PDB, EMDB AND EMPIAR: Public Archiving of Cryo-EM Data

Osman Salih
Scientific Database Curator

@PDBeurope
@EMDB_EMPIAR
Overview

- Where can I access EM Data?
- How do I evaluate the quality of EM Data?
- How can I visualise EM Data?
- How can I deposit EM Data?
- What’s next?

http://www.ebi.ac.uk/pdbe/entry/emdb/EMD-6952
4.25 Å cryo-EM structure of human volume-regulated anion channel LRRC8
Kasuya et al., 2018
Single-Particle Cryo-EM

http://www.ebi.ac.uk/pdbe/entry/emdb/EMD-0031
3.1 Å cryo-EM structure of activated transcription complex RNA Pol II-DSIF-PAF-SPT6
Vos et al., 2018
The Resolution Revolution in Cryo-EM
Cryo-EM in the Spotlight

The Nobel Prize in Chemistry 2017 was awarded jointly to Jacques Dubochet, Joachim Frank and Richard Henderson "for developing cryo-electron microscopy for the high-resolution structure determination of biomolecules in solution."

Jacques Dubochet
Prize share: 1/3

Joachim Frank
Prize share: 1/3

Richard Henderson
Prize share: 1/3
The End of “Blob-ology”
Cryo-EM Technological Advancements (1)

- **Improved Electron Microscopy & Automation**
  - Coherent and stable electron beam
  - Resilient to external factors (noise/vibrations)
  - Load grids into cartridges, then into multi-specimen cassettes
  - Auto-filling Liquid Nitrogen system
  - Automated data collection over several days
Cryo-EM Technological Advancements (2)

- **Introduction of Direct Electron Detectors**
  - High detective quantum efficiency (DQE) – the fidelity with which different spatial frequencies are retained by the imaging system
  - Images possess both high spatial frequencies (i.e. high resolution information/fine detail), and low spatial frequencies (i.e. low resolution information/coarse detail)
  - High frame-rate – recording images as “movies” enabled beam-induced motion correction

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**DQE Plot**

Li et al., 2013 (*Nat. Methods*)

**Archaeal 20S Proteasome**

Li et al., 2013 (*J. Struct. Biol.*)

Cheng, 2018
Cryo-EM Technological Advancements (3)

- Improved Software & Algorithms
  - Samples are rarely completely structurally homogeneous
  - Implementation of a Bayesian approach to cryo-EM structure determination (RELION)
    - 3D classification - sort different compositions & conformations of a complex into more homogeneous subsets
    - User-friendly with GUI

3D Classification
Brown et al., 2015
Spring-like Sheath Contraction Mechanism

Salih et al., 2018
Cryo-EM is “Trending”

Cumulative number of maps released

Maps released per year (7967 in total)

Distribution of released maps (7967 in total) as a function of technique used

Resolution trends
Data Resources at EMBL-EBI

Genes, genomes & variation
- Ensembl
- Ensembl Genomes
- GWAS Catalog
- Metagenomics portal

Gene, protein & metabolite expression
- Expression Atlas
- Metabolights
- PRIDE
- RNA Central

Protein sequences, families & motifs
- InterPro
- Pfam
- UniProt

Molecular structures
- Protein Data Bank in Europe (PDBe)
- Electron Microscopy Data Bank (EMDB)
- Electron Microscopy Public Image Archive (EMPIAR)

Literature & ontologies
- Experimental Factor Ontology
- Gene Ontology
- BioStudies
- Europe PMC

Chemical biology
- ChEBI
- ChEMBL
- SureChEMBL

Systems
- BioModels
- Enzyme Portal
- IntAct
- Reactome

Molecular Archives
- European Nucleotide Archive
- European Variation Archive
- European Genome-phenome Archive
- ArrayExpress
- BioSamples
Data Resources at EMBL-EBI

**EMPIAR**
Electron Microscopy Public Image Archive
- Founded in 2014

**EMDB**
Electron Microscopy Data Bank
- Founded in 2002

**PDBe**
Protein Data Bank in Europe
- Involved in wwPDB since 1999

The purpose of EMPIAR is to provide easy access to raw data to facilitate methods development and validation, which will lead to better 3D structures.
2014 INCEPTION

2014 ENTRIES

2014 ARCHIVE

40 2017

79 2018

98% INCREASE

138 TB
Archive of Raw EM Image Data
- Can search, browse and download EMPIAR entries
- Can also deposit your own data
- Useful for validation, methods development, teaching & community challenges

https://www.ebi.ac.uk/pdbe/emdb/empiar/entry/10205
2.7 Å cryo-EM structure of cowpea mosaic virus empty virus-like particles (CPMV-eVLPs)
To be published

https://www.ebi.ac.uk/pdbe/emdb/empiar/
EMPIAR, the Electron Microscopy Public Image Archive, is a public resource for raw, 2D electron microscopy images. Here, you can browse, upload and download the raw images used to build a 3D structure. More ...

Deposit your data in EMPIAR to share it with the structural biology community.

Browse and download EMPIAR datasets using the table below.

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**Quick links**

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

**EMPIAR Quick tour**

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**EMPIAR citations**

Cryo-EM structure of alpha-synuclein fibrils.

Structure of the herpes simplex virus portal-vertex.

Benchmarking cryo-EM Single Particle Analysis Workflow.

Characterisation of molecular motions in cryo-EM single-particle data by multi-body refinement in RELION.
EMPIAR-10205

Combining high-resolution cryo-electron microscopy and mutagenesis to develop cowpea mosaic virus for bionanotechnology

Publication: Collection, pre-processing, and on-the-fly analysis of data for high-resolution, single-particle cryo-electron microscopy
Thompson RF, Iadanza MG, Hesketh EL, Rawson S, Ranson NA
Nat. Protoc.

Related EMDB entry: EMD-3952
Deposited: 2018-08-14
Released: 2018-08-16
Last modified: 2018-08-21
Dataset size: 351.5 GB
Dataset DOI: 10.6019/EMPIAR-10205

Image set
Corrected movies
Category: micrographs - multiframe
Image format: MRC
No. of images or tilt series: 5619
Frames per image: 1
Image size: (4096, 4096)
Pixel type: 32 BIT FLOAT

Download

- FoilHole_28141849_Data_28143362_28143363_20170228_1831_Fractions.mrc 64.0 MB
External 2D Viewer

- **Fiji (ImageJ)**
  - File – Open:
    - Single EM image
    - EM image stack
      - May require:
        - Image – Stack – Z Project
        - Projection Type: Sum Slices
  - Tomography tilt-series
    - Play movie
  - Image Adjustments
    - Image – Adjust – Brightness/Contrast
      - Adjust Sliders OR
      - Click Auto as desired

Schindelin et al., 2012
https://fiji.sc/
4 Easy Steps to EMPIAR Deposition:

1. Gather Information (Requirement: related EMDB accession code!)
   - 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-framed, 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](http://asperasoft.com)) and/or Globus ([https://www.globus.org](https://www.globus.org)) efficiently and robustly transfer large data volumes

4. Deposit your Data and Metadata
is a public repository for electron microscopy density maps of macromolecular complexes and subcellular structures
2002 INCEPTION
7,967 ENTRIES
1.2 TB ARCHIVE
1,106 2017
1,768 2018
60% INCREASE
• Archive of EM Density Maps
  • Consists of macromolecular complexes and subcellular structures
  • Covers a variety of techniques, including single-particle analysis, electron tomography and electron crystallography
  • Can search, browse and download EMDB entries
  • Can also deposit your own data
  • Useful for structural analysis and comparisons, methods development and validation, and teaching

http://www.ebi.ac.uk/pdbe/entry/emdb/EMD-4322
4.5 Å cryo-EM structure of the 26S Proteasome (s4 state)
Eisele et al., 2018
The Electron Microscopy Data Bank (EMDB) at PDBe

Quick access

Click on one of these categories:
- Ribosome
- Virus
- Phage
- GroEL
- Microtubule
- Polymerase
- Helicase
- Human
- HIV
- Entries with fitted models
- Single particle
- Tomography
- Helical reconstruction
- <SA resolution

or enter 4-digit EMDB entry number: 1001

Entry summary  Visual analysis of map  Volume viewer

https://www.ebi.ac.uk/pdbe/emdb/
Advanced EMDB search

You can search the EMDB archive using this service. Use the form below to specify your query. When you press submit, the service will display a table with summary information for the EMDB entries that satisfy your query, in a separate tab. Use the "Configure search results" section below to select the sort order for the search results, and which fields are to be displayed. There is a "Download" button on the search results page which can be used to download the search results as a text or XML file for further analysis.

All text: Grove

EMDB codes

Fitted PDB codes

Authors

Resolution: highest: A lowest: A

Molecular weight: min MDa max MDa

Submit  Reset  Expand all  Collapse all

Sample

Citation

Status

Dates

EM method

Software

Microscope

Configure search results

Submit  Reset  Expand all  Collapse all
Search Results

Scroll down to find entry of interest
Allosteric signaling of ATP hydrolysis in GroEL-GroES complexes.

Source organism: *Escherichia coli* [562]
Fitted atomic model: 2c7c
Related in-frame EM entry: EMD-1181
Related EM entry by publication: EMD-1181
3Dbiomart: available for this entry
Primary publication:
[Allosteric signaling of ATP hydrolysis in GroEL-GroES complexes. Ranson NA, Clare DK, Farr GW, Houldershaw D, Horwich AL, Saibil HR. *NAT.STRUCT.MOL.BIOL.* 13 147-152 (2006)]
PMID: 16429154

Single particle reconstruction
7.7Å resolution

Map released: 2006-02-14
Last modified: 2013-03-13

Function and Biology
- Sample name: GroEL-ATP7-GroES
- Proteins: GroEL, GroES

Experimental Information
- Resolution: 7.7Å
- Resolution method: FSC 0.5
- Applied symmetry: C7
- Reconstruction software: SPIDER
- Microscope: FEI TECNAI F20
- Detector: KODAK SO-163 FILM

Quick links
- EMD-1180 overview
- Function and Biology
- Experiments and Validation
- View
  - Downloads
  - Volume viewer
  - Volume slicer
- Visual analysis

Related entries
- By authors
- By sample
- By organism

https://www.ebi.ac.uk/pdbe/emdb/
• **Visual Analysis**
  
  • Orthogonal projections, central slices and surface views reveal:
    
    • Internal detail
    
    • Whether a mask has been used
    
    • Surface features
    
    • Appropriate contour usage

• Consistency checks
Density of voxels in the map

Author recommended threshold for viewing map

The volume to which 900 kDa corresponds

Contour level the author recommends

The given resolution (Å)

The FSC curve

The resolution is given as the point at which the FSC curve intersects a specified threshold

May provide insight into processing procedure (e.g. CTF correction, B-factor correction)
• **Fitted Model Information**

  • Orthogonal views of the atomic model fitted to the EM map reveal the quality of the fitting
  
  • Atom inclusion by residue graph highlights if there is any particular part of a model that is outside of the EM map
    
    • Green = 100 %
    
    • Red = 0 %
  
  • Atom inclusion as a function of contour level
Allosteric signaling of ATP hydrolysis in GroEL-GroES complexes.

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Volume viewer

Quick links
- EMD-1180 overview
- Function and Biology
- Experiments and Validation
- View
- Downloads
- Volume viewer
- Visual analysis

Related entries
- By authors
- By sample
- By organism
EMDB
Electron Microscopy Data Bank

EMD-1180 • Volume slicer

Allosteric signaling of ATP hydrolysis in GroEL-GroES complexes.

Sample name: GroEL-ATP7-GroES
Method: Single-particle
Resolution: 7.7Å (FSC 0.5)

Volume Slicer

- Orthogonal slices of the EM map show internal features
- Interactive 3D navigation

https://www.ebi.ac.uk/pdbe/emdb/
Allosteric signaling of ATP hydrolysis in GroEL-GroES complexes.

Function and Biology
- Sample name: GroEL-ATP7-GroES
- Proteins: GroEL, GroES

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EMDB › EMD-1180

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https://www.ebi.ac.uk/pdbe/emdb/
**Volume Viewer**

- Interactive 3D volume viewer allows visual inspection of the quality of the fit of the atomic model to the EM map
- Features include:
  - Adjustable contour level, transparency, colour and zoom level
  - On/Off toggle for associated atomic model within the EM map

The author of EMDB recommended contour level for this map is 0.608

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**Map Controls**
- Map
- Solid Surface

**Level:**
- 1.79
- 2.38
- (0.608)

**Opacity:**
- 0
- 190
- (30)

**Color:**
- #FA500

**Model(s)**
- 2C7C

**Background:**
- Light Grey

**View Controls**
- Size (Å):
  - 10
  - 530
- Depth (Å):
  - 10
  - 538

The depth control sets the Z axis depth of the viewer.
Allosteric signaling of ATP hydrolysis in GroEL-GroES complexes.

Source organism: *Escherichia coli* [562]

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**Function and Biology**

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**Quick links**

- **EMD-1180 overview**
  - Function and Biology
  - Experiments and Validation
- **Downloads**
  - Experimental metadata (xml)
  - Bundle (tar.gz)
  - Bundle (zip)
- **Volume viewer**
- **Volume slicer**
- **Visual analysis**

**Related entries**

- By authors
- By sample
- By organism
External 3D Viewer (Part 1)

- UCSF Chimera
  - File – Open:
    - EM map
    - Atomic Model
  - Favorites – Open
    - Model Panel
    - Side View
  - Change Step
  - Input Contour Level
  - Adjust Clipping Plane
  - Customise
  - File – Save Image

Pettersen et al., 2004
https://www.cgl.ucsf.edu/chimera/
External 3D Viewer (Part 2)

- **UCSF ChimeraX**
  - **File – Open:**
    - EM map
    - Atomic Model
  - **Tools – Toolbar – Density Map Toolbar**
  - **Tools – General – Side View**
  - **Change Step**
  - **Input Contour Level**
  - **Customise**
  - **File – Save Image**
Generating Images (ChimeraX)

UCSF CHIMERA
an Extensible Molecular Modeling System

Goddard et al., 2018
http://www.rbvi.ucsf.edu/chimerax
.. is a public repository for atomic coordinates of biological macromolecular structures derived by X-ray crystallography, NMR and EM
INCEPTION: 1999

ENTRIES: 150,861

ARCHIVE: 353 GB

2017: 11,085

2018: 11,224

INCREASE: 1.25%
• Archive of Atomic Models
  • Consists of experimentally determined structures of biological macromolecules
  • Covers all the major structure-determination techniques, including X-ray crystallography, Nuclear Magnetic Resonance (NMR) spectroscopy and cryo-electron microscopy
  • Can search, browse and download atomic models
  • Can also deposit your own data
  • Useful for structural analysis and comparisons, methods development and validation, and teaching

http://www.ebi.ac.uk/pdbe/entry/emdb/EMD-0077
3.2 Å cryo-EM structure of the narrow filament from Pick’s disease
Falcon et al., 2018

https://www.ebi.ac.uk/pdbe/
Browse for more information on entry
- Function and biology
- Structural analysis
- Validation
- View molecular images
- Interactively view structure online (LiteMol) or download

https://www.ebi.ac.uk/pdbe/
Sub-2 Ångström Ewald Curvature-Corrected Single-Particle Cryo-EM Reconstruction of AAV-2 L336C

Source organism: Human adenovirus 2

Primary publication:
- Sub-2 Å Ewald curvature corrected structure of an AAV2 capsid variant.
  Tan YZ, Aiyer S, Mietzsch M, Hull JA, McKenna R, Grieger J, Samulski RJ, Baker TS, Agbandje-McKenna M, Lyumkis D
  PMID: 30194371

Related structures: EMD-9012

Function and Biology

Biochemical function:
- structural molecule activity

Biological process:
- viral process

Cellular component:
- virion

Sequence domains:
- Parvovirus coat protein VP2
- Capsid/spike protein, ssDNA virus
- Parvovirus coat protein VP1, N-terminal
- Parvovirus coat protein VP1/VP2

Ligands and Environments

No bound ligands

No modified residues

Experiments and Validation

Resolution: 1.86 Å

Relevant EMDB volumes: EMD-9012

Expression system: Spodoptera frugiperda

https://www.ebi.ac.uk/pdbe/
• Validation Report
  • Overall quality assessment of the structural data
  • Includes:
    • Summary sliders
    • Residue-property plots
    • Experimental information
    • Summary tables for geometry (e.g. bond lengths and angles, chirality and planarity, backbone and side-chain torsion angles, outliers, steric clashes, and linkage issues)

https://www.ebi.ac.uk/pdbe/
Summary Sliders

- Give succinct summary of key quality indicators
- Scored by comparison to all other structures in the archive

Residue-property plots

- Summarizes quality information per chain, per residue, indicating the fraction of residues that contain outliers
- Colour-coded according to the number of geometric quality-criteria outliers (e.g. bond length/angle outliers):
  - Green = 0
  - Yellow = 1
  - Orange = 2
  - Red = 3 or more
  - Grey = unmodelled

https://www.ebi.ac.uk/pdbe/
PDBe › 6e9d

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PMID: 30194371

Related structures: EMD-9012

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Biochemical function: structural molecule activity

Biological process: viral process

Cellular component: virion

Sequence domains:
- Parvovirus coat protein VP2
- Capsid/spike protein, ssDNA virus
- Parovirus coat protein VP1, N-terminal
- Parovirus coat protein VP1/VP2

Ligands and Environments

No bound ligands
No modified residues

Experiments and Validation

Metric Percentile Ranks Value
Clasicores 5
Ramachandran outliers 0
Sidechain outliers 0

Resolution: 1.86 Å

Relevant EMD volumes: EMD-9012

Expression system: Spodoptera frugiperda
Visualising Validation Data

Validation displayed on interactive components

View EM maps and atomic structures

View geometric validation on the structure
1.86 Å cryo-EM structure of an adeno-associated virus serotype 2 variant (AAV2)
Tan et al., 2018

http://www.ebi.ac.uk/pdbe/entry/emdb/EMD-9012
A unified deposition portal for structural data
5 Easy Steps to Deposition with OneDep:

1. Check Sample Sequence
   - Sequences should contain all residues, including expression tags and disordered residues. Check against a reference database with BLAST (UniProt/NCBI BLAST)

2. Check Ligands
   - Are your ligands already in our Chemical Component Dictionary (CCD)? Check at PDBeChem (pdb.e.org/chem). If yes, provide the 3-character code. If no, provide a SMILES or 2D chemical diagram

3. Prepare Data
   - Generate coordinate file in PDBx/mmCIF format (e.g. directly from PHENIX, REFMAC) – captures maximum metadata. EM maps must be in either CCP4 or MRC format

4. Validate!
   - Check your structure using the standalone validation server (validate.wwpdb.org) – provides detailed reports. Please attempt to fix any major issues highlighted

5. Deposit your Structural Data and Metadata (deposit.wwpdb.org)
What's next?
Cryo-EM Data Validation

- Use high-resolution maps in EMDB for systematic structural data-mining
  - Derive canonical 3D density motifs for various features
    - Side-chain densities, main chains and ligands
  - Examine these density motif libraries
    - Ascertain how they vary with resolution and local environment, and compare to corresponding X-ray density
  - Potential new approach for comparative EM validation

What's next?
Fully-Automated Deposition to EMPIAR

- Current deposition system for EMPIAR is web-based and interactive
  - Deposition of each entry requires human interaction
- Developing fully-automated depositions through integrated pipelines from electron microscopy centres
  - Raw image data and meta-data can be ‘pushed’ directly into EMPIAR
- Three depositions from different electron microscopy centres (including EMBL-Heidelberg) have been collected through this pilot pipeline already

![Diagram of the deposition process]

1. Finish the measurement and store data
2. Send POST JSON with EMPIAR entry metadata to API endpoint
3a. Notify the user about the submission
3b. Send the entry ID and upload directory name
4. Initiate Aspera transfer to the received directory
5. Submit the entry
The Future: BioImage Archive

- Two distinct types of biological databases:
  - Data archives – a record of scientific data and experiments
  - Added-value databases – are synthetic; enrich and combine different datasets through comparative analysis and expert curation
    - Provides integrated biological information for a wide community of users
- Central BioImage Archive proposed
  - Comprises archival layer and added-value layer
    - Allows rapid data aggregation and cross-discipline comparisons

Ellenberg et al., 2018
PDBe
Protein Data Bank in Europe

What's next?
PDBe - KB
Protein Data Bank in Europe Knowledge Base

- A community-driven resource managed by the PDBe team
  - Collates functional annotations and predictions for structural data in the PDB archive
- A collaborative effort between PDBe and a diverse group of bioinformatics resources and research teams (e.g. Pfam, UniProt, CATH, Phyre2)
- Projects include SIFTS (Structure Integration with Function, Taxonomy and Sequence) and FunPDBe
  - Aimed at placing structures from the PDB into their biological context

https://www.ebi.ac.uk/pdbe/pdbe-kb/
Collaborations and Acknowledgements

- Birkbeck College (Elena Orlova, Maya Topf, Helen Saibil)
- Baylor (Wah Chiu)
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- CNB Madrid (Jose Maria Carazo)
- Dundee (Jason Swedlow)
- EMBL-EBI (Helen Parkinson, Alvis Brazma, Ugis Sarkans)
- Francis Crick (Lucy Collinson, Raffa Carzaniga, Peter Rosenthal)
- Osaka University (Genji Kurisu)
- MRC-LMB (John Briggs, Paula da Fonseca, Wanda Kukulski, Garib Murshudov)
- RCSB (Cathy Lawson)
- STFC (Martyn Winn)
- University of Manchester (Alan Roseman)

- Websites:
  - https://www.ebi.ac.uk/pdbe/
  - https://www.ebi.ac.uk/pdbe/emdb/
  - https://www.ebi.ac.uk/pdbe/emdb/empiar/