EMDB
Deposition and validation

What to expect

CCP-EM Icknield Model Building Course

Kyle L. Morris

EMDB team leader

Icknield Model Building Course 2024

RAL/DLS | Oxfordshire UK

EMBL-EBI

Thank you!

Organisers

&

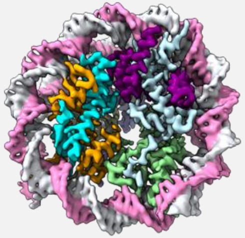
Speakers

Participants

What is it all about?

Archiving

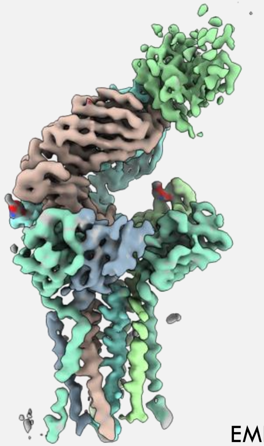
DNA histone complex



EMD-18778
Wapenaar et al

Verification

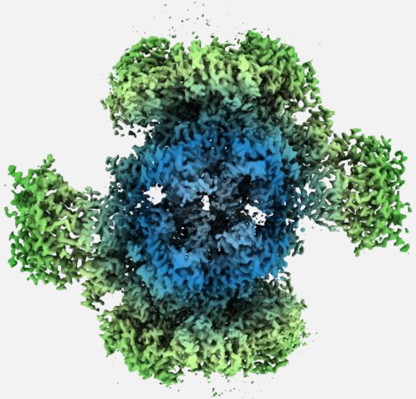
Antigen presentation



EMD-45166
Notti et al (2024) bioRxiv

Data reuse

DNA replication complex



EMD-13619
Saleh et al (2022) Nat Comm

EMDB

What is it all about?

Verification

Facilitate the scientific review process

Archiving

Every published structure must be findable

EMDB

Data reuse

Data has value beyond the primary scientific conclusions

EMDB @ EMBL-EBI

2024: EMDB Team

Lucas

Neli

Sanja

Jack

Amudha

Zhe

Miao

Outline

The EMDB

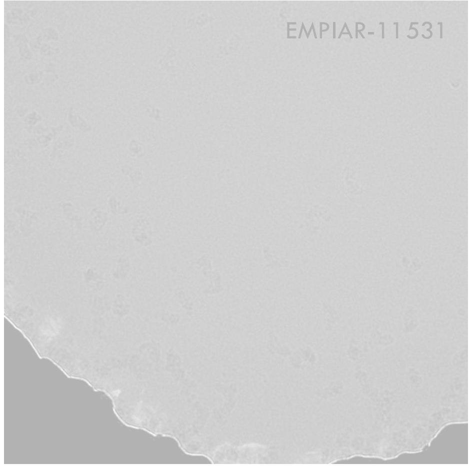
The wwPDB

Deposition

Validation

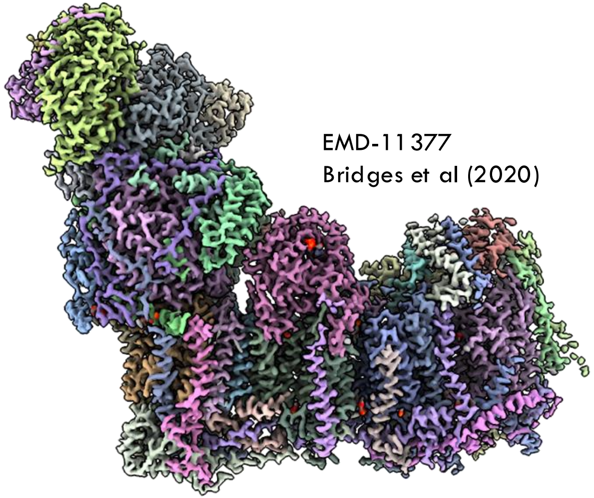
Related archives

EMPIAR


EMPIAR-11531

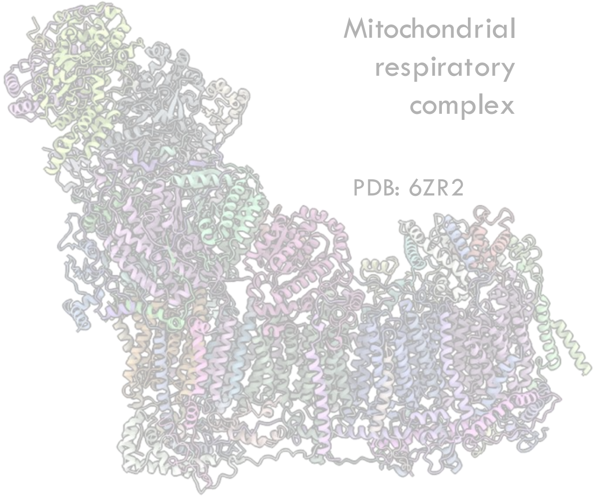
Matthew Hartley
Also, Bioimage Archive

EMDB
Electron Microscopy Data Bank


EMD-11377
Bridges et al (2020)

Kyle Morris

PDBe
Protein Data Bank in Europe


Mitochondrial respiratory complex

PDB: 6ZR2

Sameer Velankar
Also, AlphaFoldDB

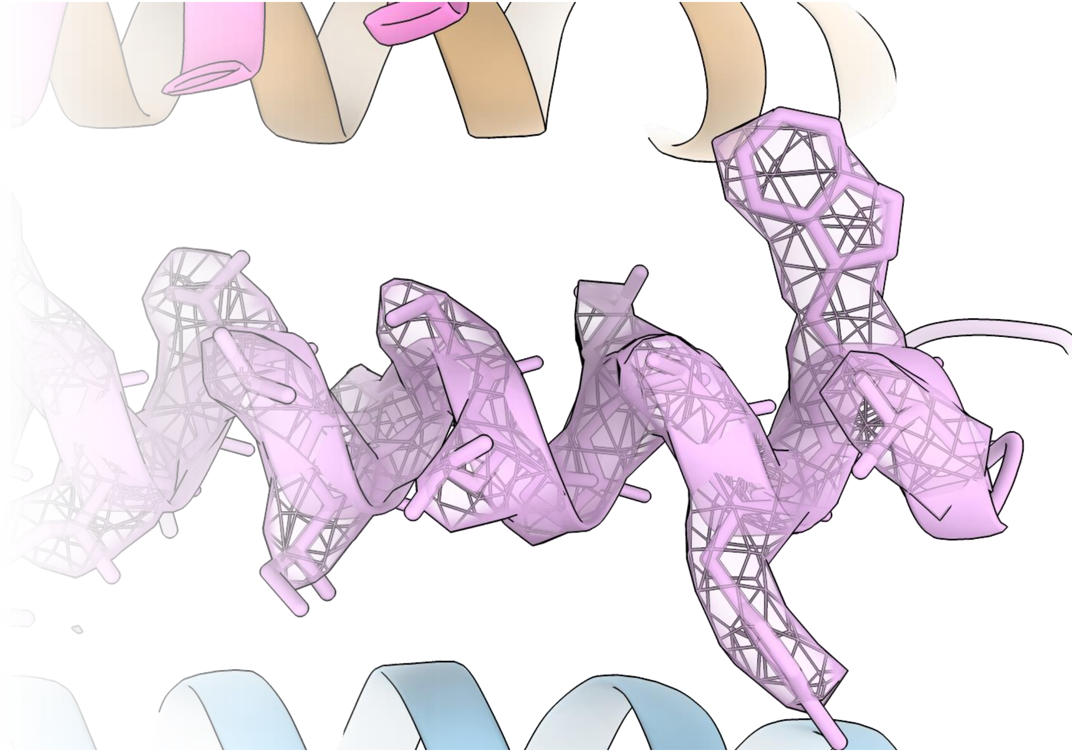
Information encoding

What is cryoEM density?

- Coulomb potential map

What is encoded in density?

- Atomic positions

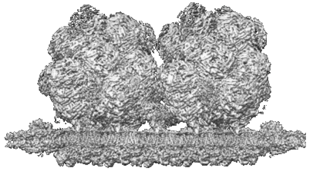


EMD-11377: Bridges et al (2020) Nature Communnications

Methodologies

Single Particle

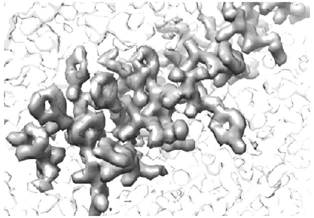
Double-PBS-PSII-PSI-LHCs megacomplex



EMD-33658 (You, 2023)

Subtomogram Averaging

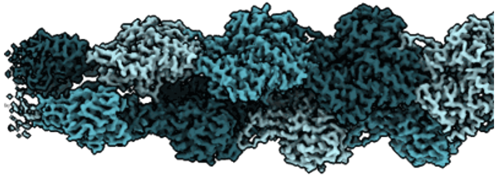
Apoferritin



EMD-16032 (Obr, unpublished)

Helical Reconstruction

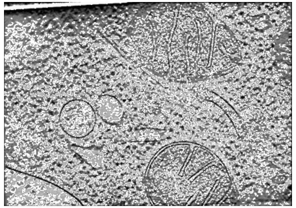
Actin 1



EMD-41583 (Hvorecny, 2024)

Tomography

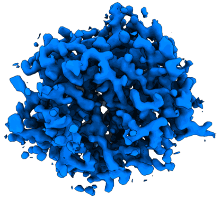
Mitochondria from cryo-FIB



EMD-43049 (Fry, 2024)

MicroED

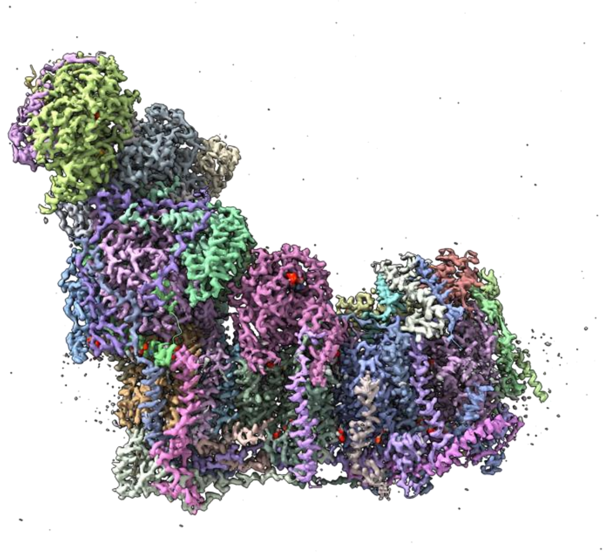
Proteinase K



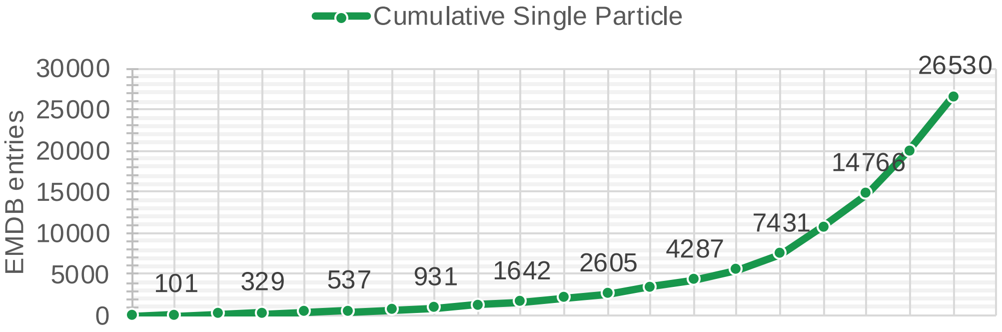
EMD-40351 (Gilman, 2023)

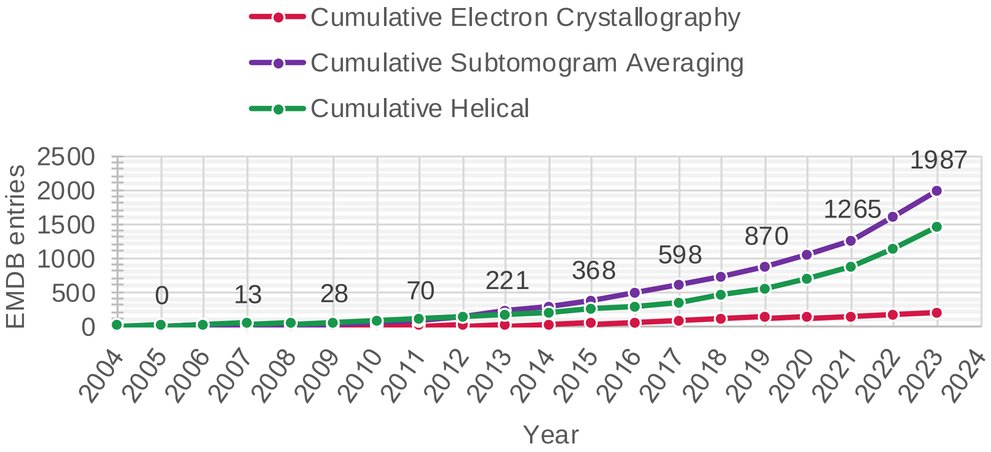
Credit: Jack Turner

EMDB holdings



EMD-11377





EMD-11377: Bridges et al (2020) Nature Communnications

Getting there…

The EMDB

The wwPDB

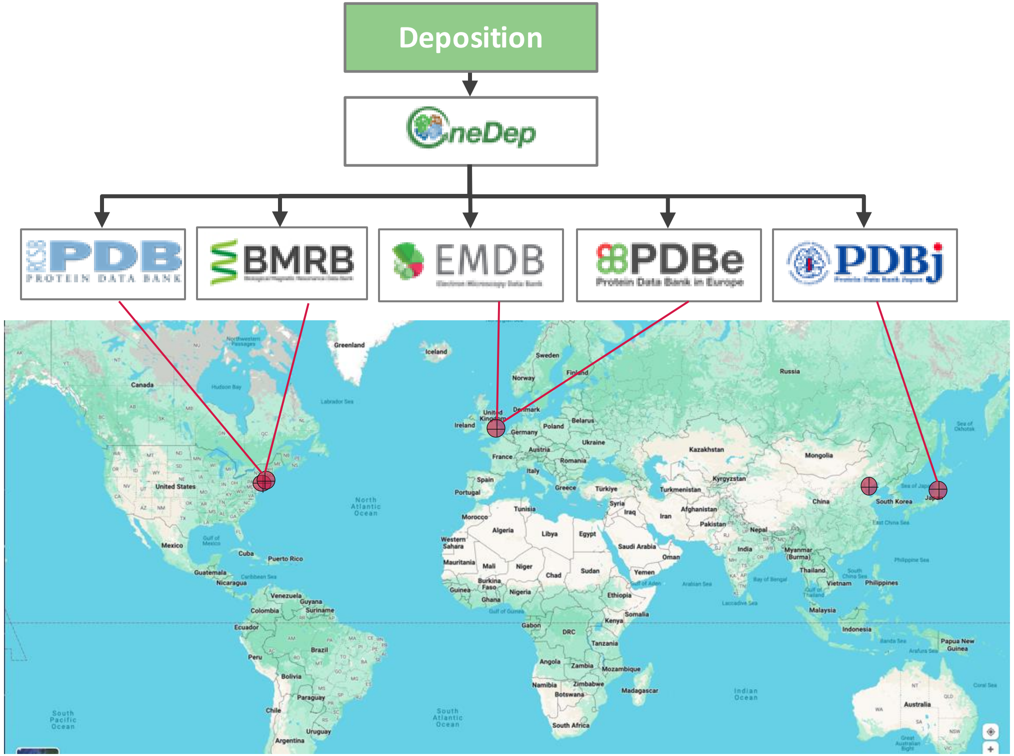
Deposition

Validation

Global partnership on archiving

Deposition

Curation



+ PDBchina

Archive becomes structured by:

OneDep deposition
&
EMDB pipeline

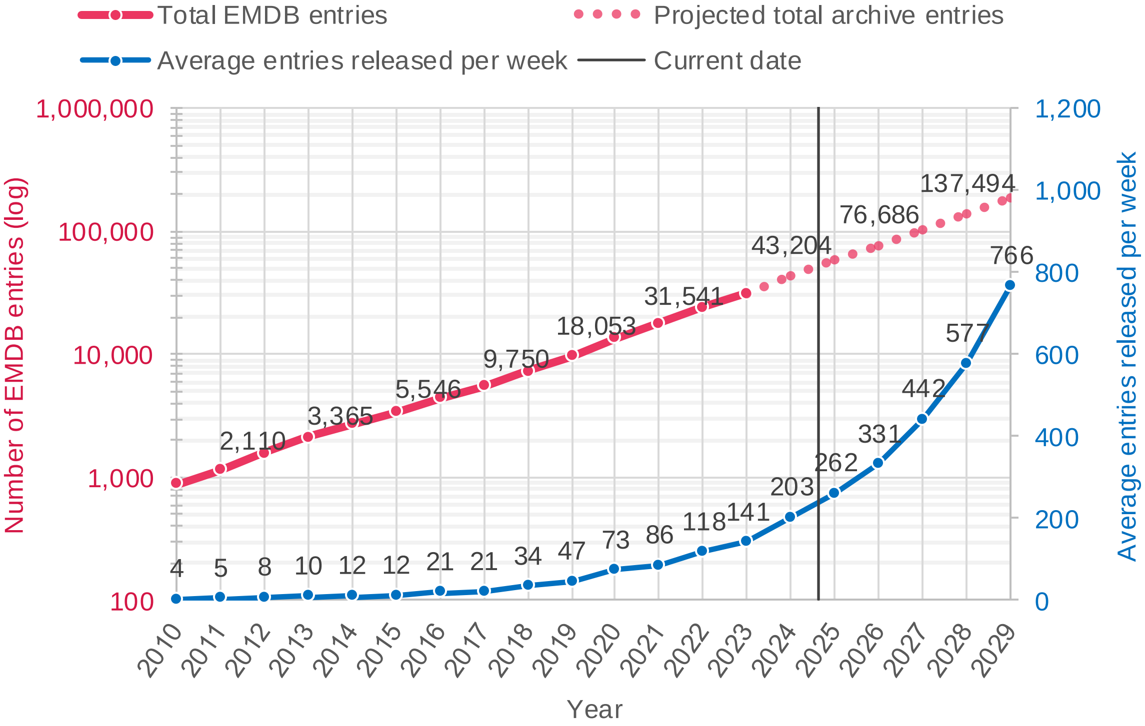
Curation procedures are:

Shared across wwPDB

Metadata model is:

Shared across wwPDB

10 year projections

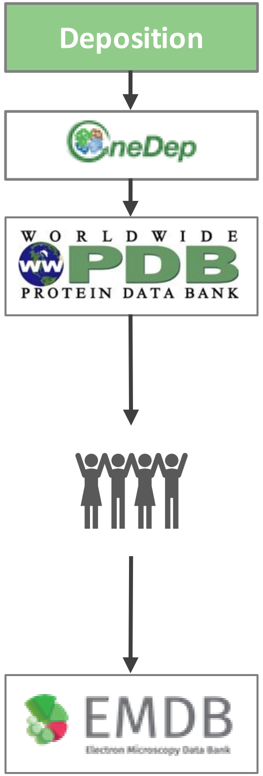


Automation and efficiency

Deposition

Curation

Archiving



Improving OneDep experience

- ORCID login (delivered)
- *Upload code redesign*
- *Deposition files*
- *Deposition API*

Improving curator efficiency

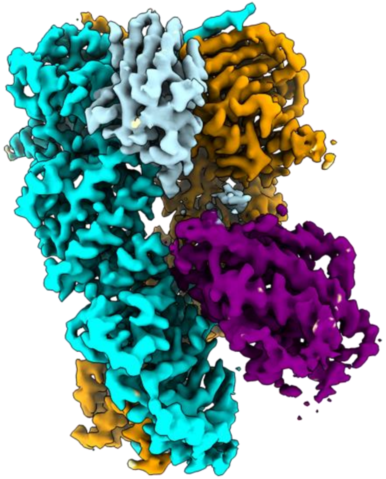
- *Automated curation checks*
- *Automated data quality advisories*

Improving archiving and release efficiency

- Upgrade global file synchronisation (delivered)
- *Archiving pipeline redesign*

At your service

Hsp90 chaperone



EMDB-23004
Noddings et al (2022) Nature

Getting there…

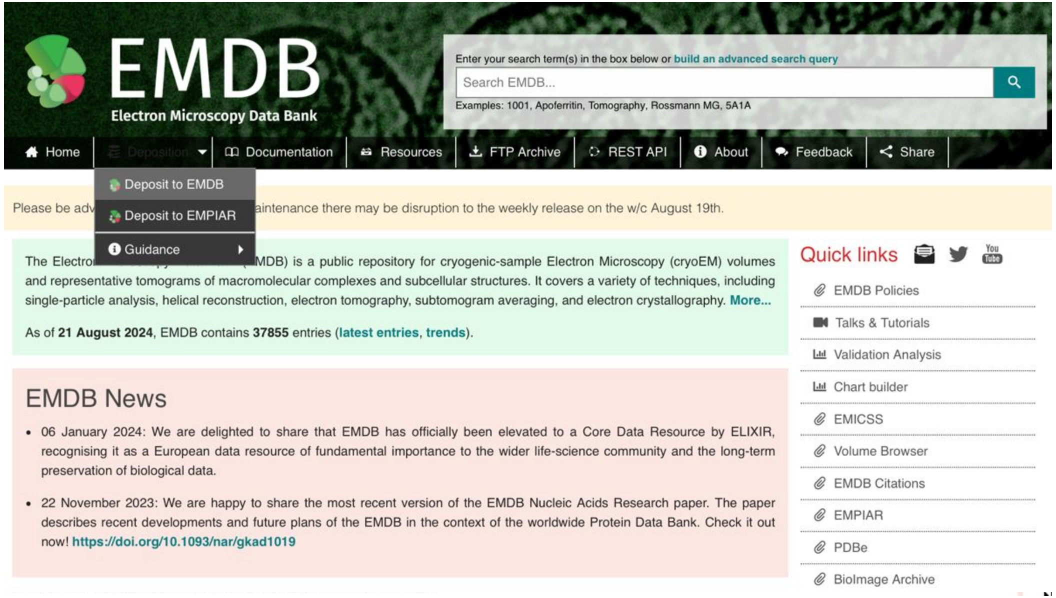
The EMDB

The wwPDB

Deposition

Validation

OneDep



EMDB
Electron Microscopy Data Bank

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

Search EMDB...

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

Please be adv aintenance there may be disruption to the weekly release on the w/c August 19th.

The Electro MDB) is a public repository for cryogenic-sample Electron Microscopy (cryoEM) volumes and representative tomograms of macromolecular complexes and subcellular structures. It covers a variety of techniques, including single-particle analysis, helical reconstruction, electron tomography, subtomogram averaging, and electron crystallography. More...

As of **21 August 2024**, EMDB contains **37855** entries (latest entries, trends).

EMDB News

- 06 January 2024: We are delighted to share that EMDB has officially been elevated to a Core Data Resource by ELIXIR, recognising it as a European data resource of fundamental importance to the wider life-science community and the long-term preservation of biological data.
- 22 November 2023: We are happy to share the most recent version of the EMDB Nucleic Acids Research paper. The paper describes recent developments and future plans of the EMDB in the context of the worldwide Protein Data Bank. Check it out now! https://doi.org/10.1093/nar/gkad1019

Advice

- Try a deposition without submitting

  Why?
- Note the info you need to record before doing the experiment / collection / processing
- Know where your experimental / collection / image processing metadata is stored

  Why?
- There is a lot of information in there
- We are working with the community on harvesting of metadata for deposition

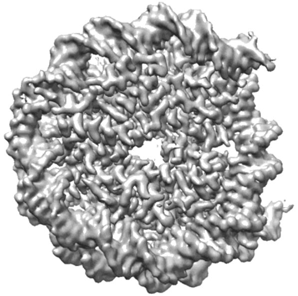
Further unsolicited advice

Save a bit of energy for the last milestone , or pack snacks

Deposition - Types

Map Only

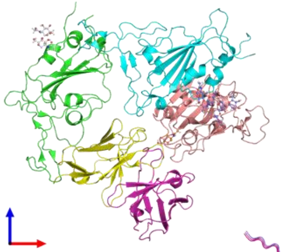
EMD-16202



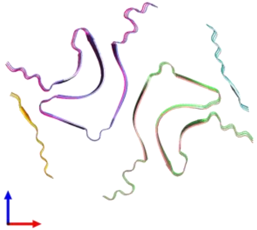
EMD-29854

All Methodologies

Model Only



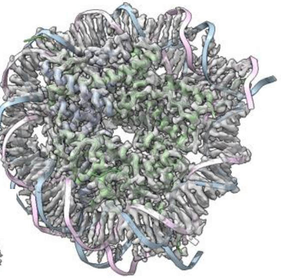
7X93



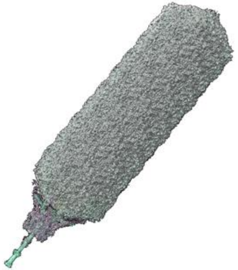
7YK8

All methodologies except Tomography

Map + Model



EMD-29837



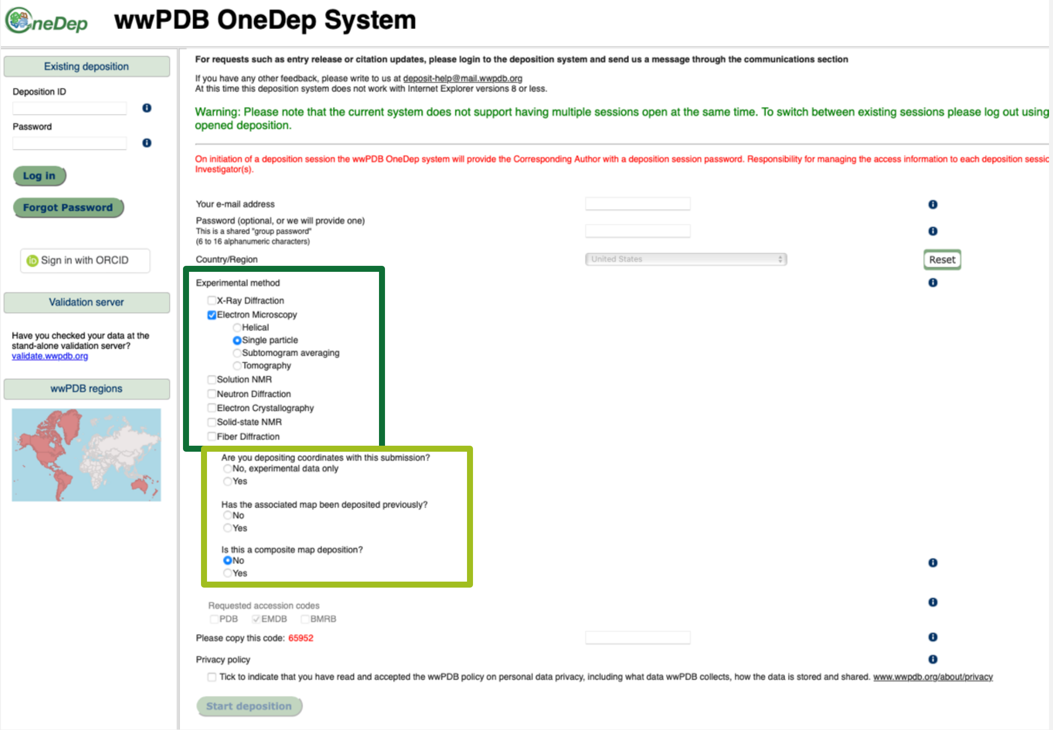
EMD-14492

All methodologies except Tomography

Must have associated map!

Credit: Jack Turner

Deposition – Brain Page



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 log out using
opened deposition.

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 sessic
Investigator(s).

Deposition ID

Password

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

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

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

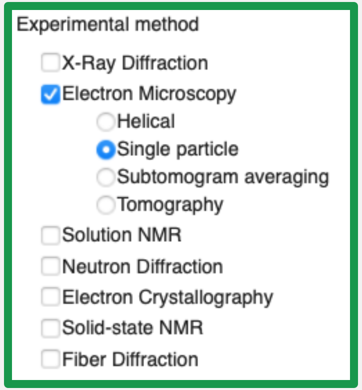
Has the associated map been deposited previously?
○ No
○ Yes

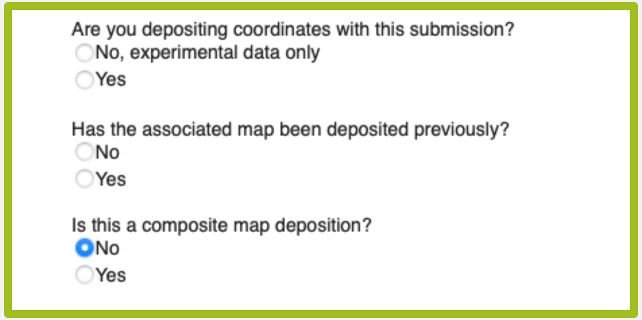
Is this a composite map deposition?
● No
○ Yes

Requested accession codes
☐ PDB ☑ EMDB ☐ BMRB

Please copy this code: 65952

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


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

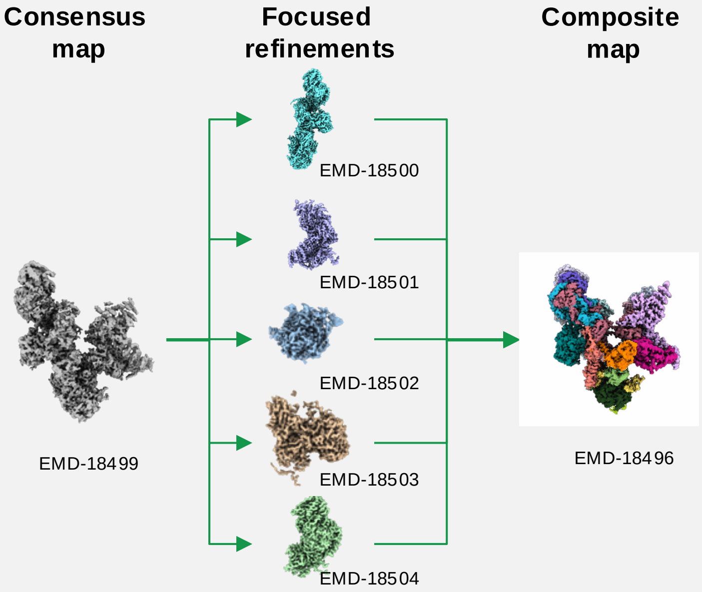
Has the associated map been deposited previously?
○ No
○ Yes

Is this a composite map deposition?
● No
○ Yes

Credit: Jack Turner

Deposition – Composite Map

Section 1.3 of EMDB Policy



Consensus map

Focused refinements

Composite map

EMD-18499

EMD-18500

EMD-18501

EMD-18502

EMD-18503

EMD-18504

EMD-18496

Please be adv aintenance there may be disruption to the weekly release on the w/c August 19th.

The Electro -sample Electron Microscopy (cryoEM) volumes

- Composite map:

Generated by combining multiple focused refinements

- Focused refinement:

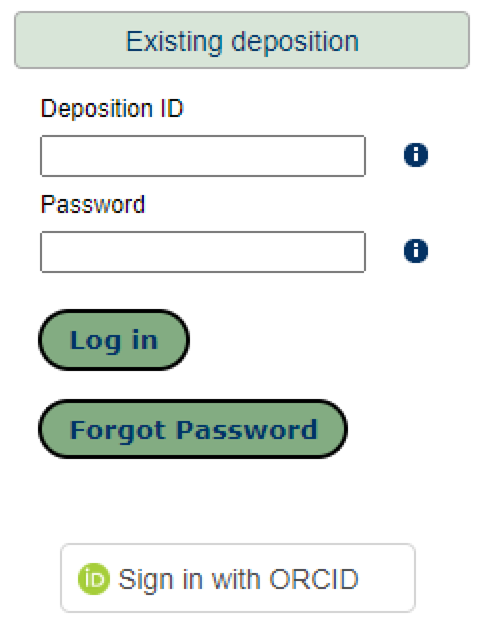
A refinement focused on an area of map

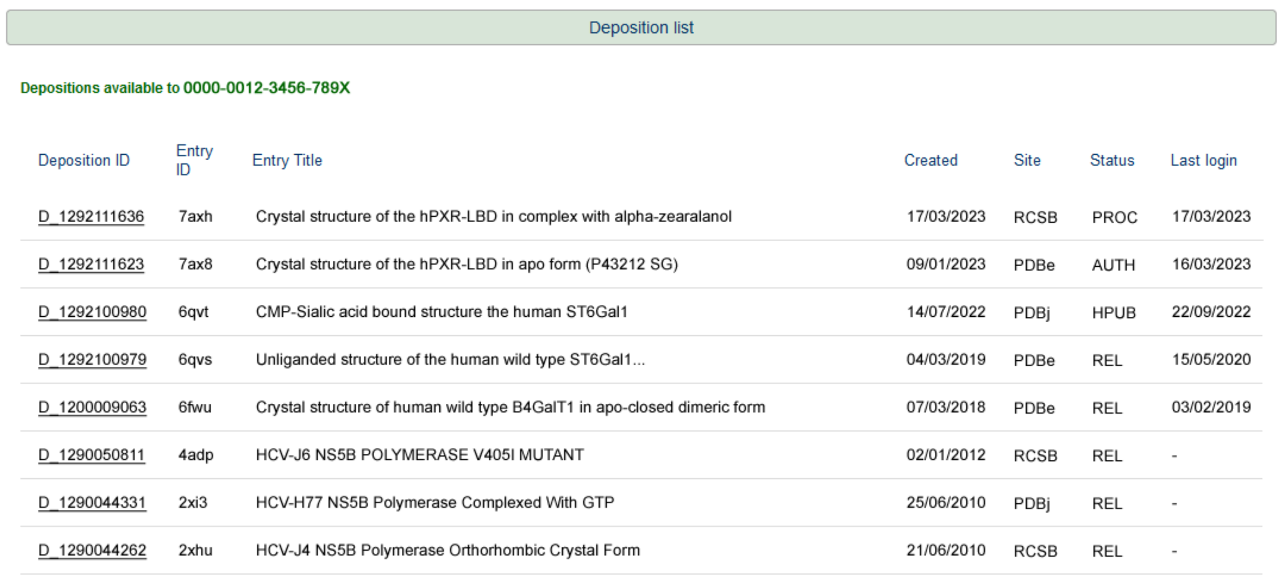
- Consensus map:

A refinement of the whole map without focusing on any region

Credit: Jack Turner

Deposition - ORCID Login



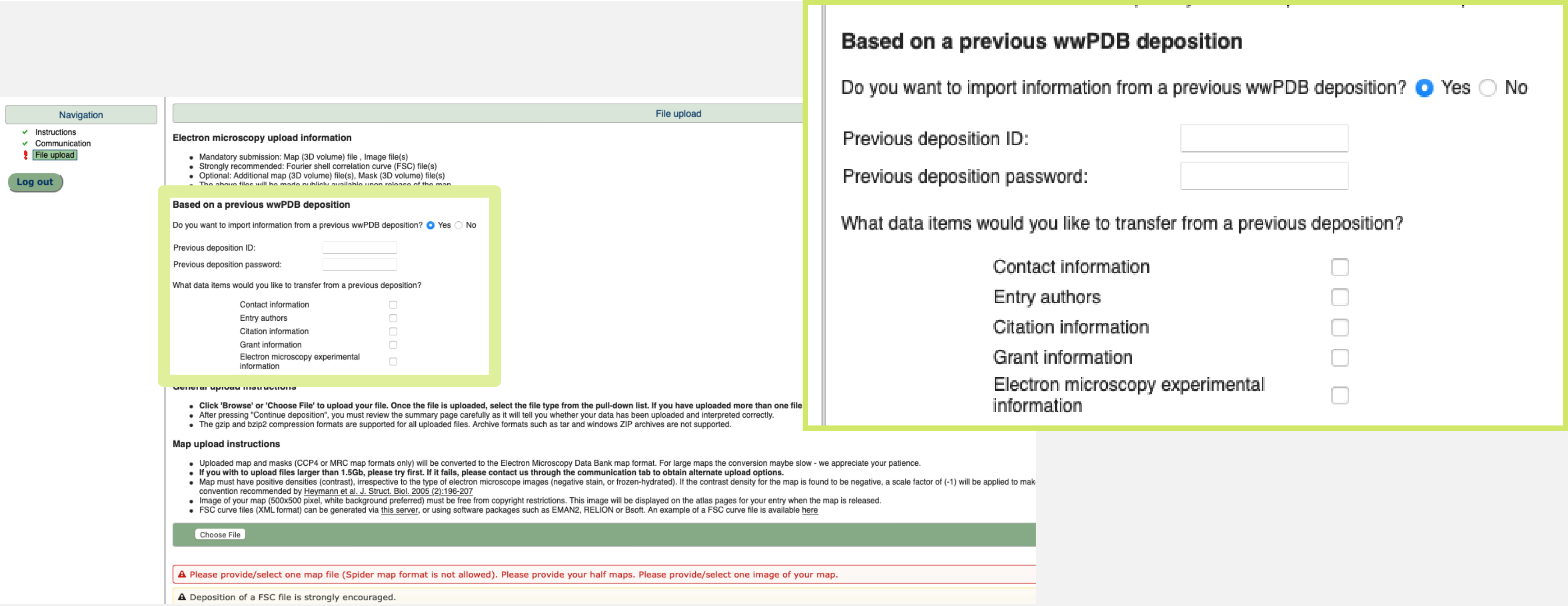


Depositions available to **0000-0012-3456-789X**

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	-

Credit: Jack Turner

Deposition – File Upload Page



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	☐
Entry authors	☐
Citation information	☐
Grant information	☐
Electron microscopy experimental information	☐

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 with 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 mak 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

⚠ 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:

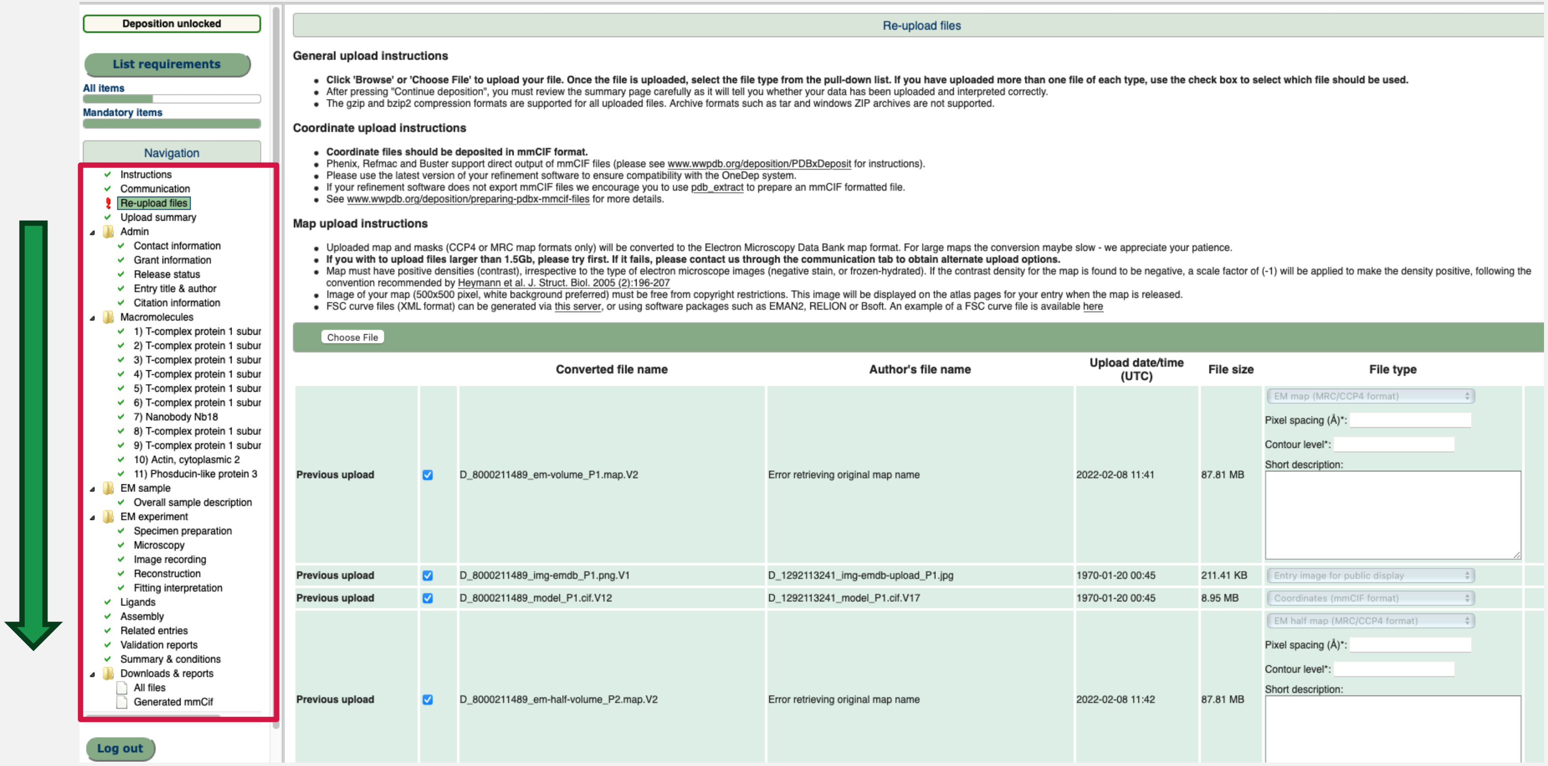
Previous deposition password:

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

Contact information ☐
Entry authors ☐
Citation information ☐
Grant information ☐
Electron microscopy experimental information ☐

Credit: Jack Turner

Deposition – Deposition Interface



- ✓ 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

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

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- **If you with 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.**
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- 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

		Converted file name	Author's file name	Upload date/time (UTC)	File size	File type
Previous upload	☑	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)*: Contour level*: Short description:
Previous upload	☑	D_8000211489_img-emdb_P1.png.V1	D_1292113241_img-emdb-upload_P1.jpg	1970-01-20 00:45	211.41 KB	Entry image for public display
Previous upload	☑	D_8000211489_model_P1.cif.V12	D_1292113241_model_P1.cif.V17	1970-01-20 00:45	8.95 MB	Coordinates (mmCIF format)
Previous upload	☑	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)*: Contour level*: Short description:

EMBL Staff Association

EMBL-EBI

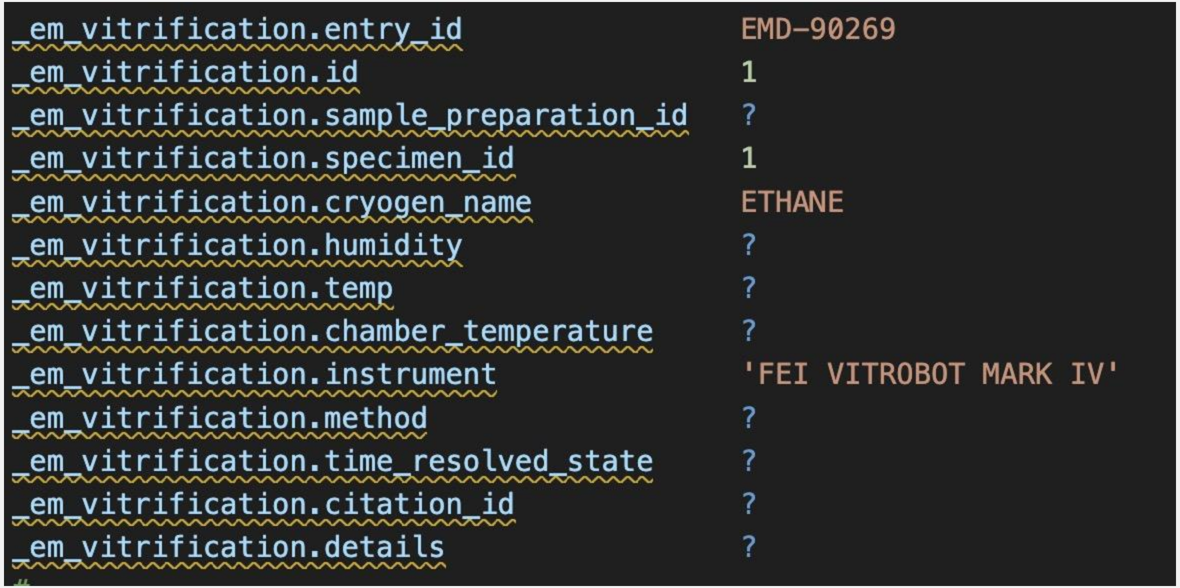
Credit: Jack Turner

Deposition - mmCIF file

```
#
_em_imaging.entry_id                        EMD-90269
_em_imaging.id                              1
_em_imaging.astigmatism                     ?
_em_imaging.electron_beam_tilt_params       ?
_em_imaging.residual_tilt                   ?
_em_imaging.sample_support_id               1
_em_imaging.detector_id                     1
_em_imaging.scans_id                        1
_em_imaging.microscope_id                   ?
_em_imaging.microscope_model                'FEI TITAN KRIOS'
_em_imaging.specimen_holder_type            ?
_em_imaging.specimen_holder_model           'FEI TITAN KRIOS AUTOGRID HOLDER'
_em_imaging.details                         ?
_em_imaging.date                            ?
_em_imaging.accelerating_voltage            300
_em_imaging.illumination_mode               'FLOOD BEAM'
_em_imaging.mode                            'BRIGHT FIELD'
_em_imaging.nominal_cs                      2.7
_em_imaging.nominal_defocus_min             2000
_em_imaging.nominal_defocus_max             4000
_em_imaging.calibrated_defocus_min          ?
_em_imaging.calibrated_defocus_max          ?
_em_imaging.tilt_angle_min                  ?
_em_imaging.tilt_angle_max                  ?
_em_imaging.nominal_magnification           ?
_em_imaging.calibrated_magnification        ?
_em_imaging.electron_source                 'FIELD EMISSION GUN'
_em_imaging.citation_id                     ?
_em_imaging.temperature                     ?
_em_imaging.detector_distance               ?
_em_imaging.recording_temperature_minimum   ?
_em_imaging.recording_temperature_maximum   ?
_em_imaging.alignment_procedure             'COMA FREE'
_em_imaging.c2_aperture_diameter            50
_em_imaging.specimen_id                     1
_em_imaging.cryogen                         NITROGEN
#
```

When you're finished this is where all the data you entered ends up.

mmCIF is a metadata file format and holds atomic coordinates.



```
_em_vitrification.entry_id               EMD-90269
_em_vitrification.id                     1
_em_vitrification.sample_preparation_id  ?
_em_vitrification.specimen_id            1
_em_vitrification.cryogen_name           ETHANE
_em_vitrification.humidity               ?
_em_vitrification.temp                   ?
_em_vitrification.chamber_temperature    ?
_em_vitrification.instrument             'FEI VITROBOT MARK IV'
_em_vitrification.method                 ?
_em_vitrification.time_resolved_state    ?
_em_vitrification.citation_id            ?
_em_vitrification.details                ?
```

https://mmcif.wwpdb.org/

Credit: Jack Turner

Deposition – Common advisories

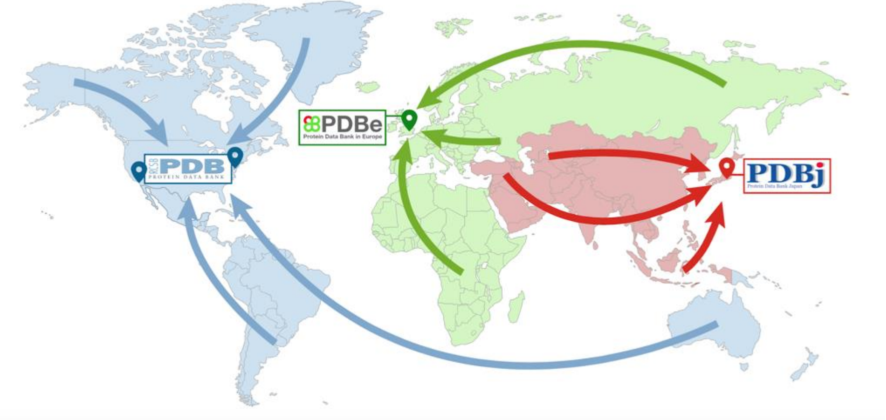
- Sequence: full sequence, including unmodeled.
- Primary map: represent the map you modelled into.
- Additional maps: maps that supported your modelling.
- Half-maps: unmasked, unfiltered and unsharpened.
- Maps/models: same coordinate space and overlay.
- Defocus: nanometres, provided as positive values.

- Please reach out if you wish to deposit variability analysis data (cryoDRGN, 3Dflex, etc)

- What about density modified maps? AI/ML or otherwise
  - Personally, I view these maps as assisting modelling i.e. additional maps
  - Validation should be run against the unmodified primary map
  - So, although density modified maps can help modelling the primary map should still support and validate against the model

EMDB Deposition Summary

- Five methodologies
  - Single Particle
  - Subtomogram Averaging
  - Helical Reconstruction
  - Tomography
  - Electron Crystallography
- Composite map depositions must follow section 1.3 of EMDB Policy
- ORCID Login
- mmCIF files are metadata files



EMBL-EBI

Credit: Jack Turner

Nearly there…

The EMDB

The wwPDB

Deposition

Validation

Map

- Validate resolution: FSC, visual inspection
- Is there anisotropy: 3DFSC, FSO, visual inspection
- Assess resolution range: Local resolution

- Look at the map, is it consistent with the resolution and being isotropic?

Model

- Validate global model fit: map-model FSC, CCC
- Validate map-model fit per residue: Many tools available
- Validate model stereochemistry: Molprobity etc

Any structure that is published in the literature must be archived

The wwPDB does not enforce depositor data quality standards
This is for the scientific review process

Make information to the scientific community so it can self-regulate data quality

Community

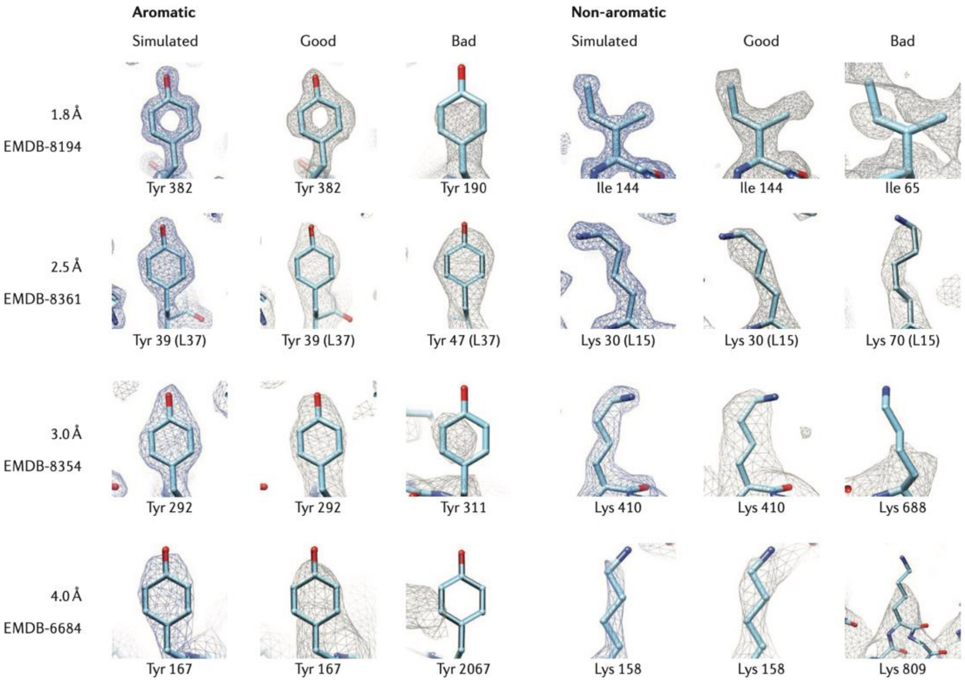
Scientist

Reviewer

Scientist

- You want your data to support your scientific conclusions
- You want your data to stand the test of time

- Look at your map
  - Do the features you see support the resolution that your refinement claims?
- Look at your model in your map
  - Is there sufficient information in your map to support what you are modelling?



Renaud et al (2018) Nature reviews drug discovery

Employer:

Look at every residue in your structure.

Scientist:

But my structure has 7,536 residues.

Employer:

“This is the way.”

Scientist:

But I solved 42 of these structures

Employer:

….

Provide a service to scientific review

Reviewer

Pre-publication

wwPDB validation reports
map
model

Validation reports: map assessment

wwPDB EM Validation Summary Report ⓘ

Aug 15, 2024 – 10:17 AM EDT

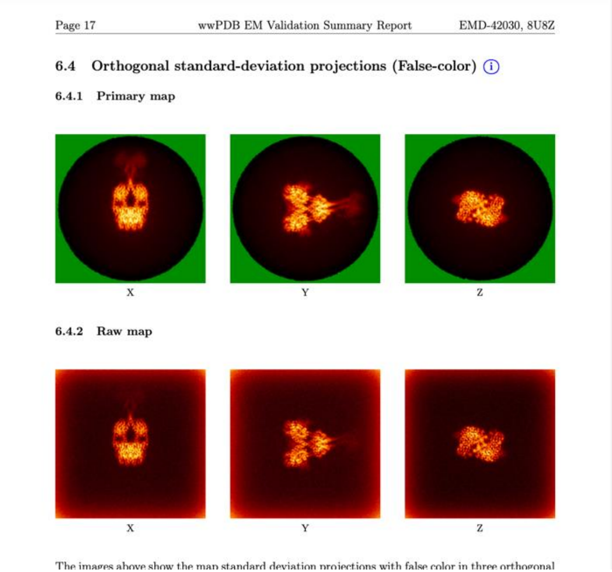
PDB ID : 8U8Z
EMDB ID : EMD-42030
Title : Cryo-EM structure of PsBphP in Pr state, extended DHp
Authors : Basore, K.; Burgie, E.S.; Vierstra, D.
Deposited on : 2023-09-18
Resolution : 3.25 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

Qualitative map assessment



Page 17 wwPDB EM Validation Summary Report EMD-42030, 8U8Z

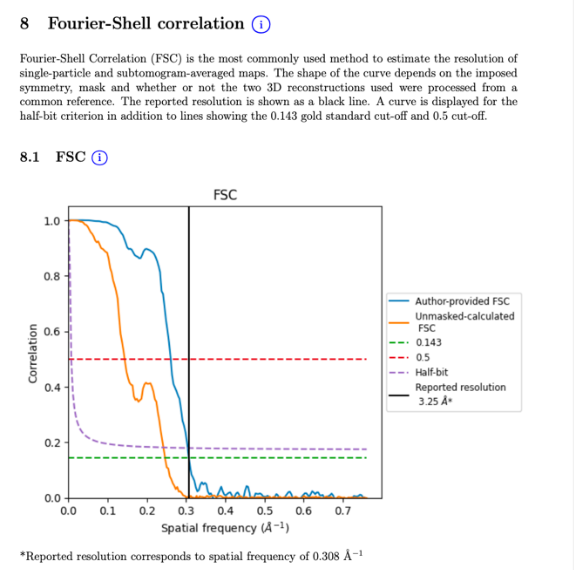
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map

6.4.2 Raw map

The images above show the map standard deviation projections with false color in three orthogonal

Quantitative map assessment



8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ

*Reported resolution corresponds to spatial frequency of 0.308 $Å^{-1}$

Look at these reports, they are likely to be the first thing a reviewer sees!

Validation reports: map assessment

WORLDWIDE PDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Aug 15, 2024 – 10:17 AM EDT

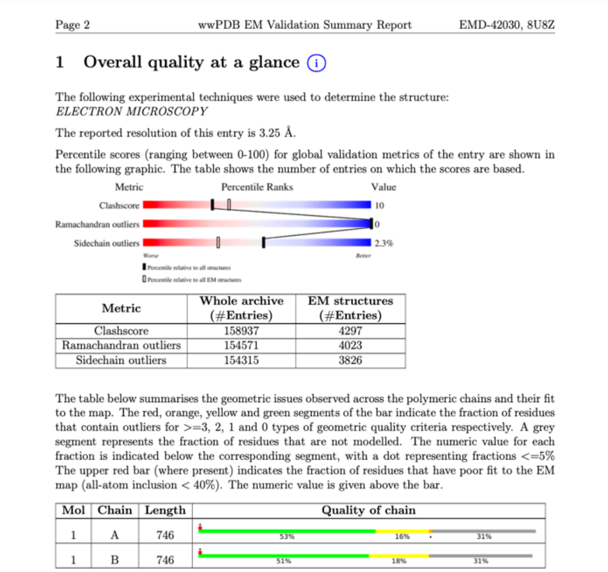
PDB ID : 8U8Z
EMDB ID : EMD-42030
Title : Cryo-EM structure of PsBphP in Pr state, extended DHp
Authors : Basore, K.; Burgie, E.S.; Vierstra, D.
Deposited on : 2023-09-18
Resolution : 3.25 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

Quantitative model assessment



Page 2 wwPDB EM Validation Summary Report EMD-42030, 8U8Z

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 Å.

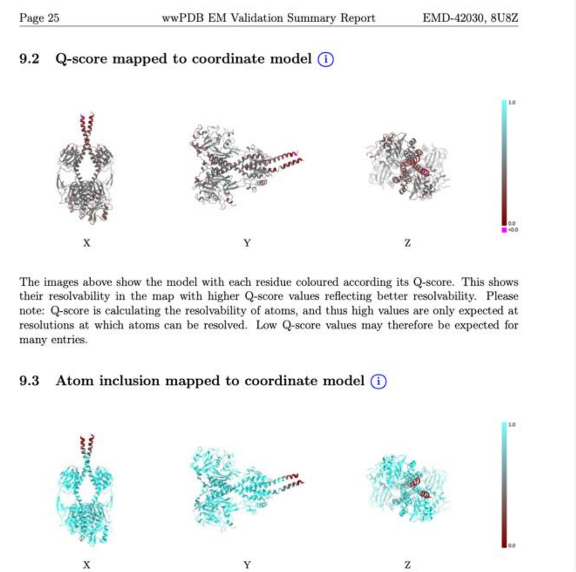
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

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 <=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	746	53% 16% • 31%
1	B	746	51% 18% 31%

Quantitative map-model assessment



Page 25 wwPDB EM Validation Summary Report EMD-42030, 8U8Z

9.2 Q-score mapped to coordinate model ⓘ

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model ⓘ

Look at these reports, they are likely to be the first thing a reviewer sees!

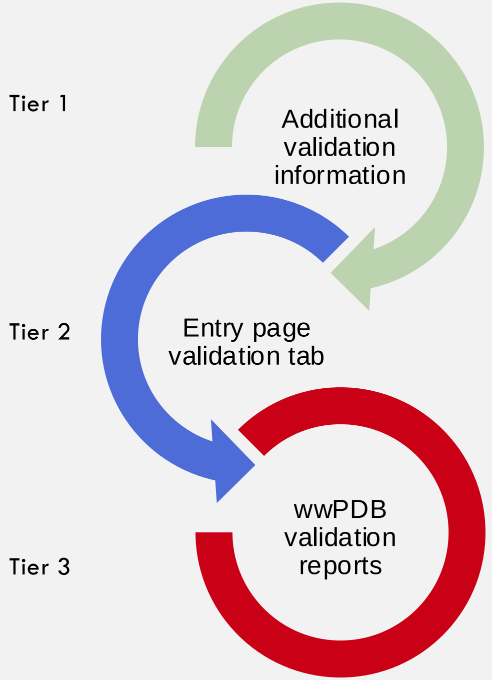
Provide a service to scientific review

Community

Post-publication

Website entry pages with validation

Provide a service to scientific review



Tier 1

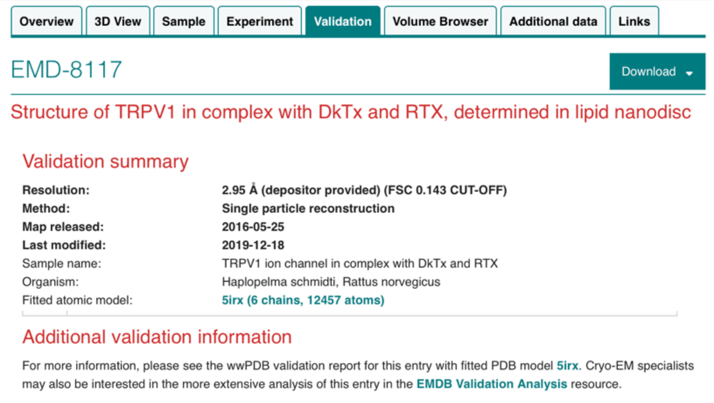
Additional validation information

Tier 2

Entry page validation tab

Tier 3

wwPDB validation reports



EMD-8117

Structure of TRPV1 in complex with DkTx and RTX, determined in lipid nanodisc

Validation summary

Resolution:	**2.95 Å (depositor provided) (FSC 0.143 CUT-OFF)**
Method:	**Single particle reconstruction**
Map released:	**2016-05-25**
Last modified:	**2019-12-18**
Sample name:	TRPV1 ion channel in complex with DkTx and RTX
Organism:	Haplopelma schmidti, Rattus norvegicus
Fitted atomic model:	**5irx (6 chains, 12457 atoms)**

Additional validation information

For more information, please see the wwPDB validation report for this entry with fitted PDB model **5irx**. Cryo-EM specialists may also be interested in the more extensive analysis of this entry in the **EMDB Validation Analysis** resource.

wwPDB EM Validation Summary Report

Validation: maps

EMD-11145

Single-particle
2.85 Å

Deposition: 07/06/2020
Map released: 30/09/2020
Last modified: 15/03/2023

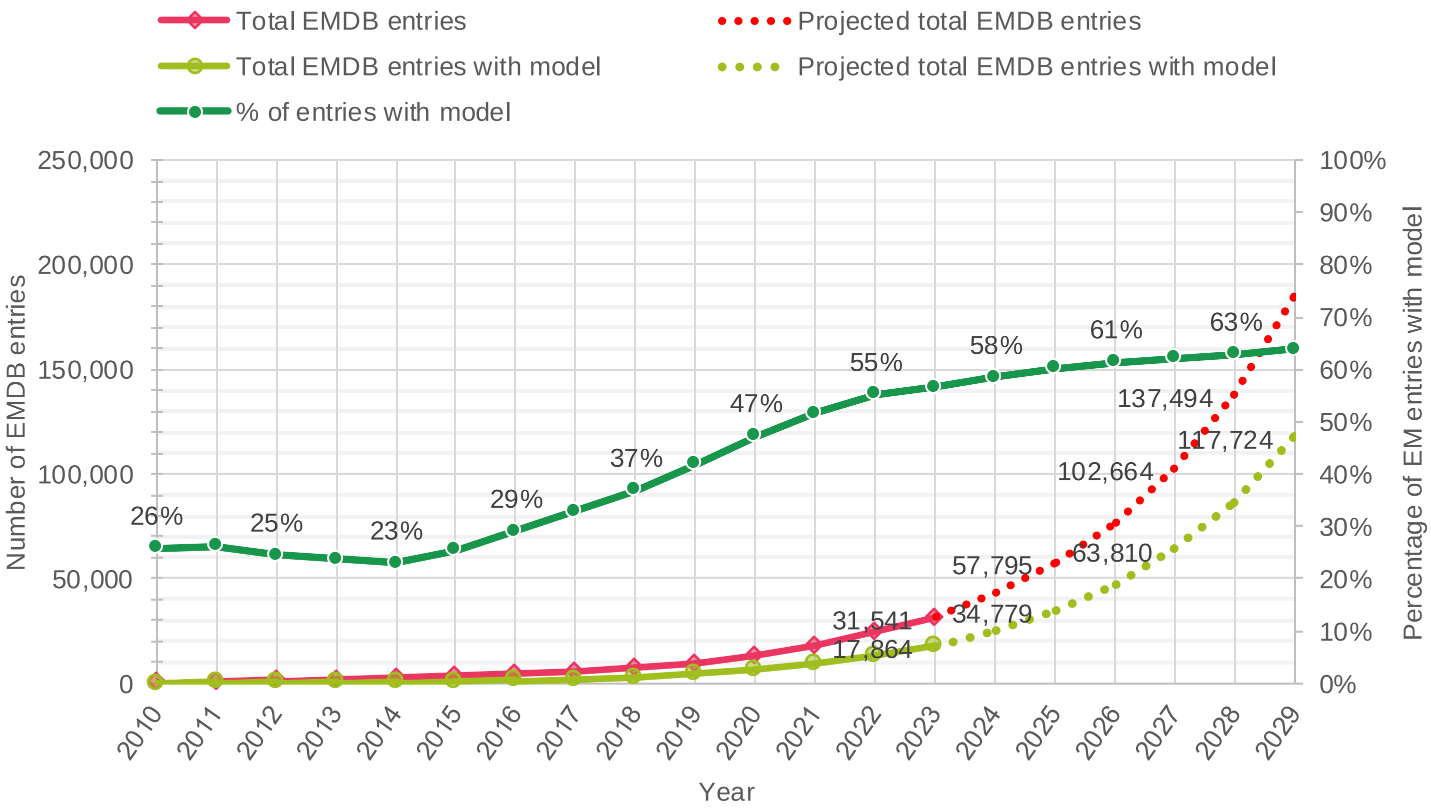
Calculated FSC measurements use a mask determined by EMDB using Relion

	Calculated resolution(Å)	Provided resolution(Å)
FSC 0.143	3.05	2.84
FSC 0.5	3.50	3.11
FSC half-bit	3.10	2.87
Local min	2.82	-
Local max	20.85	-

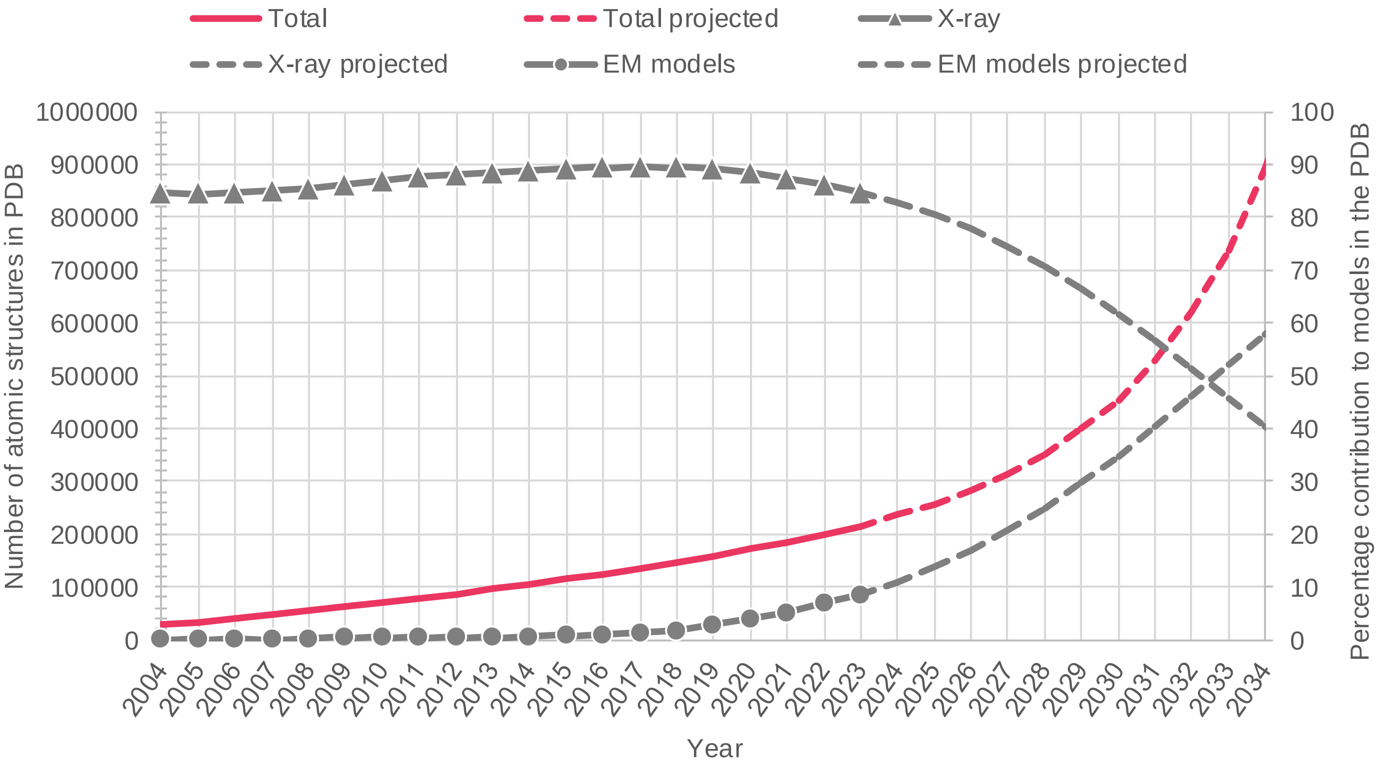
Author provided FSCs

Implementing better EMDB provided masked FSC for comparison

Model depositions

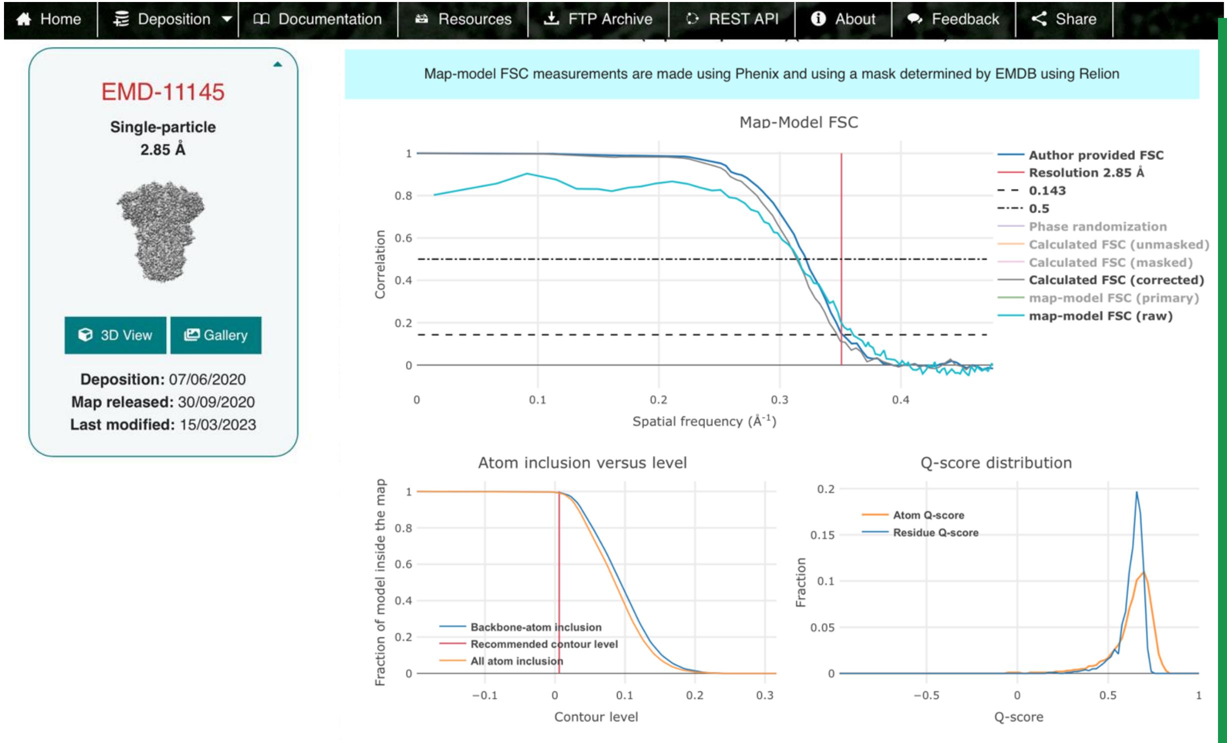


Model depositions



Kyle Morris

Model-map FSC



EMD-11145

Single-particle
2.85 Å

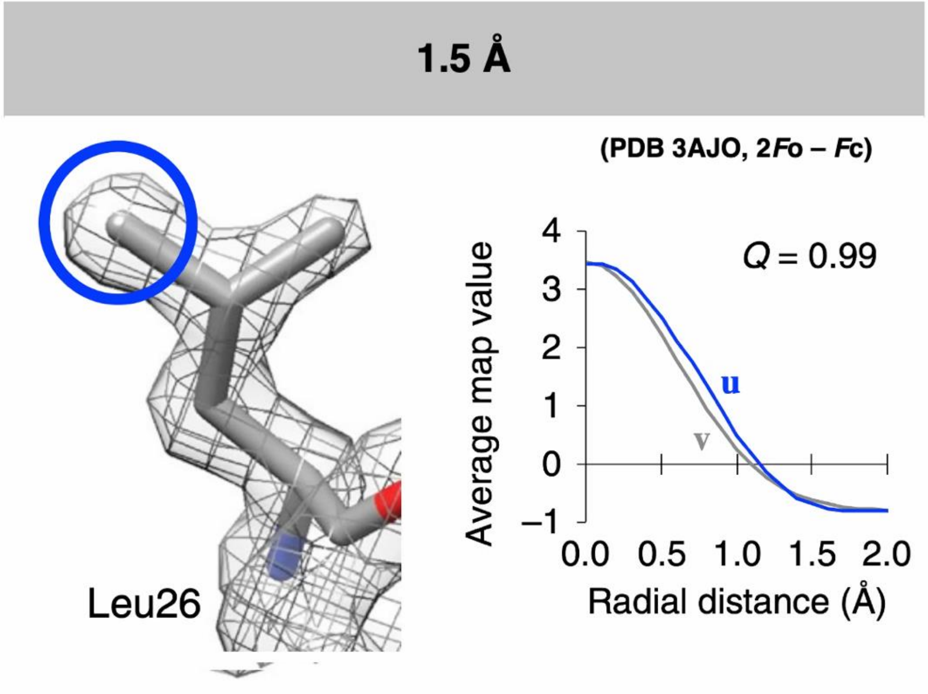
Deposition: 07/06/2020
Map released: 30/09/2020
Last modified: 15/03/2023

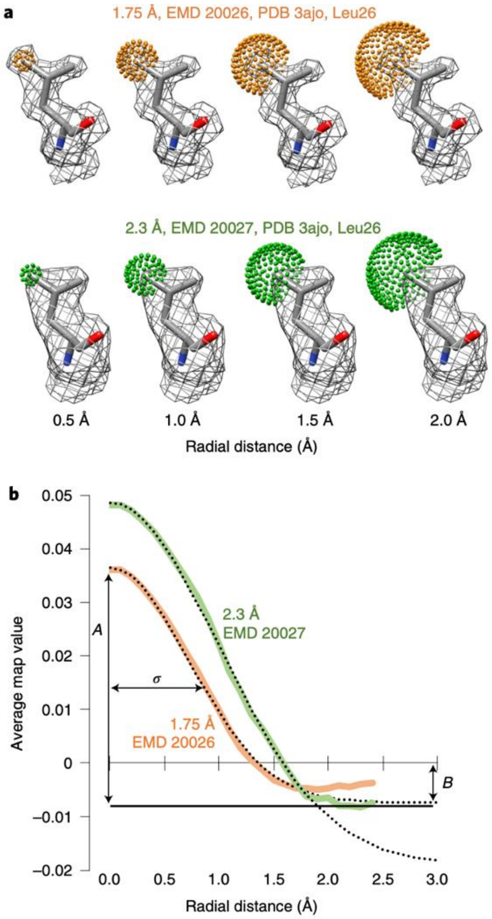
Map-model FSC measurements are made using Phenix and using a mask determined by EMDB using Relion

Implementing model-map FSC

EMBL-EBI

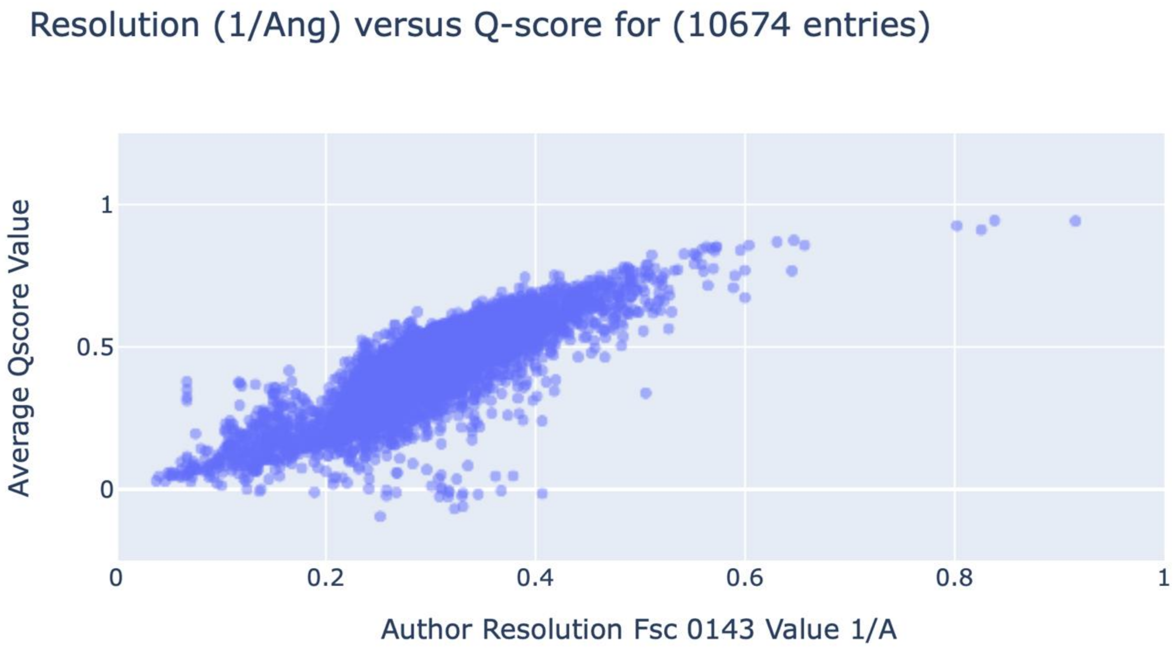
Q-score





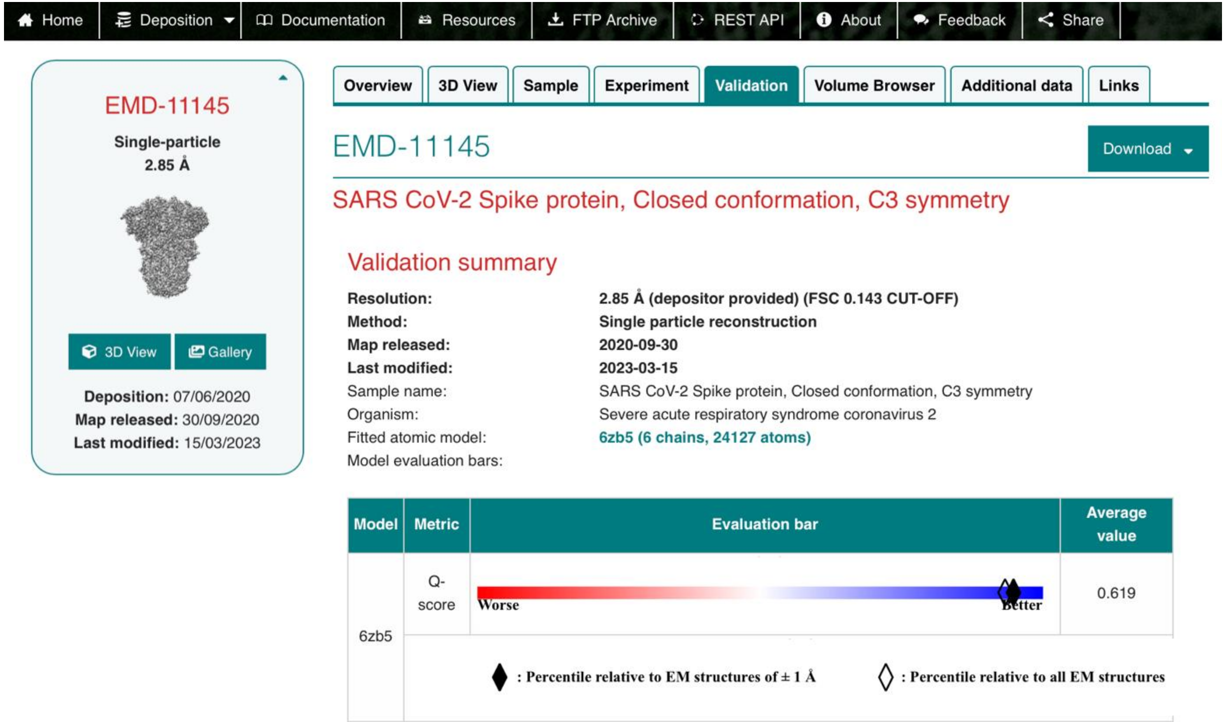
Pintilie et al (2020) Nature Methods

Validation: models



Read about the Q-score method here: Pintilie, G., et al. (2020). Nature Methods.

Validation: models



EMD-11145

Single-particle
2.85 Å

Deposition: 07/06/2020
Map released: 30/09/2020
Last modified: 15/03/2023

EMD-11145

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

Validation summary

Resolution:	**2.85 Å (depositor provided) (FSC 0.143 CUT-OFF)**
Method:	**Single particle reconstruction**
Map released:	**2020-09-30**
Last modified:	**2023-03-15**
Sample name:	SARS CoV-2 Spike protein, Closed conformation, C3 symmetry
Organism:	Severe acute respiratory syndrome coronavirus 2
Fitted atomic model:	**6zb5 (6 chains, 24127 atoms)**
Model evaluation bars:	

Model	Metric	Evaluation bar	Average value
6zb5	Q-score	Worse … Better	0.619

◆ : Percentile relative to EM structures of ± 1 Å   ◇ : Percentile relative to all EM structures

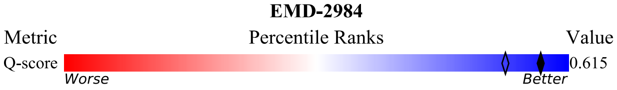
In production on website

- New evaluation bar (live)
- Based on entry average of per-residue map-model q-scores

Validation: models

Deposited files

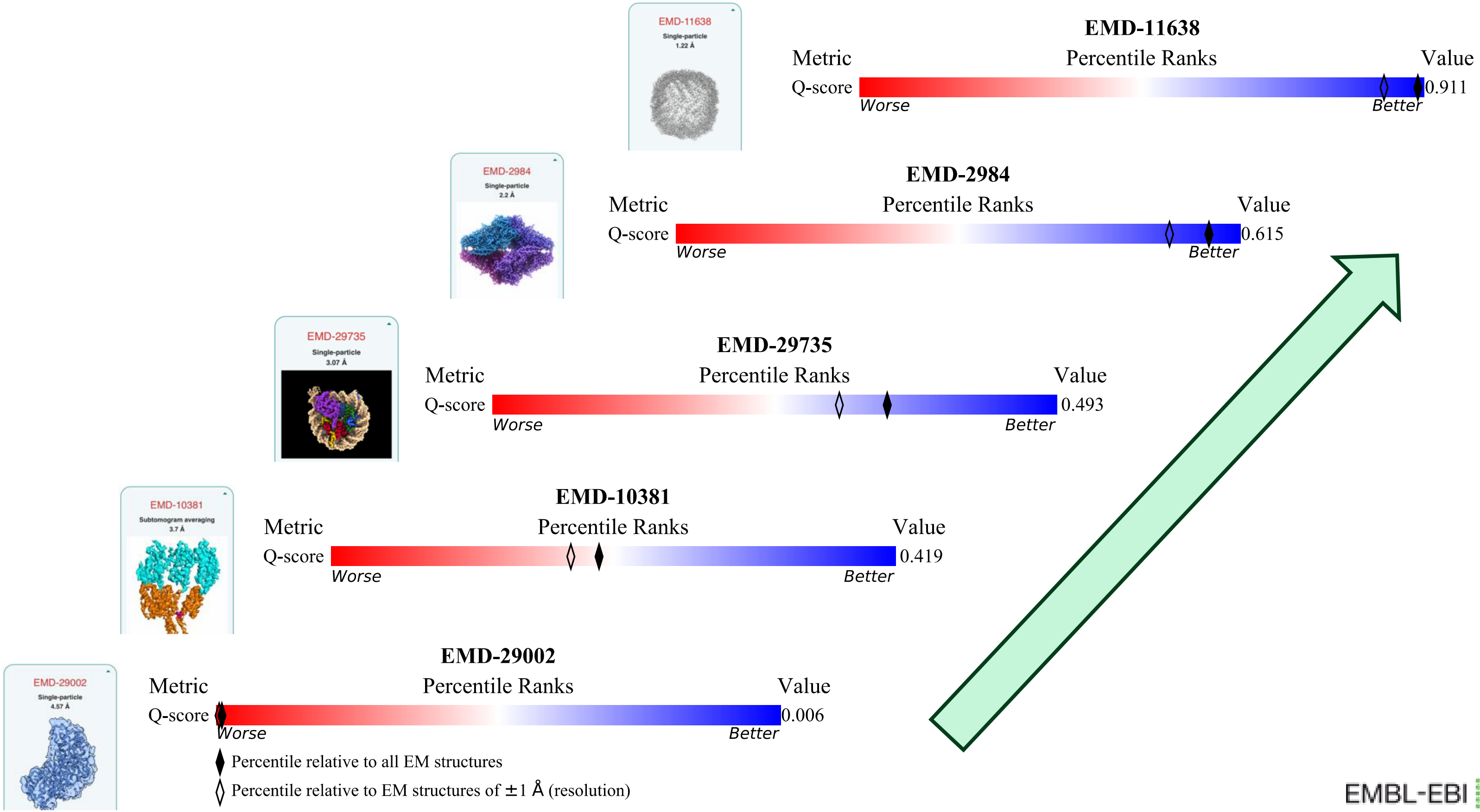
File	Category	Contour level	Toggle	Settings
emd_2984.map.gz	Primary map	0.05	●	⚙
5a1a.cif	Model	-	●	-



In production on website

- Validation visualisation

Validation: models



We made it!

The EMDB

The wwPDB

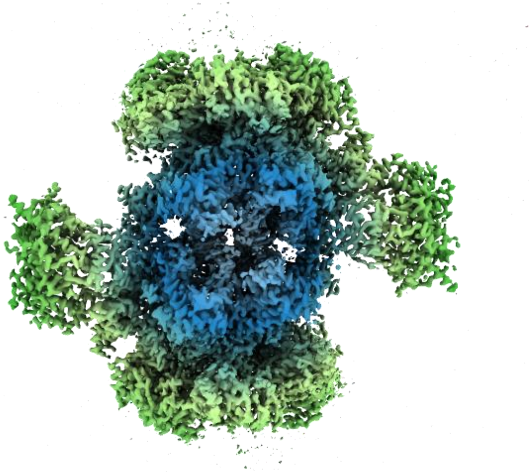
Deposition

Validation

Map re-use ♲

Biological reuse

DNA replication complex



EMDB-13619
Saleh et al (2022) Nat Comm

Map data reuse

2024: Cryo2StructData

Giri, N., et al. (2024). Nature: Scientific Data.

2024: ModelAngelo

Jamali, K., et al. (2024). Nature.

2024: Blush algorithm in Relion

Kimanius, D., et al. (2024). Nature Methods.

2023: CryoRes

Dai, M., et al. (2023). JMB.

2021: DeepEMhancer

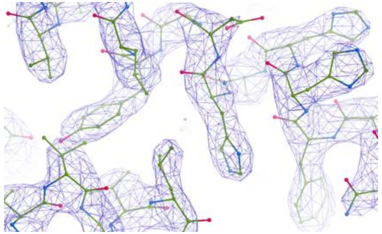
Sanchez-Garcia, R., et al. (2021). Comm Biol.

2019: crYOLO

Wagner, T., et al. (2019). Comm Biol.

EMBL-EBI

Model re-use ♲



Experimental structures

>200,000

(10% from EM)

Prediction

~200,000,000

Good luck in your projects

See you in archive soon

Write to us from inside OneDep or email, if you need help during deposition:

emdbhelp@ebi.ac.uk

deposit-help@mail.wwpdb.org

Acknowledgements

@EMDB_EMPIAR
@emdb_empiar

EMDB
Electron Microscopy Data Bank

The Electron Microscope Databank

Amudha

EMICSS & EMHarvest developement

Jack

Biocuration, scientific programming, cryoEM specialist

Neli

Operations, website, back-end

Miao Ma

Biocuration

Zhe

Validation developer

Sanja

OneDep Project lead

Lucas

OneDep developer

EMDB citation

The wwPDB consortium. (2023). "EMDB—the Electron Microscopy Data Bank." NAR

EMBL-EBI

Acknowledgements

EMDB
Electron Microscopy Data Bank

Funding

EMBL

wellcome

EBI infrastructure

IT services
Storage systems
HPC systems

Collaborators

WORLDWIDE PDB PROTEIN DATA BANK

EMPIAR

PDBe
Protein Data Bank in Europe

CCP-EM

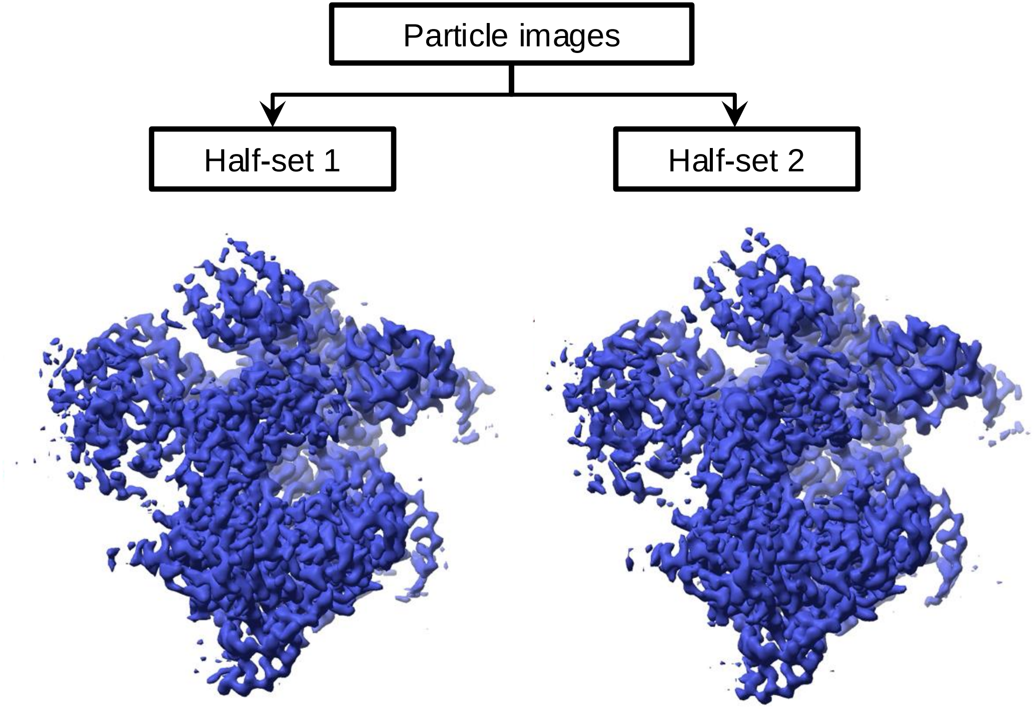
diamond

EMBL

This is the end

Jim Morrison

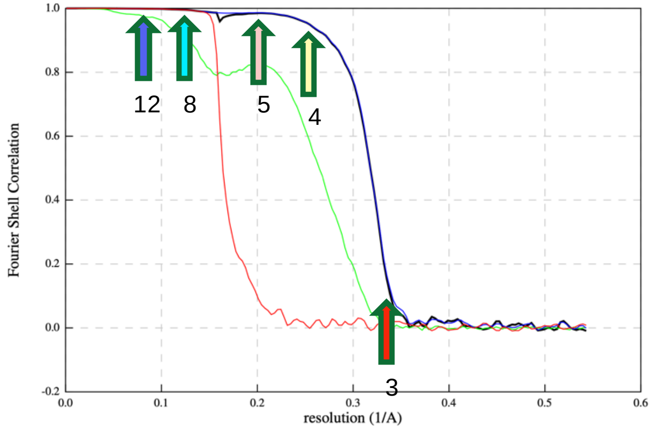
Fourier Shell Correlation



Particle images

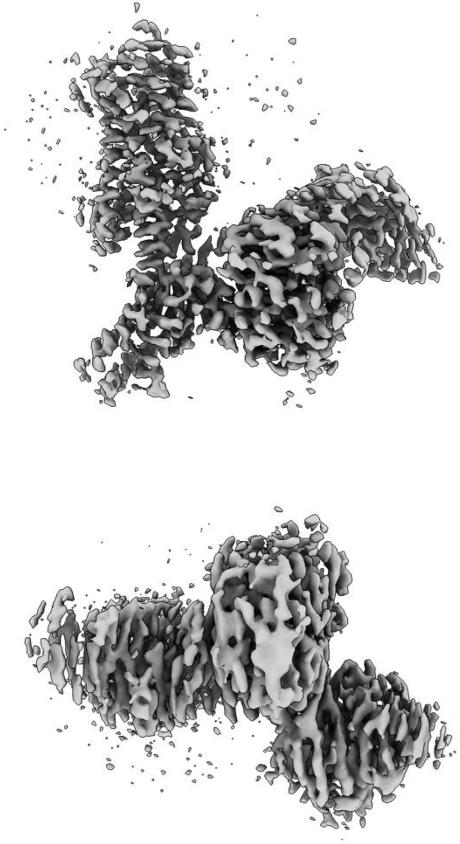
Half-set 1

Half-set 2

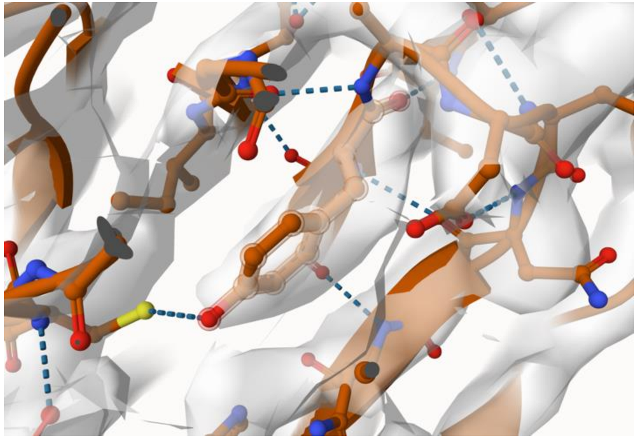


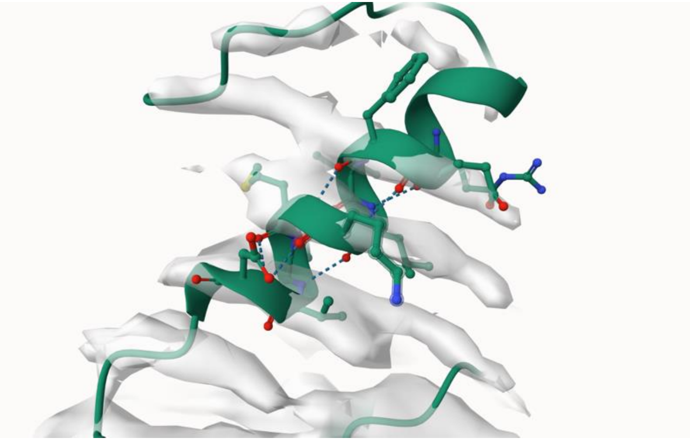
Performed automatically at every step of refinement
Should be carefully checked by a human at the end of refinement
Can be useful to check in local areas

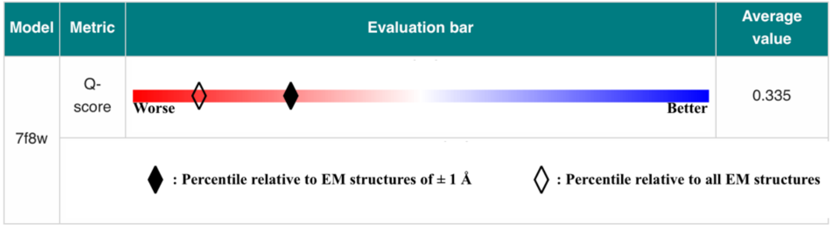
Anisotropy



EMD-31494







Model	Metric	Evaluation bar	Average value
7f8w	Q-score	Worse ◊ ♦ Better	0.335
		♦ : Percentile relative to EM structures of ± 1 Å ◊ : Percentile relative to all EM structures	

EMBL-EBI

Local resolution