial block-face scanning electron microscopy (like the Gatan 3View system)
 - iii. SXT - image data collected using soft x-ray tomography
 - iv. FIB SEM - image data collected using focused ion beam scanning electron microscopy
 - v. IHM - integrative hybrid modelling data
 - vi. CLEM - correlative light-electron microscopy
 - vii. CLXM - correlative light X-ray microscopy
 - viii. MicroED - microcrystal electron diffraction
 - ix. ATUM-SEM - Automated Tape-collecting Ultramicrotome Scanning Electron Microscopy
 - x. Hard X-ray/X-ray microCT - Hard X-ray/X-ray micro-computed tomography
 - xi. ssET - serial section electron tomography

EMPIAR Deposition Setup

EMPIAR

EMPIAR home | **Deposition** | Annotation | REST API | FAQ | About EMPIAR | Policies | Feedback | Share

Please sign in to get started.
Proceed to the [login page](#) or [register an account](#).

License:

Quick links

- Browse EMPIAR
- Sample-Preparation Widget
- Volume Browser
- Claim entries to your ORCID
- Talks and Tutorials
- EMPIAR Quick tour
- Publications
- Re-use case study
- Statistics
- EMPIAR in the news
- Contact us
- COVID-19 Data Portal
- EMDB

EMPIAR deposition system
Begin/Continue an EMPIAR deposition

Annotate a segmentation
Create and annotate an EMDB-SFF segmentation

SPW deposition system
Begin/Continue an SPW deposition

- CHEMICAL FIXATION
- STAINING
- DEHYDRATION
- RETRIDING
- INFILTRATION
- INCUBATION
- OVEN CURING
- UV POLYMERISATION
- FREEZE SUBSTITUTION

<https://www.ebi.ac.uk/empiar/deposition/choose-action/>

EMPIAR Deposition Overview Page

EMBL-EBI Services Research Training About us

EMPIAR

EMPIAR home Deposition Annotation REST API FAQ About EMPIAR Policies Feedback Share

EMPIAR deposition system

You are logged in as EMPIAR_Depositor

- Edit profile
- Helpdesk
- Deposition manual
- Invite reviewers
- Get empiar-depositor API token
- Log out

Deposition-related tasks

- Deposition overview
- Deposition help

You have exclusive access for editing the deposition. This will expire automatically after 1707 seconds unless the "Save" or "Save & Validate" buttons are pressed.

Release Lock

Deposition ID: 627

Overview

Deposition image

Please provide an image (smaller than 10 MB, minimum 400 x 400 in png or gif format) that will be used to represent your entry on the EMPIAR web-pages.

Choose a file

Save Save & Validate Submit entry

Fill in data from deposition You do not have other depositions in the EMPIAR system

Citations

1	DOI:	10.1016/j.cell.2015.10.055	Get citation from ID ⓘ N/A
	PubMed ID:	26548953	Get citation from ID ⓘ N/A
	Citation type:	<input checked="" type="radio"/> journal <input type="radio"/> non-journal	
	Published:	<input type="radio"/> yes <input type="radio"/> no	
	Title:	Cryo electron tomography of herpes simplex virus during axonal transport and secondary envelopment in primary neurons ⓘ	
	Preprint:	<input type="radio"/> yes <input type="radio"/> no	
	Journal:	Nature Methods ⓘ N/A	
	Journal abbreviation:	Nat. Methods ⓘ N/A	
	Country:	
	Issue:	10 ⓘ N/A	
	Volume:	2 ⓘ N/A	
	First page:	635 ⓘ N/A	

Deposition manual available if you get stuck

Citation can be pulled from DOI or PubMed ID

Grey = Optional
Orange = Mandatory
(N/A is clickable for optional fields)

EMPIAR Deposition - File Upload

- Aspera
- Globus
- FTP (Not recommended)

Deposition ID: 650

Upload data

▲ Removal of the uploaded files is available only by [request](#).

▲ Aspera upload may be blocked by your system's firewall. If your upload via Aspera fails, then please make sure that your system has SSH allowed and that your UDP port 330001 is open. More information on setting up firewall for Aspera [here](#).

▲ If you have already **finished uploading** your files, please proceed [here](#) to associate the image sets with the data, where you can also **check the success of the upload** (whether the uploaded data and the data stored on your side are the same).

Options for upload:

 Globus



1. Please follow the [official guide](#) to register (this is free) and set up Globus.

2. [Open Globus transfer interface](#).

IMPORTANT: Login into it before proceeding to the next step.

3. Once logged into Globus, [access the EMBL-EBI upload endpoint](#).

4. Now you will be prompted for a username and password for the EMBL-EBI endpoint:

- Username: 
- Password: 

5. Once logged into the endpoint, [open your EMPIAR directory](#).

6. **Make sure** that the Globus Path you are in does not contain "tmp" in it, as the temporary directory is visible to others. If you see "tmp", please try following instructions above again before [contacting the EMPIAR team](#).

7. You will need to select the data source endpoint as per the official guide in step 1. Please follow it to initiate the transfer from your endpoint into your EMPIAR directory. Globus will send you an email when the transfer has been completed.

 Aspera command line

 Aspera web interface

EMPIAR Deposition - Overview

1. Gather Information

- EMPIAR accepts various types of data, including multi-frame micrographs, frame-averaged micrographs, particle stacks and tilt series, as well as auxiliary files (*e.g.* particle selection coordinates)
 - Make a note of dataset details (*e.g.* # of images (or tilt-series), raw or processed, single or multi-frame, image format and dimensions, pixel spacing and type)

2. Organise your Data!

- Each data-type must be located in a separate directory (*e.g.* one for micrographs and one for particle stacks) and please sub-divide directories possessing more than 10,000 files

3. Setup Data Transfer Programs

- Aspera (<http://asperasoft.com>) and Globus (<https://www.globus.org>) efficiently and robustly transfer large data volumes (empiar.org/faq)

4. Deposit your Data and Metadata (empiar.org/deposition)

Questions!

EMDB Website



<https://www.ebi.ac.uk/emdb/>

EMDB Chart Builder



<https://www.ebi.ac.uk/emdb/statistics/builder>

Feedback

